Real Time Optimization of Chemical Processes — A Comparison of Closed Versus Open Form Equations Using Commercial Simulation Packages

by

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Real Time Optimization of Chemical Processes — A Comparison of Closed Versus Open Form Equations Using Commercial Simulation Packages

Abstract

Real time optimization (RTO) is the continuous reevaluation and alteration of operating conditions of a process so that the economic productivity of the process is maximized subject to operational constraints. Current industrial real time optimizers are generally designed and coded manually for each application, using a programming language such as FORTRAN, PASCAL or C. in order to solve the optimization problem within a reasonable period of time. Recently, computers have become powerful enough to allow the use of chemical process simulation packages in real time optimization. Process simulation packages have the advantages of providing user friendly interfaces, a library of pre-built and tested unit operation models, rigorous property libraries and built in optimization algorithms. Therefore, real time optimization applications can be developed more easily and quickly, and are easier to maintain than those developed by direct coding.

The main objective of this research was to compare the use of closed and open form equation based process simulation packages as the process models in real time optimization. Currently, both closed form equation based, or sequential modular, and open form equation based, or equation-oriented, process simulators have been suggested for use in real time optimization, but not implemented.

Two real time optimizers were developed for an industrial refinery stabilizer-splitter process using ASPEN PLUS, a sequential modular process simulator, and SPEEDUP, an equation-oriented process simulator.

After testing the two real time optimizers, it was concluded that neither ASPEN PLUS nor SPEEDUP in their present form were robust enough for an industrial on-line application. The equation-oriented simulator, how-
ever. was able to find better objective function values using approximately half as many cycles of the real time optimizer than the sequential modular simulator. The sequential modular simulator had difficulty in converging the economic optimization problem when inequality constraints became violated. Problems were also encountered converging the tear stream blocks in ASPEN PLUS for some operating conditions. The SPEEDUP real time optimizer required weighting factors in the objective functions for both data reconciliation and economic optimization due to a lack of tuning parameters for the SRQP optimization algorithm and possible flowsheet variable scaling problems.

From the development of the two real time optimizers, it was concluded that sequential modular simulators are quicker and easier to use than equation oriented simulators. However, they are not as flexible with respect to the choice of manipulated variables for optimization and convergence of flowsheet recycle loops and tear streams. The development of the real time optimizers also provides a "test bed" for future research into real time optimization.

Overall, despite the added difficulty in developing and converging an equation-oriented process flowsheet model, the added flexibility in terms of variable specification, robust and rapid tear stream convergence and more powerful optimization algorithms make the equation-oriented process simulator a more attractive tool for real time optimization, provided the problems encountered can be overcome. Equation oriented process simulation packages have also already been used in advanced model based control, scheduling and process operation analysis which has the advantage of providing the same user-interface and models for all process modelling performed.

Several other runs were performed with the ASPEN PLUS real time optimizer testing changes in the economic objective function parameters and the effect of process disturbances. Also, a sensitivity study of the economic objective function stream prices was performed which showed that in every case tested, the real time optimizer was able to find a better operating point after a change in economic parameters.
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Chapter 1

Introduction

1.1 Objectives

The main objective of this research is to compare the use of closed and open form equation based process simulation packages as the plant models in real time optimization. By developing real time optimization systems in both closed (sequential modular) and open (equation-oriented) form equation process simulators, this research will also help to determine the feasibility of using an "off the shelf" process simulation package as the process model in real time optimization. Development of the two real time optimization systems will provide "test beds" for further research on real time optimization applications and performance. This research will also help to close the gap between industry and research in this field as there is very little literature available on real time optimization.

Two other areas of real time optimization will also be studied in this research:

1. Determine the effect of changes in the financial model on the real time optimizer;

2. Demonstrate the effects of process disturbances on the operation of the real time optimizer.
These two areas will help to illustrate the benefits of performing real time optimization on a chemical process.

1.2 Real Time Optimization

The terms real time optimization (RTO) and on-line optimization are used to indicate the continuous reevaluation and alteration of operating conditions of a process so that the economic productivity of the process is maximized subject to operational constraints [56]. Optimization of process operations is of considerable interest in industry due to increasing global competition and tightening product requirements [32, 34]. Real time optimization is an appealing concept because it is at the level of the control hierarchy at which business decisions are integrated into the operation (see Section 1.2.1 for more detail). Advances in the speed and power of computers at lower costs are making on-line optimization a more cost effective method of improving plant performance.

Latour [62] lists the benefits from steady-state real time optimization as:

- Improved product yields and/or quality;
- Reduced energy consumption and operating costs;
- Increased capacity of equipment, stream factors;
- Less maintenance cost and better maintenance of instrumentation;
- More efficient engineers and operators as a tool for process troubleshooting and operation;
- Tighter, lower cost process designs if new plant designs include a real time optimizer.

However, not all processes will benefit from real time optimization. Processes that experience a wide range of operating conditions due to variability in
product prices and material costs, large variations in ambient conditions, or economic trade-offs and constraints will benefit the most from real time optimization. Some examples of suitable processes are steam utility plants, fluidized catalytic cracking units and downstream gas separation units [87].

A real time optimizer will perform the following general steps:

1. Detect when the plant is sufficiently close to steady state to perform optimization:

2. Perform data rectification on the process data (data reconciliation and possibly gross error detection);

3. Read the data into the process model and optimize the set points for the plant using an economic objective function and operational constraints:

4. Download the new set points into the plant's process control system and return to step 1.

Details on how each of these steps can be performed and the methodologies being used at present are covered in Chapter 2.

1.2.1 Real Time Optimization and Control Hierarchy

Figure 1.1 graphically represents the hierarchy of process control applications. At the base of the pyramid is regulatory control. This is a basic requirement for all for all further applications higher up the pyramid as they all require the availability of current on-line data from the plant [52].

Advanced regulatory control is used mostly in situations where where the process is unstable and requires stability. Advanced regulatory control is mostly applied using the DCS (distributed control system) hardware or with a higher level device such as an application module.

Advanced control is the application of software and control algorithms to do some predictive analysis and local optimization of the process. Some model based multivariable control techniques include generic model control
Figure 1.1: Hierarchy of process control applications [52].
(GMC) [22, 64], dynamic matrix control (DMC) [33], model algorithmic control (MAC) [90] and internal model control (IMC) [46]. Advanced controllers generally provide control strategies for one or two process units.

Wide area or real time optimization involves multiple process units, complex units or several areas within a plant. The goal is to maintain an optimum over a wider area of the plant and thus assumes that the combination of advanced and regulatory control can implement and maintain any set point requested by the optimizer.

Finally, at the top of the pyramid is "what-if" analysis. This includes production planning and scheduling as well as off-line analysis of the process.

1.2.2 Current Real Time Optimization Systems

Industrial real time optimization systems operating today are generally designed and coded specifically for each application. These large scale real time optimization systems are difficult to develop and maintain, requiring extensive development periods by highly skilled staff before implementation. The process models used in the real time optimizer are usually coded manually in open form equations, using a programming language such as FORTRAN 77, PASCAL or C. Typically, the process model will require in the order of 10,000 variables and equations to represent a chemical process. Subsequent maintenance of this process model is also difficult and highly specialized, often requiring recoding of sections of the process model. Historically, this method of development has been necessary to ensure that a cycle of the real time optimization can be completed within an acceptable amount of time on the computers available, typically between 1 and 3 hours.

Recently, computers have become powerful enough to allow the use of higher level programming and modelling techniques to be used in real time optimization. Several authors have proposed the use of process simulation packages for performing real time optimization [20, 45, 71, 105] (see Section 2.2.1 for further details). Both closed form (sequential modular) and open form (equation-oriented) equation process simulation packages have
been proposed. However, there are no known industrial applications of real
time optimizers using process simulators. Historically, the reason for this was
that the additional computational time required to complete real time opti-
mization using a process simulation package was too great. With the recent
advances in computer processor power and speed, this additional computa-
tional overhead is no longer a barrier to the use of process simulation packages
in real time optimization systems. Process simulation packages also offer the
advantages of built in unit operation models, powerful nonlinear optimization
software and user friendly interfaces.

Several process simulation companies are working on the development of
real time optimization and on-line modelling systems. These systems are
summarised in Table 1.1. All of these systems are currently being imple-
mented on chemical processes in conjunction with other companies, however
it appears that these implementations are being used to assist in the devel-
opment and testing of these packages. At the time of writing, none of these
real time optimization systems had been released as commercial packages.

1.3 Process Simulation

Chemical process simulation, or process flowsheeting, is used to enable an
engineer to model the behaviour of a plant, or parts of it, under defined
conditions and so produce the heat and material balances for the process. In
mathematical terms, the requirement is to solve the large number of nonlinear
equations that represent the performance of the unit operations and the
behaviour of the chemical components [104]. Process simulators are typically
used in design, analysis and optimization of chemical processes [88].

Process flowsheeting architectures used to solve the nonlinear equations
generated fall into two main categories: the sequential modular and the
equation-oriented approaches. These two approaches and their advantages
are discussed in the following subsections.
Table 1.1: Commercial real time optimization systems in development.

<table>
<thead>
<tr>
<th>Company</th>
<th>Product</th>
<th>Process Modelling Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aspen Technology [14]</td>
<td>RT-OPT</td>
<td>Open form equation models. possibly based on SPEEDUP process simulation models.</td>
</tr>
<tr>
<td>Honeywell Hi-Spec Solutions [52, 53]</td>
<td>RT-EXEC (Previously OPTIMIZER)</td>
<td>Based on open form equation MASSBAL process simulation models.</td>
</tr>
<tr>
<td>Simulation Sciences [94]</td>
<td>ROM</td>
<td>Originally based on closed form equation PRO/II process simulation models, may now use open form equation models.</td>
</tr>
<tr>
<td>Treiber Controls</td>
<td>CRO</td>
<td>Open form equation models.</td>
</tr>
</tbody>
</table>
1.3.1 Sequential Modular Process Simulators

The sequential modular approach to process simulation implements unit operation blocks as computer subroutines, or modules, that calculate the output variables as functions of the input variables [67]. These computer subroutines are stored as library models which are matched to the various unit operations in the flowsheet. An executive program calls each subroutine in turn, using the output stream data from one unit as the input data for the next unit. Since most continuously operated plants involve multiple recycles, the executive program needs to manage the iterative calculation around the loops until a satisfactorily converged solution is achieved. Calls for physical properties are standardized so that consistent data are available throughout the program [104]. Thus, the basic components of a sequential modular simulation system are the executive, the model library and the physical properties system as summarised in Figure 1.2. The executive program accepts input data, determines the process flowsheet, derives and controls the calculation sequence for the unit operations in the flowsheet. The executive passes control to unit operations for the execution of the modules.

The level of model complexity is internalized within each model in a sequential modular simulation allowing the substitution of shortcut with rigorous unit models requiring only minor changes to the simulation program. Also, special purpose solution strategies can be constructed for each different unit type without altering the overall approach to the flowsheeting program. Liu et al. [67] list the advantages of sequential modular simulators as:

- the approach is conceptually easy for process engineers to understand;
- there is a large body of computer software organized in the form needed by the sequential modular approach;
- it is possible to include convergence heuristics developed by experience over the years (e.g., good initialization procedures);
- in case of an error, it easy to give understandable error messages.
Figure 1.2: Structure of a sequential modular process simulator [18].

However, the input/output nature of the unit operation modules leads to difficulties as well. Problems occur when the recycle structure of the flowsheet and any external design specifications create awkward iteration loops, or tear streams, in the calculation sequence. Iteration loops are also required when any indirect unit specifications or design constraints are used [18].

Most of the more widely used flowsheeting systems such as Simulation Science's PRO/II, Aspen Technology's ASPEN PLUS and HyproTech's HYSIM employ the sequential modular approach (see Biegler [18] for a more comprehensive list of process simulation packages). The sequential modular approach has had wide acceptance due to the ease of building process flowsheets and the reliability of their solution.

Recently, some sequential modular process simulators have gradually added simultaneous modular methods. Unit operation modules remain intact, however the flowsheet stream connections are solved simultaneously using application of Broyden-type or quasi-Newton methods. This has allowed complicated recyclers and flowsheet constraints to be solved together producing much faster convergence rates.
1.3.2 Equation-oriented Process Simulators

The basic idea of equation-oriented approaches to process simulation is to collect all of the equations describing the flowsheet together, and solve them as a large system of nonlinear algebraic equations. Mathematically this problem can be stated as [67]:

\[
\text{solve } f(x, u) = 0 \\
\text{subject to } g(x, u) \leq 0
\]  

(1.1)

where \( x \) = the vector of state (dependent) variables; 
\( u \) = the vector of decision (independent) variables; 
\( f(x, u) \) = the set of process model equations; 
\( g(x, u) \) = the set of inequality or equality constraints.

The decision variables include all of the input variables and the feed stream variables. The state variables include all the intermediate and product stream variables, internal variables within each unit operation block, and output performance variables from each block.

The crucial difference between sequential modular and equation-oriented process simulators is that the process equations, no matter how they are collected, are treated by general purpose solution strategies (e.g., Newton-Raphson) and are often solved simultaneously. The basic components of an equation-oriented process simulator are summarised in Figure 1.3. As seen in Figure 1.3, the executive performs a slightly different function to the executive for a sequential modular simulation (see Figure 1.2) in that it organises the equations and controls the general purpose equation solver.

Equation-oriented simulators are far more flexible than sequential modular simulators in terms of solving problems with nested tear recycle loops and additional design constraints at the flowsheet level. Also, the accessibility of derivative and function information within the equation oriented simulator allows for the application of more sophisticated optimization strategies. However, the solution of several thousand equations that represent a typical industrial scale process is a much more complex mathematical task than that
posed by a sequential modular approach, where the equations are segregated into smaller sets in the unit operation routines. Equation-oriented flowsheeting problems require large scale numerical algorithms, good initialization strategies and reliable options to prevent convergence failures [18, 54, 104].

Equation-oriented process simulation packages are not as widely used as sequential modular simulators. Two commercially used packages are Aspen Technology’s SPEEDUP, originally developed by Imperial College, and Honeywell Hi-Spec Solutions’ MASSBAL, commonly used in the pulp and paper industry. Neither of these packages are “purely” equation-oriented as they incorporate procedures at the lowest levels to promote convergence. In particular, physical properties are determined using procedures rather than including large sets of nonlinear property equations in the simulation.

1.4 Scope of this Research

Current large scale real time optimizers implemented in industry usually suffer from a lack of user friendliness. Both Lojek and Whitehead [68], and
Darby and White [34] emphasize the importance of good man-machine interfaces required to facilitate the use and maintenance of a real time optimizer. One method of simplifying the development and subsequent maintenance of a real time optimization system is to use process simulation packages. Several process simulation packages already have the features required to implement a complete real time optimization system, including the ability to perform the process modelling, data reconciliation, economic optimization and data transfer required. In addition to simpler modelling environments, process simulation packages also offer the advantages of rigorous property calculations, choice of convergence algorithms and, with some packages, graphical user interfaces.

Process simulation packages also offer the advantage of providing a standardized modelling environment for several areas of the process control hierarchy shown in Figure 1.1. As well as providing the models for economic optimization and data reconciliation in real time optimization, the models could also potentially be used in advanced control and "what-if" analysis. For example, process simulator models can be used in Generic Model Control (GMC) as demonstrated by Douglas et al. [36] and Lee [65] who both used the SPEEDUP simulations package as the model. The same models used in the real time optimizer and advanced control can also be used by process engineers for general process simulation and trouble shooting. These same models may also be used for nonlinear modelling of entire plants for scheduling and production planning purposes. For example, McLellan [75] and Picaseno-Gamiz [86] both used SPEEDUP to present systematic non-linear approaches to scheduling for continuous processes.

The purpose of this research is to compare the use of the two main types of process simulation package in real time optimization applications. The two main types are closed form equation, or sequential modular, and open form equation, or equation-oriented, process simulators. Both types of process simulator were used to develop a real time optimizer for the same chemical process to compare the development and operation advantages of each
package.

The two process simulation packages chosen were ASPEN PLUS v9.2 [8, 9] and SPEEDUP v5.5d [11, 12]. A newer version of ASPEN PLUS, version 9.3 was used for some real time optimizer testing, however, unless otherwise stated in the thesis, version 9.2 of ASPEN PLUS was used. These packages were chosen as being representative of their respective types of process simulator and for their extensive optimization capabilities.

ASPEN PLUS is a sequential modular process simulator with some simultaneous modular convergence options. It also has a wide range of unit operation models with tailored convergence methods for best performance. An SQP (successive quadratic programming) algorithm is available for optimization problems (see Section 4.2.1 for more detail on SQP) and user defined FORTRAN blocks can be added to a process flowsheet. The process flowsheet is specified either using the MODEL MANAGER graphical user interface or by editing a keyword based text file.

SPEEDUP is an equation-oriented process simulation package with procedure base property calculations. SPEEDUP contains a library of pre-coded simple unit operation models which can be combined to form more complex units. Both MINOS and SRQP (successive reduced quadratic programming) optimization algorithms are included with SPEEDUP (see Section 4.3.1 for more detail on SRQP). User defined models may be added using both SPEEDUP’s modelling code and additional FORTRAN procedures if required. The process flowsheet is specified by editing a keyword based text file, with a text based user interface providing syntax checking, result display and several error diagnosis tools.

The chemical process chosen for testing both real time optimizers was a stabilizer-splitter process at Shell Canada’s Sarnia refinery. This process is used to remove the light ends from a hydrocracked stream in the stabilizer column, and then remove the petroleum products in the splitter fractionation column. For a detailed description of this process, see Section 3.1.2. The stabilizer-splitter was chosen as being a suitably complex industrial process
for testing a real time optimizer, while being small enough to be optimized within a reasonable period of time using the computing resources available.

The basic structure of the real time optimizer to be developed using both types of process simulator is summarised in Figure 1.4. Both real time optimizers were developed in four stages:

1. The process model to be used in both the data reconciliation and economic optimization was simulated. The development of the process model is discussed in Chapter 3.

2. The data reconciliation optimization was added to fit the measured data to the process model using a least squares objective function optimization. Gross error detection was not performed on the process data. See Chapter 4 for details of the data reconciliation development.

3. The economic optimization using a profit objective function was developed. This optimization development is discussed in Chapter 5.

4. Finally, the above components were linked together to form the real time optimizer as shown above the dashed line in Figure 1.4. The plant, shown below the dashed line in Figure 1.4, provides process measurements either from real process data supplied by Shell, or from a steady state process simulation with noise added to the results. See Section 6.1 for details on the formation of the real time optimizers.

The testing of and results obtained from the two real time optimizers are also discussed in Chapter 6.

The development of the two real time optimization applications will also provide "test beds" for future on-line optimization testing and research. To date, most research into real time optimization has been conducted in industry, and there has been very little academic research into this area. The availability of a working real time optimization application should help close the gap between industry and research in the field of real time optimization.
In addition to comparing the two types of process simulators in real time optimization applications, two further areas of real time optimization were studied. The first is to study the effects of changes in the economic objective function on the real time optimizer. The results of this study is presented in Section 6.3. The second area is to demonstrate the effect of process disturbances on the operation of the real time optimizer (see Section 6.4 for details). The study of these areas will help to illustrate the benefits of performing real time optimization on this process when changes in either economic or process conditions occur.

1.5 Conventions Used in this Thesis

Real time optimizers and process simulators perform several different types of iterations during their operation. To prevent confusion about which type of iteration is being discussed, the following conventions will be used:
• "Cycle" will be used to indicate a full cycle of the real time optimizer. This is one complete run through the flow chart given in Figure 1.4. that is the measured data is read from the plant, data reconciliation is performed on this data, then the process is optimized before the set points are passed back to the plant.

• "Iteration" will normally refer to an iteration of an optimization algorithm (either SQP in ASPEN PLUS or SRQP in SPEEDUP). Iterations occur in both the data reconciliation optimization and the economic optimization steps of a real time optimization cycle.

• Flowsheet "passes" refer to one evaluation of the entire process flowsheet by the simulator. Multiple flowsheet passes are usually made on an iteration of an optimization algorithm.

• "Tear stream iterations" are required in ASPEN PLUS to converge a tear stream. To prevent confusion with optimization algorithm iterations, these will always be referred to in full as tear stream iterations. Several tear stream iterations are required on each flowsheet pass to converge a tear stream.
Chapter 2

Literature Review

2.1 Components of a Real Time Optimizer

A general structure for real time optimization based on the one shown in Hanmandlu et al. [49] is given in Figure 2.1. This structure is also similar to those presented in several other papers [17, 34, 38, 43, 44, 56, 68, 70, 83, 93].

The general steps taken in one cycle of the real time optimizer pictured in Figure 2.1 are:

1. Steady State Detection: This detects when the process is close enough to steady state to allow the real time optimizer to model the process with reasonable accuracy. When the plant is determined to be at steady state, data from the process is passed onto the optimizer.

2. Data Reconciliation and Gross Error Detection: All measured data are subject to error. Data reconciliation adjusts the measured variables (e.g., energy, mass, etc.) and, if possible, estimates any unmeasured variables for the process so that they satisfy the balance constraints. Gross error detection takes suitable corrective actions to rectify any gross errors found in the process data [101]. This adjusted data from the plant is then passed onto the next step.
Figure 2.1: General structure for model based real time optimization.

3. **Parameter Estimation**: The process of updating the model parameters to the adjusted process data available. These model parameters are then used in the process model for the optimization of the set points.

4. **Process Model**: The model of the process which represents the effects of changes made to the process by the optimization algorithm while it is iterating to an optimum solution.

5. **Optimization**: The optimization algorithm used to determine the optimum set points for the process given an objective function and process constraints.

6. **Updating of Process Set Points**: The optimum set points for the process found by the optimizer are returned to the plant. Once the plant has returned to steady state, another cycle of the real time optimizer is performed to keep the plant operating at its optimum.

Some of the above steps are detailed further in the following subsections.
2.1.1 Steady State Detection

Steady state is one of the most important assumptions made when designing a real time optimizer because the plant is being represented by a steady state model [82]. The steady state model is used to perform data reconciliation and parameter estimation on the raw data from the plant. If unsteady or transient data is used, the reconciled results may not accurately reflect the operation of the plant, and therefore the subsequent optimization of the plant may not yield a realistic optimum for the current operating conditions. For this reason, a method of checking for steady state is required before real time optimization can proceed.

In any steady state detection algorithm, two questions must be answered [87]:

1. Which measured variables should be used to determine if the process is at steady state? Not every measured variable should be analysed in assessing the state of the plant. The variables used to assess the plant condition should be chosen from the measured variables considered to be the most representative of the state of the plant. These choices are usually made based on operational experience within the plant.

2. How much variability in the measurements is allowed before the process is deemed unsteady? This question is also answered from plant operating experience. When the plant is considered to be at steady state over a period of time, the variances of the key variables can be estimated. These base variances can then be used to determine the plant's "steadiness" when compared to the future observed variances. Generally, on-line tuning of the steady state detection algorithm will be required over a period of time to ensure that the state of the plant is being predicted accurately.

Two methods for determining the condition of the plant have been proposed in the literature; the successive means test and examination of residuals. The successive means test offers a more statistically valid method of checking for steady state, while the examination of residuals method has a
higher degree of tunability. Figure 2.2 shows a general steady state detection program algorithm.

**Successive Means Test:**

Two papers by Narasimhan et al. [80, 82] detail the successive means test method. This test involves the calculating the means and variances of the key variables over two time periods. These two periods are then compared statistically to determine if there is a significant difference between the two means. This statistical test is based on the mathematical theory of evidence and is calculated using the following calculation [80]:

$$t_{1,i}^2 = \frac{(\bar{x}_{2,i} - \bar{x}_{1,i})^2}{\frac{s_{1,i}^2 + s_{2,i}^2}{N}}$$  \(2.1\)

where \(t_{1,i}^2\) = a random variables obeying Hoteller's \(T^2\) distribution with numerator degrees of freedom 1 and denominator degrees of freedom \(2N - 2\).

\(N\) = number of measurements in each period.

\(\bar{x}_{1,i}\) = mean value of variable \(i\) in the first time period.

\(\bar{x}_{2,i}\) = mean value of variable \(i\) in the second time period.

\(s_{1,i}^2\) = sample variance of variable \(i\) in the first time period.

\(s_{2,i}^2\) = sample variance of variable \(i\) in the second time period.

A level of significance, \(\alpha\), is chosen, and \(T^2(\alpha)\) is calculated to be the upper quantile of the \(T^2\) distribution. Two cases are now possible:

**Case I:** \(t_{1,i}^2 \leq T^2(\alpha)\), and therefore the plant is presumed to be at steady state with respect to variable \(i\).

**Case II:** \(t_{1,i}^2 > T^2(\alpha)\), and therefore the plant is presumed to not be at steady state.

The following assumptions are made in using this method:
Figure 2.2: General steady state detection program flowchart [87].
1. A process undergoes a change in steady state if the true values of one or more of its variables change.

2. Measurements of process variables only contain normally distributed random errors with mean \( 0 \) and covariance matrix \( Q \).

3. A time period consists of \( N \) successive measurements. The process state can change from one period to another, but within a period the process is assumed to be in a steady state.

4. Successive measurements are mutually independent.

5. \( Q \) is unknown. It is diagonal and constant from one period to another.

**Examination of Residuals:**

Examination of residuals is based on a confidence region approach to determine if the process is at steady state. A maximum residual value is chosen for each variable. The number of violations of this maximum residual are determined from the sample of \( N \) measurements over a given period. If the number of violations for a variable exceeds the maximum violations allowed, then the plant is assumed to not be at steady state. If the maximum violations allowed is not exceeded then the plant is presumed to be at steady state with respect to that variable. Figure 2.3 illustrates how the examination of residuals method determines both steady and non-steady state variables.

**2.1.2 Data Reconciliation and Gross Error Detection**

The key features of the process data problem are as follows:

1. All measurements are subject to errors. Random errors are assumed to be normally distributed and have zero mean. Gross errors are caused by non-random events such as instrument biases, malfunctioning measuring devices, inaccurate or incomplete process models and process
Figure 2.3: Examination of residuals test [52].

leaks [66, 73, 101]. Figure 2.4 gives an illustration of the probabilities involved for random and gross errors.

2. Not all process variables are measured for reasons of cost, inconvenience or technical infeasibility.

3. There is data redundancy in the sense that there are more measurements (or data) available than needed if the measurements were not subject to errors. This is also referred to as spatial redundancy [28, 73, 76].

4. Since most process data are being sampled continuously and regularly at great frequencies, there is also data redundancy if the process conditions are truly at steady state. This is usually referred to as temporal redundancy.

The adjustment of measured variables for random errors and, if possible, the estimation of unmeasured variables so that they satisfy the balance
Figure 2.4: Error probability distribution for process measurements [101].

constraints is known as the data reconciliation problem. Detection of the presence of any gross errors so that suitable corrective actions can be taken is known as the gross error detection problem [99]. Collectively, these two problems are sometimes called data rectification [100]. The objectives of data rectification are to improve confidence in the measurements, estimate unmeasured streams, identify meter faults and to identify process losses [63]. A simplified view of the three basic steps to data rectification is shown in Figure 2.5. The first step, variable classification, involves determining which variables are observable and/or redundant [66]. In practice, steps two and three are often used iteratively to reconcile the data and remove gross errors.

**Linear, Steady State Data Reconciliation:**

The simplest case is linear, steady state data reconciliation. This is covered by Mah [73] and Crowe et al. [31]. The basic model used for the data reconciliation in the absence of gross errors [73] is:

\[ y = x + \varepsilon \]  \hspace{1cm} (2.2)
where $y = (s \times 1)$ vector of measured variables:
\[ x = (s \times 1) \text{ vector of true variable values:} \]
\[ \varepsilon = (s \times 1) \text{ vector of random measurement errors.} \]

It is usually assumed that:

1. the expected value of $\varepsilon$, $E(\varepsilon) = 0$;

2. the successive vectors of measurements are independent. i.e.,
\[ E(\varepsilon_i \varepsilon_j^T) = 0, \text{ for } i \neq j; \]

3. the covariance matrix is known and positive definite. i.e.,
\[ \text{cov}(\varepsilon) = E(\varepsilon_i \varepsilon_i^T) = Q, \text{ and } Q \text{ is positive definite and known.} \]

The linear constraints are formed by stoichiometric constraint, energy, mass and other balances. In this case they are linear and homogeneous, and given by:

\[ Ax = 0 \quad (2.3) \]
where $A = (n \times s)$ coefficient matrix representing the linear process model ($A$ is of full row rank).

If we assume that the measurement errors are normally distributed, the data reconciliation problem may be formulated as the following constrained least squares estimation problem:

$$\min_x \left[ (y - x)^T Q^{-1} (y - x) \right]$$
subject to $Ax = 0$ \hspace{1cm} (2.4)

The solution is given by:

$$\hat{x} = y - QA^+ (AQA^+)^{-1} Ay$$ \hspace{1cm} (2.5)

Crowe et al. [31] use a projection matrix to obtain a reduced set of balance equations (equation (2.3)), and also include a statistical test for the removal of gross errors. Mah [73] also covers the decomposition and solution of these equations in detail.

**Nonlinear, Steady State Data Reconciliation:**

Nonlinear, steady state data reconciliation is the extension of the above method to include nonlinear constraints. These occur when variables are measured indirectly by other physical properties, e.g., concentration by density, pH or thermal conductivity. Bilinear constraints occur when variables appear in two balances, e.g., temperatures measured along with concentrations will appear in both energy and component material balances. Bilinear constraints also occur when a stream is split into two or more streams of the same temperature and composition. No general analytical solution is available to bilinear and nonlinear data reconciliation problems. Nonlinear constraints also make it more difficult to determine whether unmeasured variables may be estimated, and how to decompose a problem with missing measurements [73].
One simple method of solving the nonlinear data reconciliation problem is to extend the linear case to handle the nonlinear constraints [87]:

\[
\min_x [(y - x)^T Q^{-1} (y - x)]
\]

subject to \( h(x) = 0 \) \( g(x) \geq 0 \) \( (2.6) \)

where \( h(x) = \) the set of equality constraints representing the process model:

\( g(x) = \) any inequality constraints present in the process model.

There is no longer an analytical solution to the problem given in equation (2.6) and the problem must be solved using an optimization algorithm. In practical applications of this method, weights are added to the least squares objective function to place emphasis on key measured variables. A large weighting factor for a given variable will force the optimization to reduce the degree of adjustment for that variable. These weights are usually chosen based on operational experience. The objective function for the nonlinear data reconciliation then becomes:

\[
\min_x \left[ \sum_{i=1}^{n} w_i \left( \frac{y_i - x_i}{s_i} \right)^2 \right]
\]

subject to \( h(x) = 0 \)

\( g(x) \geq 0 \) \( (2.7) \)

where \( w = \) weighting factor associated with each measured variable:

\( y = \) the measured variable:

\( x = \) the true variable value:

\( s = \) the standard deviation of the measurements (usually the standard deviation of the measurement transmitter).

Crowe [26] handles the nonlinear constraints by extending the method outlined in Crowe et al. [31] by applying two successive projection matrices to the equations defining conservation laws and other constraints. Also, no restrictions are placed on the location of measurements, nor upon what is
measured in any one stream. The construction of the projection matrices is direct and each requires the inversion of a matrix that is also needed for subsequent steps in the solution.

A paper by Serth et al. [89] adds details on the choice of regression variables used in nonlinear data reconciliation by defining primary and secondary variables. Total flow and component flows are examples of primary and secondary flows respectively. Since material balances are linear in secondary variables, they can be exploited to develop a particularly efficient data reconciliation procedure [26]. However, they do not yield maximum likelihood estimates for the true values of primary measured variables. This in turn could affect the error detection procedure, tending to increase the number of Type I errors (Definition of Type I error is given in the Gross Error Detection section).

Data reconciliation using process simulation software has been looked at by both Macchietto et al. [70] and Stephenson and Shewchuk [95]. Both used equation based simulation packages. Macchietto et al. [70] used both SPEEDUP and a package using simplified process models called DEBIL. SPEEDUP was found to be slower and use more computational resources, but was more flexible. Stephenson and Shewchuk [95] detail the methodology by which MASSBAL solves the data reconciliation problem. Applications to a pulp mill screening and cleaning system are described.

Takiyama et al. [98] outline the use of SEBDARM (Sensor Based Data Reconciliation Method). The method is based on the direct use of measurement variables rather than using balanced variables (conventional method). This has the advantage of having the reconciled data not being influenced by the number of reduced balance equations. Their method, however, has only been tested on pilot plants to date.

**Dynamic Data Reconciliation**

This is relatively new area of research in the field of data reconciliation. In many practical situations the process conditions are continuously undergoing
changes and steady state is never truly reached. Generally the data reconciliation problem in this case is reduced to a discrete Kalman filter for a quasisteady-state problem [35].

Darouach and Zasadzinski [35] develop a new dynamic algorithm based on steady state reconciliation leading to a recursive scheme useful for real time processing of data. The method was shown to reduce computational problems associated with discrete Kalman filters, especially for singularities and round off error situations. Rollins and Devanatham [89] refine the method proposed by Darouach and Zasadzinski [35] to reduce the computational time required, while preserving its properties of unbiased estimation. Liebman et al. [66] use nonlinear programming to help solve systems in highly nonlinear regions where the Kalman filter method may be inaccurate. The method given was found to be a more robust means for reconciling dynamic data, especially in the presence of inequality constraints. The method is demonstrated on a reactor example.

Gross Error Detection

Gross errors in the data invalidates the statistical basis of reconciliation due to their non-normality. One gross error present in a constrained least squares reconciliation will cause a series of small adjustments to other measured variables. For these reasons, gross errors need to be identified and removed before data reconciliation is carried out. The most common techniques for detecting gross errors are based on statistical hypothesis testing of the observed or measured data. For any gross error detection method to work, there must be at least two alternative ways of estimating the value of a variables, for instance, measured and reconciled values [73]. Crowe [27] and Mah [73] give detailed accounts of typical statistical gross error detection algorithms.

Two measures of the effectiveness of a gross error detection scheme are the terms Type I and Type II errors made by the detection scheme. Type I errors refer to wrongly identifying truly random errors to be gross errors. Type II errors refer to wrongly finding truly gross errors to be random errors [27].
In devising the tests for a gross error, the probability of a correct detection must be balanced against the probability of mispredictions.

The Maximum Power (MP) test for Gross Errors is detailed in two papers by Crowe [29, 30]. The maximum power test has the greatest probability of detecting the presence of a gross error without increasing the probability of Type I error than any other test would on a linear combination of the measurements. Crowe [29] only deals with the linear case, while Crowe [30] extends the method to the bilinear case and retests the original constraints used.

The Generalized Likelihood Ratio (GLR) approach is detailed by Narasimhan and Mah [81] and Mah [73]. The previously discussed methods only deal with gross errors from measurement or sensor biases. The GLR approach provides a framework for identifying any type of gross errors that can be mathematically modeled. This can be very useful for identifying other process losses such as a leak. The method and examples of its use are detailed reasonably fully by Narasimhan and Mah [81]. Narasimhan [78] shows that the Maximum Power Test detailed above is equivalent to the GLR approach for simple steady state models.

Serth and Heenan [91] tested 3 different methods of gross error detection on the same steam metering system. These methods were:

1. Measurement test (MT) method. This method proposed by Mah and Tamhane [74] uses a test which possesses maximal power properties for detecting the presence of a single outlier (gross error) of the least squares residuals. The main problem with this method is that the least squares procedure tends to spread the gross errors over all the measurements, thereby creating large residuals corresponding to good measurements [91]. Two modifications of the MT have also been proposed: the iterative measurement test (IMT) method, and the modified iterative measurement test (MIMT) method. The IMT method simply applies the MT method iteratively removing one gross error at each iteration until none remain. IMT, however, can predict sets of recon-
ciled variables which may contain negative flow rates or absurdly large values. The MIMT adds bounds to the reconciled variables to prevent negative flows and absurdly large values.

2. Method of pseudonodes (MP). This method proposed by Mah et al. [72] is based on a nodal imbalance test applied to each node and also to aggregates of two or more nodes, which are called pseudonodes. This method predicts potentially bad streams (i.e. may contain gross errors) and then treats these streams as being bad. Therefore this method will tend to err on the side of treating good streams as containing gross errors [91]. A modified method of pseudonodes (MMP) fixes a problem which arises in MP when no potentially bad streams are predicted, but one or more nodes are bad. Practically, this modification has very little effect on the performance of this method.

3. Combinatorial method. The basic idea behind this method proposed by Serth and Heenan [91] is to identify combinations of gross errors that are consistent with the observed pattern of nodal imbalances. The Combinatorial method was found to be less susceptible to error cancellation than MP or MMP as the algorithm does not work with aggregates of nodes. However, this method can result in an extremely large combinatorial problem, even on on a system of moderate size. The Screened Combinatorial (SC) method was proposed to alleviate this problem by using the MMP method as a screening procedure to reduce the size of the combinatorial problem.

From the results of their testing, Serth and Heenan [91] concluded that both the screened combinatorial (SC) and modified iterative measurement test (MIMT) methods constitute effective and reliable methods for gross error detection and data reconciliation in steam metering systems. MIMT was found to be computationally more efficient than the SC method. Both the MT method and MP were found to perform very poorly.
Combined Data Reconciliation and Gross Error Detection Methods

Two papers by Narasimhan and Harikumar [50, 79] give details of incorporating bounds into data reconciliation. Most approaches to data reconciliation do not impose inequality constraints because the solution can no longer be obtained analytically, and the statistical analysis of the measurement residuals for gross error detection is difficult. This leads to an iterative cycle of data reconciliation and gross error detection phases to complete the data rectification. Narasimhan and Harikumar [79] develop the algorithm for solving the data reconciliation problem with bounds and produce the constraint and measurement residuals. In the second paper [50], the gross error detection procedures are detailed and the whole method is compared to existing methods. Their results indicate that their method performed better than currently available methods.

Tjoa and Biegler [101] develop a simultaneous data reconciliation and gross error detection method. They minimize an objective function that is constructed using maximum likelihood principles to construct a new distribution function. This distribution takes into account both contributions from random and gross errors. This method gives unbiased estimates in the presence of gross errors. Therefore simultaneously a gross error detection test can be constructed based on the new distribution functions without the assumption of linearity of constraints. This method is particularly effective for nonlinear problems.

Serth et al. [92] show how the choice of regression variables can adversely affect the performance of an associated gross error detection algorithm. The principal effect is an increased tendency of the algorithm to make Type I errors. Their study was carried out on two sets of variables: primary or total flow variables, and secondary or components flow rates. They conclude that for systems with relatively small numbers of variables and constraint equations, data reconciliation should be performed by regressing the primary variables. For large systems where computational efficiency has a high priority, the best approach may be to regress on the secondary variables and
to use the primary residuals for gross error identification.

Terry and Himmelblau [100] detail the use of Artificial Neural Networks (ANN) for Data reconciliation and gross error detection. The ANN is "trained" or "learns" to perform the data rectification based on a given model and constraints. The method is still being researched and the results look promising compared to models built from first principles.

2.1.3 Parameter Estimation

Parameter estimation, or model parameter updating, involves updating of any process parameter in the model which changes slowly over time, usually due to wear and tear of the equipment or catalysts. Process parameters include heat transfer coefficients, column efficiencies and loading factors, and reactor effectiveness factors. The real-time updating of a model's parameters permits realistic models to be provided for an optimization system. Another benefit of parameter estimation is the ability to track the condition of equipment in the plant with time (e.g., heat exchanger fouling, catalyst activity etc.) [32].

A simple method of updating process parameters is to include them in the objective function during data reconciliation. Since these parameters should not vary significantly between each cycle of a real time optimizer, movement from the previous parameter value should be penalized. This can be achieved by setting the weight associated with a parameter to a large value (e.g., two or three orders of magnitude larger than the weights associated with measured variables) [87]. In this case, the nonlinear constrained data reconciliation problem given in equation (2.7) becomes:

\[
\min_{x, p} \left[ \sum_{i=1}^{n} w_i \left( \frac{y_i - x_i}{s_i} \right)^2 + \sum_{j=1}^{m} v_j \left( p_j' - p_j \right)^2 \right]
\]
subject to \( h(x) = 0 \)
\( g(x) \geq 0 \)

where \( v = \) weighting factor associated with each parameter to be estimated;
\[ p' = \text{the previous estimated parameter value}; \]
\[ p = \text{the estimated parameter value.} \]

MacDonald and Howat [71] propose two different methods of combined data reconciliation and parameter estimation. The first method is a sequential, "decoupled" procedure that reconciles the data to satisfy the material and energy balances, and then estimates the process parameters using maximum likelihood estimation. The second method is a "coupled" procedure that simultaneously reconciles the data to satisfy the constraints and estimates the process parameters. Both methods were tested on a single stage flash. It was found that the decoupled procedure was computationally faster and more easily adapted to existing reconciliation algorithms. However, the coupled procedure was more statistically rigorous and gave better parameter estimates.

Krishnan et al. [59] present a two step method for the design of a robust parameter estimation scheme that may be used to update the process model employed in on-line optimization. This method is summarized in Figure 2.6. The first step involves determining the "key" model parameters (i.e. those having a significant effect on the calculated optimum). The second step involves finding the "best" set of measurements to estimate these parameters. This is achieved by using structural analysis, singular value analysis and calculation of parameter confidence regions. A case study using this method is detailed in a later paper [60].

Stewart et al. [96] provide an extensive review of Bayesian and likelihood approaches to parameter estimation from various types of multiresponse data with an unknown covariance matrix. They found that these methods are preferable to weighted least squares and to use of a specified covariance matrix, since they estimate the covariance and parameters optimally from the data provided. Several software programs were described for performing both least squares and multiresponse parameter estimation. Some multiresponse applications were also reviewed.
Figure 2.6: Methodology for selecting a robust parameter estimation scheme [59].
2.1.4 Process Model

The process model used in real time optimization must represent changes in the manipulated variables of the process given the updated set points calculated by the optimization algorithm. The model approximates the effect of these variables on the dependent variables, which are usually those that are constraints or those that have a significant economic impact, such as yields, material balance or utility usage. In virtually all practical cases, the model is based on steady state (rather than dynamic) relationships and is non-linear [34]. The choice of measurements to be used for matching the model parameters to the plant operations must be made carefully to avoid an infeasible problem. Bailey et al. [17] chose their variables so that each piece of equipment had enough associated specifications for the available degrees of freedom. Development of process models for optimization is covered in detail by Edgar and Himmelblau [37].

Fatora and Ayala [38] discuss the application of open equation-based models. Instead of posing an equation in its closed form, for example equation (2.9), the equation should be formulated in its open residual format as shown in equation (2.10).

\[ Q = mC_p(T_2 - T_1) \]  \hspace{1cm} (2.9)

\[ R = Q - mC_p(T_2 - T_1) \]  \hspace{1cm} (2.10)

A simultaneous equation solving and optimization package will manipulate the unknowns such that the residual terms, \( R \), are driven to zero. This method gives the same results as the closed form equation. The advantage of open form equations is that the model formed from them are more easily maintained than closed form models. Such models are easily modified to account for process changes in the plant since the convergence scheme is separated from the model. The maintenance staff need not recode the convergence scheme each time the model is changed. The open equation-based
approach to process simulation has been used successfully in industry for several years with the proper mathematical tools available.

Two papers by Forbes et al. [43, 44] give some criteria for helping choose a model adequate for real time optimization. The quality of the model has a large effect on the success of the real time optimization system. They give a point-wise model adequacy criterion as the ability of the model to have an optimum that coincides with the true plant optimum. Analytical methods for checking the point-wise model adequacy were developed using reduced space optimization theory, and from these more practical numerical methods were developed for use on industrial problems [44]. A later paper by Forbes and Marlin [42] extends the point-wise model accuracy criteria to yield a set of necessary conditions which must be met for a given real time optimization system to exhibit zero-offset in the manipulated variables with respect to the plant optimum. They also introduce the idea of Design Cost as a framework within which real time optimization design decisions can be made. The Design Cost metric consists of two terms: one for offset from the plant optimum manipulated values and one for the covariance of the model based predictions of the optimal manipulated variables. A systematic method for selecting which parameters should be adjusted by the real time optimizer based on Design Cost is presented.

Bailey et al. [17] briefly cover some modeling issues affecting their non-linear optimization of a hydrocracker fractionation plant. They found that large equation-based models are sensitive to scaling. However choosing appropriate units avoided numerical problems, even if the resulting units were unusual (e.g., TJ per day). Numerical stability of the model can also be a problem and care should be taken to avoid division as an operator. Also, during the optimization, bounds must be placed on certain variables to prevent the solution from moving too far from the starting point. This is because it takes a finite amount of time to move the plant to a new operating point, therefore the set points should not be moved a great deal on each run of the optimizer. They suggest choosing bounds on the variables to reflect the
allowable change in 1 to 3 hours. The maximum change should depend on the length of time it would take the control system to take the maximum step and bring the plant back to steady state.

A common method for more rapidly computing the optimum is an “inside-out” algorithm first proposed by Boston and Britt [21] to solve a single stage flash algorithm. In this method the major iterations deal with updating the parameters for the simplified models and matching their properties with a rigorous model. Therefore since the more computationally expensive model is only evaluated in the outer loop, considerably less effort is required than with a conventional procedure. However, Biegler et al. [19] and Forbes et al. [44] point out that when this method is applied to optimization problems, this approach based on simplified models can converge to a solution that may not necessarily correspond to the optimum predicted when only rigorous methods are used. They give two observations to help avoid this problem when the “inside-out” type of algorithm is used:

1. A necessary condition for an appropriate simplified model for optimization is that it recognizes the rigorous model optimum as a Karush-Kuhn-Tucker (KKT) point, that is an optimal point.

2. A sufficient condition for an appropriate simplified model is that it matches all the gradients of the rigorous at all points of interest.

Several papers cover the use of commercially available process simulation packages used as the process model, although there is no evidence to date of this method being used in industry. Two types of simulation packages are available. The first are open form, equation oriented or simultaneous process simulation packages, for example, SPEEDUP and MASSBAL. Although these simulators are more flexible, they generally require a high level of expertise to learn and use, have poor user interfaces, and are not widely used in industry. The second type is the closed form or sequential modular process simulation packages, for example, ASPENPLUS, PRO II and HYSIM. These packages are widely used in industry due to their proven reliability and ease
of use, however, they are less efficient with respect to speed and computer processing power required [45]. In addition they require special techniques and insights to develop and change the optimization strategies for on-line operation due to the sequential modular architecture.

Gallier and Kisala [45] used ASPEN, a sequential modular package, in their study of real time optimization. They cover two methods where the simulator is treated as a "black-box" and as an infeasible path optimization using the SQP method. It was found that the latter is preferable as the constraints at each iteration need not be satisfied. This allows the optimization of the process model to be completed in as few as five simulation time equivalents. Macchietto et al. [70] used the equation-based SPEEDUP process simulation package as the process model and also to perform the data reconciliation, gross error detection and optimization steps. Dynamic real time optimization is also possible using the SPEEDUP package. Shewchuk and Morton [93] outline the use of SACDA's MASSBAL process simulation packages as the model in their OPTIMIZER package. This package is also capable of both steady state and dynamic optimization.

2.1.5 Optimization

Objective Function

The objective function is derived from the plant model, and is to be either maximized or minimized through changes in the independent variables. The objective function for real time optimization normally represents the economic model of the process, usually limited to variable effects and ignoring fixed costs such as labour, overheads, etc. A typical objective function given in Darby and White [34] is:

\[
\text{Objective} = \text{Product value} - \text{Feed costs} - \text{Utility costs} + \text{Other variable economic effects}
\]  

(2.11)

Bailey et al. [17] cover objective function development in detail. Feed
and product prices must be chosen carefully since different values are often associated with the same material. For example the product might have a contract price, spot market price and also be an intermediate stream sent to another part of the plant for further processing. The case of a stream being an intermediate stream and a product is particularly difficult to determine an accurate value for an inter-process stream, as many planning models only consider feeds and finished products. One remedy for this problem is to include a simple model of the finishing process in the objective function thereby giving an approximate value to the inter-process stream.

Since the optimizer will be estimating derivatives of the objective function with respect to operating variables, it is important that the objective function be continuous. Discontinuities arising from streams with multiple prices should be treated specially (e.g., the stream has a contractual price and a spot price). Often an average price for the stream is not acceptable, and the discontinuity caused needs to be handled by a method such as an integer programming technique.

Bailey et al. [17] also show how they developed their objective function for the real time optimization of a hydrocracker fractionation plant in some detail. Edgar and Himmelblau [37] cover the development of objective functions including methods for measuring profitability and cost estimations.

**Optimization Algorithm**

The optimization algorithm uses the process model and the objective function to solve for the new optimum set points for the plant. The important considerations in choosing an optimizing algorithm are computational requirements, number of objective function evaluations and robustness. The general form of the constrained optimization problem using the process model
and the objective function [38] is:

\[
\min_{z} \text{ (or max)} [F(z, p)]
\]

subject to \( f(z, p) = 0 \) \hspace{1cm} (2.12)
\[ z_{l} \leq z \leq z_{u} \]

where \( F(z, p) \) = the objective function;
\( f(z, p) \) = the vector of \( n \) equality constraints (from the process model);
\( p \) = fixed variables or parameters (e.g., fouling factors, cost coefficients etc., changes in these variables will change the optimum values of \( z \));
\( z \) = the process variables which can be varied to optimize \( F \) (the number of these variables must be greater than \( n \));
\( z_{l}, z_{u} \) = the lower and upper bounds on the variables \( z \) respectively (which give the inequality constraints on the model).

Methods on how to solve the above constrained optimization problem are covered in several texts [37, 40, 47]. A great deal of literature is available on optimization algorithms, and generally is considered to be a mature area of mathematics.

Presently, the most common type of algorithm reported in the literature for solving this type of problem are Sequential (or Successive) Quadratic Programming (SQP) techniques. The SQP method approximates the objective function by a quadratic function, and the constraints by linear functions, so that quadratic programming can be used recursively to find a search direction minimizing the objective function. At each outer iteration (or quadratic program solution) the SQP method constructs these approximations using information about the values of the variables and their derivatives with respect to the decision variables [37, 40, 69, 93, 103]. Edgar and Himmelblau [37] provide a table of the sources of computer codes for SQP methods. Lucia and Xu [69] provide an extensive review of the SQP algorithms available, particularly with respect to chemical processes and large-scale problems. Fatora
and Ayala report the use of an SQP algorithm in their real time optimization with over 36,000 variables and 31,000 equations.

Bailey et al. [17] use the MINOS routine developed by Stanford. MINOS is a sequential quadratic programming technique which also makes use of the Simplex method and a projected Lagrangian algorithm. The MINOS method is detailed by Murtagh and Saunders [77], and has been shown to solve large problems of around 5000 variables and 4500 equality constraints successfully.

The DICOPT routine is discussed in a paper by Kocsis and Grossman [58]. DICOPT is an outer-approximation/equality relaxation algorithm specifically designed for process systems involving mixed-integer nonlinear programming (MINLP) due to nonlinearities in the models. The algorithm was tested successfully using problems of up to 528 variables and 1171 constraints, including 74 binary variables.

2.2 Methods of Real Time Optimization

2.2.1 Global or Centralized Approach to Real Time Optimization

This is the most common approach found in the literature. It involves optimizing the plant as a whole using one objective function, subject to constraints, and a model of the entire plant.

Several examples in the literature use very similar techniques of taking a rigorous steady state model of the process which is then optimized using a nonlinear objective function and constraints. In all the cases listed below, the model appeared to be developed specifically for the real time optimization implementation. Examples of this general form were performed on the following plants:

- Hydrocracker fractionation plant, Bailey et al. [17]. The optimization algorithm was carried out using MINOS 5.1 on nonlinear mass and energy balances models and nonlinear constraints. Comparison is made to
a rank-null space decomposition SQP (Sequential Quadratic Programming) optimization technique. The problem involved 2836 equations, 2891 variables and 10 degrees of freedom. Modeling issues were found to be problems with scaling of the problem, numerical stability, particularly when using the division operator, and minimizing the number of relinearizations of the model constraints required to find the optimum. Bounds were placed on the maximum amount any variable could be changed in a run of the real time optimizer to prevent large set point changes destabilizing the plant. Objective function development was also covered in detail.

- Olefins plant, Fatora and Ayala [38]. Rigorous, fundamental chemical engineering models were developed for the olefins plant. All of the models were written in the open equation form and were optimized using an SQP algorithm. The resulting complex nonlinear optimization problem contained over 36,000 variables and 31,000 equations, and approximately 20 minutes is taken to complete a full cycle of the real time optimizer. The real time optimizer was commissioned in February 1991, and took a total of three weeks to fully implement. The payback was less than one year. The observed benefits from installing the real time optimizer were:
  - Improvements of 5% to 10% of the value added by the process.
  - Consistently holding the process at production targets.
  - Decreased product variability.
  - Optimal handling of utility versus yield trade-off.
  - Many perceived bottlenecks were eliminated.
  - Energy savings.
  - Increased productivity by trending unit performance and monitoring of key parameters.
  - More accurate off-line planning.
• Olefins plant, Lojek and Whitehead [68]. This reference gave very few specifics on what methods they actually used in the real time optimization. They do however outline a very generalized method. The model was based on a set of modular blocks of successive plant sections. The advanced local control techniques used in the plant were also detailed in the paper.

• Hot acid leaching and strong acid leaching residue treatment plant in a zinc refinery, Krishnan et al. [60]. The purpose of this real time optimization was to show the effectiveness of the robust parameter estimation method as outlined in Krishnan et al. [59] and the development of the rigorous steady-state model required. However, the reference mentions very little about the optimization itself.

• Ammonia process, Tsang and Meixell [102]. A rigorous plant model built from first principles was used for the ammonia unit handling 1600 t/day. They found that statistical regression type models were found to have significant disadvantages to the rigorous model approach. The model was performed in Exxon Chemical’s Equation Manager and Solver (EMS) package using 5500 equations with 160 tear streams taking two person years’ effort to set up.

• Packed-bed immobilized-cell reactor, Hamer and Richenburg [48]. Used a recursive least squares algorithm and high pass filtering of the data to estimate the parameters in the discrete-time dynamic model which was optimized by a full Newton optimization algorithm using the objective function’s curvature information. The process was relatively small compared to most of the other plants listed, although it did involve very noisy process data.

• Refinery power plant, Wellons et al. [103]. The MESA nonlinear simulator was selected to model the power plant unit as it was specifically developed for power plants. Mobil’s proprietary SQP optimiza-
tion technology, MOPT, was used as the optimization algorithm. They ran the real time optimization algorithm every 30 minutes, but have the option of execution on demand. The system averages 20 updates to the plant per day. From an audit of the on-line power plant optimizer, savings of approximately $2.1 million/year or a 3% saving in fuel consumption were found.

- Pulp refining process, Strand et al. [97]. They found that the model based control technique was dependent on three main factors:
  
  1. Robust, mechanistic models which accurately describe the effects of process conditions over a wide range of operating conditions.
  2. Tuned parameters for the refiner models so that the equations accurately represent the real process.
  3. Optimization and control techniques which allow the refiner models to be applied in a systematic fashion.

They found the weaknesses of their optimization system were maintaining the flow of information to the model and ensuring the correct information is available. Maintenance of the system was found to require a dedicated effort from both the mill and vendor.

- Refinery hydrogen plant, Bussani et al. [23]. On-line data reconciliation, gross error detection and optimization were carried out on the hydrogen plant. A sequential modular modelling approach was used. The model contained 27 units and 51 streams, including 8 recycle streams. The optimization was solved using a feasible path/black box method based on SQP. The paper covers the development of the data reconciliation and optimization steps in some detail.

- High-pressure low-density polyethylene (LDPE) tubular reactor, Kiparissides et al. [57]. Parameter estimation, modelling and optimization issues specific to the LDPE tubular reactor are discussed in this paper
in some detail. Unfortunately very few numerical or structural details of the real time optimizer are given. It was found that real time optimization of this process offers large economic gains due to its high volume and extreme operating conditions on one hand, and tight profit margins and quality specifications on the other.

Jang et al. [56] took a two-phase approach to the global real time optimization method. The problem of plant operation is based on the idea of a moving time horizon. The method uses the present measurements and the measurements taken during the past period of time, together with a partial knowledge of the plant's physical and chemical principles governing the plant, to give an optimal time plan for the manipulation of the set points for a future period of time. The plant is modeled by either a steady state or dynamic model depending on how stable the plant is. The two phase approach is summarized in Figure 2.7. The identification phase of the method is only carried out when the process has been significantly disturbed from the previous steady state.

Several authors have proposed using process simulation packages for performing real time optimization and data reconciliation of chemical processes:

• Zhang et al. [105] used a combination of ASPEN PLUS for process optimization and parameter estimation, and GAMS/MINOS for data reconciliation and gross error detection to form a real time optimizer for a Monsanto sulphuric acid plant. The data reconciliation and gross error detection method used was the bivariate approach proposed by Tjoa and Biegler [101]. The data reconciliation involved 39 process measurements, 29 of which were required to determine the state of the process. Parameter estimation in ASPEN PLUS used a least squares optimization to determine the 22 key parameters. Other details such as data validation and simulation errors were also covered in this paper. A profit improvement of 17% was achieved, as well as a 25% reduction in stack gas emissions over the previous operating conditions.
Figure 2.7: Two phase approach to on-line optimization [56].
• Gallier and Kisala [45] use process simulation as the process model using a SQP optimization algorithm to solve for the optimum. Their steps to create the real time optimizer, given the model of the plant, were to:

1. identify the objective function.
2. identify the degrees of freedom for the optimization.
3. identify the constraints.

They found the SQP method was very efficient at finding the optimum of the ammonia synthesis example they tested. However, they did not extend the method to a real plant situation nor mention the use of data reconciliation or gross error detection in their method.

• Bossen et al. [20] discuss the use of the equation oriented simulator GHEMB for simulation, optimization and data reconciliation of chemical processes. They found that the equation oriented approach was better suited for handling complex and highly integrated process flowsheets. Examples of data reconciliation and optimization were performed on an ammonia process containing 5 recycle streams using a SQP optimization algorithm.

• Macchietto et al. [70] used a an equation oriented simulator, SPEEDUP, a data screening program called DEBIL and the SPEEDUP External Data Interface (EDI) as a communication mechanism to form a real time optimizer. Figure 2.8 gives an outline of plant/control/simulator system. SPEEDUP has an advantage of having both SQP and MINOS optimization routines built into the simulator. They conclude that the SPEEDUP flowsheet optimizing package, using the built in external data interface, can be used successfully on-line with a plant control system. Only case studies are presented in the paper, and no evidence of an industrial application of this method of real time optimization was given.
Figure 2.8: Integrated plant/control/simulator system [70].
Several process simulation companies are also developing real time optimization and on-line modelling systems. Honeywell Hi-spec Solutions is developing a system called RTEXEC (previously called OPTIMIZER) based on their equation oriented process simulator MASSBAL [51, 52, 93]. Aspen Technology is also currently developing an equation oriented real time optimization system called RTOPT [14]. Simulation Sciences is developing a rigorous on-line modelling system called ROM which will also be capable of real time optimization [94]. Hyprotech and MDC Technologies are also developing a real time modelling and optimization package called HYSYS.RTO+ [55]. At the time of writing, there were no known industrial applications of these three packages as real time optimizers.

2.2.2 Distributed Approach to Real Time Optimization

The distributed approach breaks down the overall optimization into several local optimizations which are coordinated by a unit optimization/coordination model. Figure 2.9 contrasts the distributed approach to the centralized or global approach [34]. The aim of the distributed approach is to decompose the large scale plant into subsystems thereby reducing the complexity of the original optimization problem [3]. The distributed approach is also sometimes referred to as modular or hierarchical optimization. Distributed real time optimization has been likened to a "bottom-up" implementation of optimization as opposed to the "top-down" centralized approach.

Darby and White [34] give a proposed overall control systems structure to deal with the distributed real time optimization shown in Figure 2.10. Some short examples are given to illustrate that the distributed approach will lead to the same answer as the global approach, but very little detail on implementation of the method is given.

Arkun and Stephanopoulos [3] give a very detailed method of how to perform optimization on a plant decomposed into its subsystems with functional
Figure 2.9: Centralized vs. distributed optimization [34].
Figure 2.10: Overall process control systems structure [34].
uniformity and common objectives in terms of economics and operation. The subsystems are not independent of each other so interconnections between the subsystems are defined. Local optimizing controllers are designed for each subsystem, $S_i$, of the plant. If the plant has $N$ subsystems, then the subproblem $S_i, i = 1, \ldots, N$ is subject to the system constraints, as given by:

$$\min_{u_i, m_i} l_i = \Phi_i(x_i, m_i, u_i, d_i) - \lambda_i u_i + \sum_j \lambda_j^T Q_{ji} y_i$$  \hspace{1cm} (2.13)$$

where $d_i$ = vector of disturbances entering the subsystem $S_i$;

$l_i$ = sub-Lagrangian for a subsystem $i$;

$m_i$ = vector of manipulated variables;

$Q_i$ = incidence matrix denoting the interconnection among the subsystems;

$u_i$ = vector of interconnection points;

$x_i$ = vector of state variables;

$y_i$ = vector of output variables;

$\lambda_i$ = Lagrange multipliers for the interconnection constraints;

$\Phi_i$ = subobjective function.

The coordinator or overall optimizing problem for the plant attempts to satisfy the interaction balance between the subsystems by satisfying:

$$u_i = \sum_{j=1}^{N} Q_{ij} y_j$$  \hspace{1cm} (2.14)$$

By performing this decomposition, and by properly formulating the subsystem control objectives, the selection of the controlled and manipulated variables can be made in a decentralized fashion. The method also deals with the sequencing of the set point changes using "Sequencing Trees" to ensure plant safety and bottlenecking are considered. The best route selected should also try to reduce the number of set point changes made and select the smoother and faster routes with respect to plant operation.
There is no agreement in the literature on whether distributed is better than global real time optimization or not. Darby and White [34] claim the following advantages for the distributed approach:

- The distributed optimization can be carried out more frequently than the global approach as the method only has to wait for steady state in each subsystem rather than the plant as a whole.

- The local optimizers can model the subsystem more accurately and completely than a global optimizer can as the individual model dimensionalities will be less restricted than the global model. Also different models can have different optimization levels.

- Local optimizers permit the incorporation of on-line adaptation or on-line parameter estimation more easily.

- Local optimizers are easier to maintain as they are less complex and hence easier to understand than a large global optimizer.

- If problems are occurring in the modeling, the local optimizer causing the problem can be taken off-line while the rest of the optimizers continue to function. A global optimizer would have to be completely turned off to be restructured.

Bailey et al. [17], however, point out two major difficulties with the distributed approach:

- The constraint information being passed between local unit optimizers to prevent conflicts is not as effective as that in a global approach.

- It is possible to get inconsistencies in the update of the parameters when only parts of the process are considered in the local optimizers.

Unfortunately no actual case studies using the distributed approach were available to help determine which approach gives better results.
2.2.3 Direct Methods (Model free approaches)

The real time optimization is performed directly on the process without explicitly using any model. Direct methods are discussed by Arkun and Stephanopoulos [2] who conclude that the method is too slow and simplistic for on-line optimization. The method is an evolutionary operation, sometimes called an on-line hill-climbing gradient search, where after each trial of set point changes, the objective function is measured at steady state and its sensitivity is used to readjust the set point. Large numbers of set point changes and on-line sensitivity measurements are required to observe the behaviour of the objective function, especially when process noise is present. The method is also slow to reach the optimum as it has to wait for steady state after each set point change. In early attempts at real time optimization, this method was used and criticized for its slowness.

2.3 Implementation

Two papers by Latour [61, 62] cover many of the issues relating to real time optimization from a business objective point of view. A list of their requirements for an on-line optimization project to be successful are:

- Select proper independent variables.
- Formulate model requirements.
- Formulate business objective functions.
- Select optimization algorithms appropriate to the nature of the problem (process and business). Always guarantee a feasible solution. Handle partial equipment failures.
- Specify sensor inputs and manual inputs.
• Define human interface for objectives, defaults, economic parameters, physical limits, laboratory analyses. The system must inform people what it is doing and why.

• Specify the interface with regulatory controls. Consider timing, move limits, output sequencing, process dynamics, stability and interactions.

• Specify computer hardware and software.

• Consider procedures for maintaining model fidelity, process and economic.

However, what an on-line optimizer will not achieve when it is implemented into the plant is:

• Determine business objectives of the plant.

• Specify the process and economic models.

• Select criteria for finding and defining the plant optimum.

• Select the best set of independent variables.

• Specify mechanical or safety limits

• Determine market requirements for product quality.

• Verify product values, fuel and feed costs, and production rate limits.

All process models are only approximations of real process behaviour. Therefore as operating conditions in the units shift with time, the model coefficients will require updating. Also new constraints may need to be added or old ones deleted at some point. Whether some model maintenance should be carried out manually or automatically is an important decision to be made in the implementation of the optimizer. Ongoing long term maintenance of the on-line optimizer must be carried out after implementation. There have
been many cases of initial successes which later floundered due to an inadequate number of trained personnel assigned to the long term maintenance of the optimizer. This often results in the real time optimizer falling into disuse.

The complexity of the process model also determines the sophistication of the maintenance required. Not all variables and constraints can be included in the process model. The art of optimization modeling is to select the variables that have the most significant effect on the economics and important constraints, while eliminating those of lesser significance [34].

It is difficult to convey to operators what the optimizer is doing and why. Generally, if the operator does not understand the results, the optimizer will be turned off at the first excuse. Simplicity and modularity in the interface to the operators will enhance understanding [34]. Campbell [24] and Hanmandlu et al. [49] both cover features of on-line optimization software. Figure 2.11 shows how an on-line optimizer interacts with other parts of the plant. Good training and documentation at both the user and system level are required to get the best results out of the optimizer.

The real time optimizer needs to be able to operate without some available process measurements. If the optimization is disabled every time a single input is off-line, then it will not be in use very much in a large plant. Methods for getting around this problem include estimating the missing input or being able to switch off that portion of the optimizer affected by the loss of the input [34].
Figure 2.11: Interaction of optimizing program in the plant system [24] [49].
Chapter 3

Process Simulation Model Development

3.1 Introduction

3.1.1 Objectives

The objective in developing the process simulation model is to represent the real stabilizer-splitter process as closely as possible. This process model will be used as the basis for both the data reconciliation of the raw plant data and the subsequent economic optimization of the process set points. Figure 3.1 highlights the part of the real time optimizer to be discussed in this chapter.

3.1.2 Process Description

The process to be modelled consists of a stabilizer column and a splitter column used to prepare the feed stream for a catalytic cracking unit in an oil refinery. A process flow diagram of the plant to be modelled is given in Figure 3.2.

The stabilizer column is fed by a hydrocracked petroleum based stream on stage 14 of a 29 stage column. Light hydrocarbons and other gases are re-
Figure 3.1: Real time optimizer process flow diagram with process model highlighted.

moved in the Vapour product stream from the stabilizer's partial condenser. The liquid product from this condenser, C_4-distillate, contains mainly C_4 hydrocarbons. The bottoms from the stabilizer are passed though a heat exchanger before being fed into the splitter column on stage 21.

The splitter column consists of a 24 stage main column with two 3 stage sidestrippers. Three product streams, Light Iso, Heavy Iso and Light Distillate, are removed from this column, and the bottoms are fed to the hydrocracker. Light Iso is a gasoline product stream removed from the total condenser on the main splitter column. Heavy Iso, also a gasoline product stream, is removed from the reboiler on the first sidestripper. This sidestripper is fed by a liquid draw from stage 15 of the main column, and returns vapour to stage 14. Light Distillate, a heating oil product stream, is removed from the reboiler on the second sidestripper. This sidestripper is fed by a liquid draw from stage 18 of the main column, and returns vapour to stage 17.

Note that the column stages are numbered from top to bottom following
Figure 3.2: Stabilizer-splitter process flow diagram. The portion of the process to be modelled is contained within the dashed box.
the convention used the two process simulation packages used. Also, the stages used in these columns are equilibrium stages. that is, tray efficiencies are not used when modelling this flowsheet.

3.1.3 Development Method

The ASPEN PLUS and SPEEDUP process simulation models were developed using the same method:

1. Choose the components and pseudo-components, and develop the rigorous thermodynamic properties. These were developed based on stream assay data provided by Shell Canada.

2. Develop the process flowsheet around the operating point provided and compare results to those generated by Shell’s real time optimizer. The point at which this simulation was run was a typical plant operating point for which the data had already been reconciled to fit mass and energy balances. The results of the simulation being developed were checked against the results of Shell’s real time optimization simulation run on the same data.

3. Validate the process model using raw data from the plant. Key variables were checked to ensure that they were being modelled correctly by the process simulation package. A great deal of experience from plant operation was required to check that the results were reasonable and consistent.

3.2 Properties

Both of the process simulation packages, ASPEN PLUS and SPEEDUP, interface with the same properties package, PROPERTIES PLUS [6, 7, 10]. Therefore the properties development for both simulators was identical.
The properties were developed using the MODELMANAGER graphical user interface [8, 9].

Hydrocracked refinery streams typically consist of a range of components from gases such as hydrogen and ammonia to hydrocarbons ranging from methane to nonane and other heavy hydrocarbons. For hydrocarbons components above pentane, many isomers with different properties may exist in the stream. Due to the large number of components present in small quantities, components above pentane are approximated using pseudocomponents. Pseudocomponents are defined in boiling point ranges, e.g., one pseudocomponent may represent all hydrocarbons boiling between 125°C and 145°C. Each pseudocomponent has an associated boiling point, specific gravity and molecular weight which are used to determine other physical and thermodynamic properties for that pseudocomponent. Pseudocomponents are then treated by the simulator in the same way as all other components [4].

The component composition of the stabilizer feed stream was determined from a light ends analysis, true boiling point (TBP) curve, stream specific gravity and stream molecular weight provided by Shell Canada. From this information, the stabilizer feed stream composition was approximated using 7 conventional components and 16 pseudocomponents. The seven conventional components were methane (C\textsubscript{1}), ethane (C\textsubscript{2}), propane (C\textsubscript{3}), i-butane (i-C\textsubscript{4}), n-butane (n-C\textsubscript{4}), i-pentane (i-C\textsubscript{5}) and n-pentane (n-C\textsubscript{5}). The sixteen pseudocomponents were used to represent true boiling point ranges of hydrocarbons larger than n-pentane. The naming convention used for pseudocomponents in both simulations is B(T\textsubscript{1})T(T\textsubscript{2}) where T\textsubscript{1} and T\textsubscript{2} give the boiling point range in degrees Celsius. For example, B205T235 represents all hydrocarbons with boiling points between 205°C and 235°C.

The Peng-Robinson equation of state is used to calculate all the thermodynamic properties required except for liquid molar volume. Liquid molar volume is calculated for conventional components using the Rackett model, and for pseudocomponents using the API method for molar volume. The Peng-Robinson equation of state is applicable to nonpolar or mildly polar
mixtures such as hydrocarbons including light gases (e.g., carbon dioxide, hydrogen, hydrogen sulphide etc.). This equation of state is recommended for refinery and other hydrocarbon applications [6].

3.3 Sequential Modular Simulation

Development of the sequential-modular process simulation model was performed using the MODEL MANAGER graphical user interface [8, 9] to produce an ASPEN PLUS input file. The input file produced is keyword-based ASCII text file which can either be edited directly, or imported into MODEL MANAGER for editing. Figure 3.3 shows how the process flowsheet given in Figure 3.2 was modelled with ASPEN PLUS.

Five models were required to model the stabilizer-splitter process. The following subsections outline the models used and the flowsheet convergence.

3.3.1 Stabilizer (C1)

The stabilizer column was modelled using the model RADFRAC, a rigorous tray by tray equilibrium-based distillation column [5]. Both a vapour product, VAP, and a liquid product, DIST-C4 are drawn from the partial condenser at stage 1 of this column. A liquid bottoms product, SPLITFEED, is drawn from stage 29. The reboiler furnace was simulated as a 2 phase pumparound reboiler with both the draw and return streams on stage 29 of the stabilizer column. To improve the column convergence efficiency and reliability in petroleum applications, the RADFRAC convergence algorithm “SUM-RATES” was chosen.

3.3.2 Heat Exchanger (E1)

The heat exchanger was modelled using the model HEATER, a simple generic heating or cooling model [5]. The preferred model for this block would have been HEATX, a rigorous heat exchanger model, which also calculates the
Figure 3.3: ASPEN PLUS stabilizer-splitter process model. The Unit models used are shown as dashed boxes.
heat transfer coefficients. However, there were insufficient measured variables around this unit in the actual process to provide the information required to use HEATX.

3.3.3 Splitter (C2, C4 and C5)

A combination of three models were used to model the splitter: PETROFRAC, FSPLIT and HEATER. The main column, condenser and sidestripper columns were all modelled using PETROFRAC. A rigorous tray by tray equilibrium based distillation column model designed specifically for petroleum applications. Another model, MULTIFRAC, could have been used in place of PETROFRAC to produce similar results. However, this is not recommended for petroleum applications [5]. The liquid product stream LT-ISO was drawn from the subcooled total condenser at stage 1. Two reboiled sidestrippers are used to remove the liquid products HV-ISO and LT-DIST. The first sidestripper, C4, is fed by a liquid from stage 15, and returns vapour to stage 14. The second sidestripper, C5, is fed by a liquid drawn from stage 18 and returns vapour to stage 17.

PETROFRAC was unable to model a 2 phase pumparound reboiler. Therefore, the C2 reboiler furnace was modelled externally using a combination of the model FSPLIT, a simple flow splitting block, and a HEATER model. Since these models generate a recycle loop in the flowsheet, a tear stream convergence block was also needed (see Section 3.3.4 below for convergence block details). FSPLIT was used to split the PETROFRAC bottoms into a liquid product stream, SSFEED, and the reboiler feed. The HEATER model was used to reboil the stream C2REBL before it was returned to stage 29 of the main splitter column.

3.3.4 Convergence

A convergence block was required to converge the tear stream created by the external pumparound reboiler on the splitter column. This tear stream was
placed on the stream C2REBL between the reboiler and the main column. The tear stream was converged using the Wegstein method to tolerance, \( tol \), of \( 1 \times 10^{-4} \) for each variable to be converged using the following expression:

\[
-tol \leq \frac{x_{\text{calculated}} - x_{\text{assumed}}}{x_{\text{assumed}}} \leq tol
\]

(3.1)

This convergence test is bypassed for all components with a mole fraction less than the trace value of \( tol/100 \). The Wegstein acceleration parameter, \( q \), was allowed to vary between 0 and -5. For a detailed description of the Wegstein method, see either the ASPEN PLUS User Guide [9] or Perry and Green [85]. Converging the tear stream on C2REBL requires iterative solution of the blocks PETROFRAC, FSPLIT, and HEATER that make up the splitter column. Typically convergence of the tear stream takes between 15 and 25 passes through these blocks. Initial guesses of the C2REBL stream flow rate, pressure, temperature and composition were also required.

To promote flowsheet convergence speed, estimates of the column temperature, vapour flow and liquid flow profiles were used. These estimates are obtained from a previous run of the process model when it is used in the real time optimizer.

### 3.4 Equation-oriented Simulation

The equation-oriented process simulation flowsheet was developed by writing a keyword based ASCII text input file. The SPEEDUP Executive is a text based interface which provides syntax checking, specification checking (degrees of freedom analysis) and some tools for run-time error diagnose [11, 12]. Figure 3.4 shows how the process flowsheet given in Figure 3.2 was modelled with SPEEDUP.

Modelling of the stabilizer-splitter flowsheet equipment in SPEEDUP required 7 macros and 24 models. Macros are groups of repeated models used to simplify construction of the flowsheet. In this flowsheet, macros were used to model sections of the distillation columns using multiple distillation tray
Figure 3.4: SPEEDUP stabilizer-splitter process model. Volume flow and other measurement blocks are not shown.
models. One user defined equipment model was used in the flowsheet as the bottom stage of columns C1 and C2 (see Section 3.4.1 below for details of the model).

In addition to the equipment models, an extra 17 user defined measurement models were required to calculate volume flow rates, C5 compositions, true boiling point temperatures and Reid vapour pressures (see Section 3.4.2 below for details of these models). Including the models used in the macros, a total of 74 models were used to simulate the stabilizer-splitter flowsheet. The following subsections outline how these macros and models were used and the flowsheet convergence.

3.4.1 User Defined Equipment Models

SPEEDUP allows user defined models to be added to the flowsheet easily. In this simulation, one user written equipment model, BTRAY_SS was used to simulate the bottom tray of columns C1 and C2. BTRAY_SS is based on the SPEEDUP Library model FTRAY_SS without a vapour inlet stream and two liquid outlet streams. This model was required because the bottom trays of columns C1 and C2 are fed by mixed vapour-liquid streams instead of vapour only inlet streams. Also, two liquid outlet streams are drawn from the bottom tray; the reboiler feed stream and the bottoms product stream.

This model was created by copying the model FTRAY_SS from the SPEEDUP Library and editing the input code. The input code (including the modelling equations) for BTRAY_SS is listed in Appendix E, Section E.8.

3.4.2 User Defined Measurement Models

Seven user defined models were created to measure the various stream properties required by the real time optimizer. These measurement models do not change or affect the flowsheet in any other way. They are included in the flowsheet in the same way as other unit models. The input code for the models outlined below is included in Appendix E, Section E.8.
Volume Flow Rates

Three models, VFLOW, LIQ_VFLOW and VAP_VFLOW, were created to measure standard and true volume flow rates for mixed phase, liquid and vapour streams respectively.

The true volume is calculated by making a property procedure call for the liquid or vapour molar density at the current pressure and temperature of the stream. The volume flow rate is then obtained by solving for the unknown volume flow $F_v$ from the known molar flow $F$ and molar density $\rho$:

$$ F = F_v \rho $$  \hspace{1cm} (3.2)

For the model VFLOW, the property calls are made separately for the liquid and vapour phases. The liquid and vapour volume flow rates are calculated separately, and then summed to give the overall stream volume flow rate.

The standard liquid volume flow rate is calculated in the same way as true volume flow, except the property procedure call for molar density is only made for the liquid phase at 60°F and 1 atmosphere. The model VAP_VFLOW also calculates a standard vapour flow using a property procedure call for molar density for the vapour phase at 60°F and 1 atmosphere.

C₅ Composition

The model C5_VFLOW is used to calculate both volume flow rates and the stream C₅ composition. The C₅ composition, C5S, is calculated simply by adding the i-pentane and n-pentane compositions together. This model is identical to LIQ_VFLOW with addition of the calculation for C5S.

True Boiling Point Temperatures

The model TBP is used to calculate both volume flow rates and true boiling point temperatures. The true boiling point temperatures are calculated at both 10% and 90% standard liquid volume distilled. A user supplied FORTRAN procedure, which linearly interpolates between the boiling point
temperatures of the pseudocomponent, is used to determine the true boiling point temperatures at both 10% and 90% of the streams standard liquid volume. This model is the same as LIQ_VFLOW with addition of the true boiling point procedure calls.

**Reid Vapour Pressure**

Unfortunately SPEEDUP does not include a built in procedure for determining the Reid vapour pressure of a stream. Therefore, two user-defined models, M2R and RVP, were created to determine Reid vapour pressure based on the methods outlined in the API Technical Data Book [1] and ASTM standard D323 [41].

The model M2R changes the stream equation of state from Peng-Robinson to ideal, and adds air as the 24th stream component. The model RVP follows the procedure outlined below with the outlet stream of M2R as the inlet stream:

1. Saturate the stream with air at 32°F.
2. Calculate the moles of air required to mix air with the stream at a ratio of 4:1 at 32°F.
3. Flash the 4:1 mixture of air and the stream at 100°F under constant volume. This pressure of this flash under these conditions gives the Reid vapour pressure of the stream.

The model RVP requires that the ideal molar density of air at 32°F and 100°F are set in the simulation operation section. This model was tested against Reid vapour pressure results produced in ASPEN PLUS simulations at several operating conditions and was found to be in close agreement (±1.0%).

**3.4.3  Stabilizer (C1)**

The stabilizer was modelled using 2 macros and 7 other models. The feed stream, STAB, was specified using MOL_FEED, a molar feed model [10].
The stabilizer column stages were modelled using two SECTION_SS macros and a FTRAY_SS rigorous feed stage model at stage 15. The SECTION_SS macros form both the stripping and rectifying sections of the column, and are made up of 14 and 12 stages respectively. Each of the stages within the macro use the model TRAY_SS, a rigorous distillation stage, which flashes the mixture of the inlet vapour and liquid streams to yield the outlet vapour and liquid steams.

The partial condenser was modelled using PCOND_SS, a rigorous partial condenser model, and RSplit, a liquid flow splitting model. The vapour product, VAP, was drawn from the partial condenser. The RSplit model divides the condensed overhead liquid into a reflux stream and the liquid product stream DIST_C4.

The reboiler and bottom stage (stage 29) of the column were modelled using the models BTRAY_SS, HEAT_COOL and TEAR. One of the liquid outlet streams from BTRAY_SS was fed to the reboiler, while the other forms the bottoms product. The reboiler was modelled by a HEAT_COOL model, a simple generic heating or cooling model. Since the pumparound reboiler creates a flowsheet recycle loop, a TEAR block was required. The TEAR block was placed on the stream from the reboiler feeding the bottom stage of the column. See Section 3.4.6 for details and convergence of the TEAR block.

3.4.4 Heat Exchanger (E1)

The heat exchanger was modelled using the model HEAT_COOL. Unfortunately a more rigorous heat exchanger model could not be used to calculate heat transfer coefficients due to insufficient measured data around this unit in the actual process.
3.4.5 Splitter (C2, C4 and C5)

The splitter columns were modelled using 5 macros and 16 other models. The main column was formed using 3 feed stage models, FTRAY_SS, 3 standard stage models, TRAY_SS, 2 liquid flow splitting models, RSPLIT, and 3 column section macros, SECTION_SS. The three feed stage models were used at stages 14, 17 and 21. Stage 21 receives the column feed from the heat exchanger E1. Stages 14 and 17 receive vapour phase feed from the sidestripper columns C4 and C5 respectively. The two RSPLIT models are used to the liquid feeds for the sidestripper columns C4 and C5 from stages 15 and 18 respectively. The 19 stage rectifying section of the C2 column is formed by 2 SECTION_SS macros, 3 TRAY_SS and 2 FTRAY_SS models. The stripping section of the column is formed using a 2 stage SECTION_SS macro.

The sub-cooled condenser was modelled using TCOND_SS, a rigorous total condenser model. Both the sub-cooled liquid product, LT-ISO, and the reflux are drawn from the total condenser. The reboiler and bottom stage (stage 24) of the column were modelled with the same models and layout used in the stabilizer column, C1.

The two sidestripper columns, C4 and C5 were formed using the same simulation models. The columns were modelled using 2 stage SECTION_SS macros. The reboilers were simulated using REBOILER_SS, a rigorous kettle reboiler model. A liquid product was removed from the reboilers and vapour was returned to the sidestripper columns. Since the sidestriers create a flowsheet recycle loop, a TEAR block was placed on the vapour stream being returned to the main column, C2.

3.4.6 Convergence

The process simulation flowsheet in SPEEDUP was solved as a large set of simultaneous equations. After translation of the input code, block decomposition of the flowsheet is performed. For this simulation, 1164 equation blocks used to solve the 6066 equations and unknown variables. These equation
blocks are formed based on the equations in the models used, and the variables set in the operation section of the input code. Only 6 of the 1164 blocks generated are nonlinear and contain more than one equation. SPEEDUP then generates the derivative code for the simulation (13.653 derivative expressions were required). The simulation is then ready for solution.

The linear equation blocks are solved by direct substitution. The 6 nonlinear blocks are solved using a Newton trust region method using a dogleg step (see Edgar and Himmelblau [37], Fletcher [40] or Gill et al. [47] for details of this method). The flowsheet is converged to an accuracy of $1 \times 10^{-5}$, that is, all the equation residuals are less than $1 \times 10^{-5}$. The residual of an equation is the difference between and left and right hand sides of the equation.

To promote flowsheet convergence, all variables not “set” in the operation section were given preset values. The values used to preset the first runs of this process model were generated by an ASPEN PLUS run of the same model to attain convergence. Later runs used presets generated from previous SPEEDUP simulations to ensure flowsheet convergence.

Tear streams in an equation-oriented simulators do not require a separate convergence scheme from the rest of the flowsheet. In SPEEDUP, a TEAR block is used to add slack variables to the recycle stream which allow for the convergence of the recycle loop. The tear model has equations for flow, temperature, pressure and each composition of the form:

$$F_{in} = F_{out} - F_{slack}$$

(3.3)

All the slack variables (e.g., $F_{slack}$) are set to zero in the input file operation section and the tear stream equations are converged using the same method as the rest of the flowsheet. Therefore, the addition of a TEAR block in this simulation means the addition of 26 equations and variables to the overall flowsheet problem. Four TEAR blocks were required for this flowsheet: two were used in the reboilers for columns C1 and C2, and two were used on the vapour returns from the two sidestrippers C4 and C5.
3.5 Discussion

The following subsections discuss various problems and modelling aspects encountered using both the sequential modular and equation-oriented process simulators. Property development issues are discussed separately as these were common to both simulation packages. A summary comparing various quantitative aspects of the process model simulation development and performance are presented in Table 3.1.

3.5.1 Properties

Property development for both of the process simulation packages took 104 hours to complete due to difficulties in matching the pseudocomponent properties to those of a hydrocracked petroleum stream. Specifically, the properties of the first two pseudocomponents, B45T65 and B65T85 (representing hydrocarbons with boiling points from 45°C to 65°C and 65°C to 85°C respectively), were the most difficult to match. This was because the properties of these components greatly affect the operation of the condensers on both columns C1 and C2. It was found with the original assay data provided that if the correct temperatures were met in the condensers of both columns, the compositions and product flows of the C4-Distillate and Light Iso streams were incorrect by up to 200%.

The cause of this problem was found to be the assumptions made by PROPERTIES PLUS when determining the specific gravities and molecular weights for each pseudocomponent from the data provided. Since only an overall specific gravity and molecular weight had been given in the assay analysis, PROPERTIES PLUS determines the pseudocomponent properties based on a typical hydrocarbon stream's specific gravity and molecular weight curves. A hydrocracked hydrocarbon stream, however, exhibits different typical property curves due to the presence of a different component mix, particularly at the ends of the curves (i.e., the light and heavy components). Using typical hydrocracked petroleum stream curves, the pseudocomponents were
Table 3.1: Comparison of both process simulators for model development.

<table>
<thead>
<tr>
<th></th>
<th>Sequential Modular Simulator</th>
<th>Equation-oriented Simulator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Development Time (hours)</td>
<td>192</td>
<td>310</td>
</tr>
<tr>
<td>(excluding property development)</td>
<td>(88)</td>
<td>(206)</td>
</tr>
<tr>
<td>Input file size (bytes)</td>
<td>10,855</td>
<td>263,366</td>
</tr>
<tr>
<td>(without preset variables)</td>
<td>(8,085)</td>
<td>(44,324)</td>
</tr>
<tr>
<td>Number of process models used</td>
<td>5</td>
<td>74</td>
</tr>
<tr>
<td>Number of tear streams</td>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>CPU time (mins)(^a)</td>
<td>1.17</td>
<td>1.51</td>
</tr>
<tr>
<td>Stabilizer column flowsheet passes</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>Splitter column flowsheet passes</td>
<td>5</td>
<td>2</td>
</tr>
<tr>
<td>Largest discrepancy from Shell process model</td>
<td>0.30%</td>
<td>2.65%</td>
</tr>
</tbody>
</table>

\(^a\)CPU time is measured for calculations only on an IBM RS 6000 Model 530H computer.
recalculated. These new pseudocomponents provided very accurate results to within 0.5% of Shell's simulated results.

3.5.2 Sequential Modular Simulation

The initial building and debugging of the process flowsheet in ASPEN PLUS was relatively straightforward. The major problems encountered were during the modelling of the two phase pumparound reboiler on the splitter column using the rigorous multiple distillation column models available, and drying up of the main splitter column during flowsheet convergence.

The model PETROFRAC was a very powerful way to model a column including sidestrippers by removing the need for flowsheet tear streams. PETROFRAC solves the recycle loops created internally within the block, thereby ensuring robust convergence and faster solution. However, PETROFRAC was not as flexible as RADFRAC in simulating the column C2 furnace reboiler. The pumparound model built into PETROFRAC is only capable handling single phase streams. Therefore, the reboiler had to be modelled externally using an FSPLIT and a HEATER model, thereby creating a recycle loop. The addition of this tear stream significantly slows convergence of the flowsheet due to the extra flowsheet passes required to converge the recycle loop. The addition of this recycle loop illustrates the effect of recycle loops on convergence of sequential modular process flowsheets.

Internal convergence of the PETROFRAC block was initially quite difficult. The main column tended to dry up around the stages where liquid was drawn to feed the sidestripper columns. This problem was fixed by adding temperature, liquid flow and vapour flow column profile estimates. Initially these estimates were guesses until convergence of the column was achieved. From then on, the column was initialized using estimates provided from a previous run of the process model. Correction of the pseudocomponent properties as discussed in Section 3.5.1 also helped this convergence problem.

Table 3.2 summarises the testing of the final ASPEN PLUS process model simulation against Shell's RTO process model. From these results and testing
performed by Shell against actual plant data, it was felt that this model adequately reflects the true process for real time optimization.

3.5.3 Equation-oriented Simulation

The initial building and syntax debugging of the SPEEDUP flowsheet input code was relatively straightforward. Obtaining flowsheet convergence, however, was very difficult for several reasons outlined below.

In building the flowsheet, several user written models were required to supplement those in the SPEEDUP model library (see Sections 3.4.1 and 3.4.2 for details). These models were easy to write and implement with the exception of the Reid vapour pressure measurement model. This model required a complex series of flashes and a different equation of state to the rest of the process flowsheet to calculate the Reid vapour pressure. It is probable that in future versions of SPEEDUP, procedure calls to PROPERTIES PLUS will be implemented for Reid vapour pressure and other petroleum specific properties.

The main problem with flowsheet convergence was caused by the large numbers of equations and variables created because of the 23 components in each stream. This resulted in a problem involving 6066 equations and unknown variables which were difficult to analyse due to number of composition variables. Also, a large percentage of these composition variables were at or close to zero. Therefore bound checking was very difficult to perform since usually over 1000 composition variables would be on their lower bound. Bounds on variables in an equation-oriented simulator are used to prevent impossible solutions, e.g., negative compositions, temperatures below absolute zero etc. Bounds can also be used to promote flowsheet convergence by preventing excessive movements in some variables which can prevent solution. However, bounds can also hinder flowsheet convergence if they restrict the movement of the equation solver too much.

Initially, flowsheet convergence was promoted by using a combination of checking the bounds after solution failure and checking the maximum resid-
Table 3.2: Discrepancies between the ASPEN PLUS process model and Shell's RTO process model.

<table>
<thead>
<tr>
<th>Stream Name</th>
<th>Molar Flow</th>
<th>Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vapour</td>
<td>0.00%</td>
<td>0.01%</td>
</tr>
<tr>
<td>C₄-distillate</td>
<td>0.00%</td>
<td>0.01%</td>
</tr>
<tr>
<td>Splitter Feed</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>Light Iso</td>
<td>0.01%</td>
<td>0.01%</td>
</tr>
<tr>
<td>Heavy Iso</td>
<td>0.00%</td>
<td>0.23%</td>
</tr>
<tr>
<td>Light Distillate</td>
<td>0.01%</td>
<td>0.30%</td>
</tr>
<tr>
<td>SS Feed</td>
<td>0.01%</td>
<td>0.00%</td>
</tr>
</tbody>
</table>

uals at the end of each iteration. When variables other than compositions hit their bounds, these bounds were widened. For variables with the highest residuals on the first iteration, estimates of the final values of those variables were provided from the results of an ASPEN PLUS process simulation in the form of “presets”. Eventually it was found that so many variables required estimates, it was decided to preset all variables using ASPEN PLUS process model results. Flowsheet convergence was then obtained. Future process model simulations were then run using presets of a previous simulation which had converged, using SPEEDUP’s ability to save results. These saved results can then be used to preset future simulations through the “Use” sub-environment.

This difficulty with flowsheet convergence shows that for very large, complex simulations using an equation-oriented process simulator, the initial values of the unknown variables dramatically affects the simulator’s ability to obtain a solution. In this case, the simplest way to provide estimates was to use the results of a sequential modular simulation. In future runs, it was found that if the process model was initialized using a feasible solution, convergence was usually obtained, even for quite large movements in operating conditions.

Another tool that was useful in promoting flowsheet convergence was
scaling of the flowsheet variables and equations. In this problem, variables ranged in magnitude from $10^{-2}$ for compositions to $10^4$ for flows. When scaling is used, the flowsheet is solved in terms of scaled variables. A scaled variable is equal to the unscaled variable divided by a user set scaling factor. The aim of scaling is to have all the scaled variables of similar magnitude to promote convergence and performance of the simulation. It was found that scaling did help convergence considerably, however presets were still required for most variables. Unfortunately, scaling has not been implemented in SPEEDUP for use in optimization runs at this time. Therefore the process model had to be able to converge without scaling.

Table 3.3 summarises the testing of the final SPEEDUP process model simulation against Shell’s RTO process model. From these results and testing performed by Shell against plant data, it was felt that this model adequately reflects the true process for real time optimization.

Table 3.3: Discrepancies between the SPEEDUP process model and Shell’s RTO process model.

<table>
<thead>
<tr>
<th>Stream Name</th>
<th>Molar Flow</th>
<th>Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vapour</td>
<td>0.00%</td>
<td>0.62%</td>
</tr>
<tr>
<td>C4-distillate</td>
<td>0.00%</td>
<td>0.62%</td>
</tr>
<tr>
<td>Splitter Feed</td>
<td>0.29%</td>
<td>0.00%</td>
</tr>
<tr>
<td>Light Iso</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>Heavy Iso</td>
<td>0.00%</td>
<td>2.65%</td>
</tr>
<tr>
<td>Light Distillate</td>
<td>0.00%</td>
<td>0.59%</td>
</tr>
<tr>
<td>SS Feed</td>
<td>0.67%</td>
<td>0.10%</td>
</tr>
</tbody>
</table>
Chapter 4

Data Reconciliation Development

4.1 Introduction

4.1.1 Objectives

The objective of data reconciliation is to adjust the measured process data to satisfy mass and energy balances. The adjustments made to the process data should be as small as possible to ensure that the reconciled data still accurately represents the true operating conditions of the process. The data reconciliation is to be performed using the process model developed in the previous chapter. Figure 4.1 highlights the part of the real time optimizer to be developed in this chapter.

4.1.2 Data Reconciliation Description

The stabilizer-splitter data reconciliation problem is a nonlinear, steady state, unconstrained data reconciliation involving 28 measurements. Figure 4.2 shows the measured temperature and flow variables available for the stabilizer-splitter process. All the variables shown in Figure 4.2 were reconciled except
Figure 4.1: Real time optimizer process flow diagram with data reconciliation highlighted.

for the stage 3 temperature, T11. The stage 3 temperature was not reconciled because the process model developed uses equilibrium stages to model the stabilizer column, therefore an accurate measurement of the true tray 3 temperature cannot be made using this process model. See Table B.2 or Table C.2 for full explanations of the measured variables by tag name. No gross error detection or parameter estimation was performed using the process data.

The data reconciliation problem was solved using a weighted least squares objective function similar to the one used by Piccolo [87]. The objective function for this problem is given by:

$$\min_x \left[ \sum_{i=1}^{28} E_i \right]$$

subject to \( h(x) = 0 \) \hspace{1cm} (4.1)

where \( E_i = w_i \left( \frac{y_i - x_i}{s_i} \right)^2 \)
Figure 4.2: Stabilizer-splitter process flowsheet including measurement variable tag numbers.
where \( E \) = least squares error term associated with each measured variable;

\( w \) = weighting factor associated with each measured variable;

\( y \) = the measured variable;

\( x \) = the reconciled variable;

\( s \) = the standard deviation of the measurement transmitter;

\( h(x) \) = the set of equality constraints represented by the process model.

The standard deviations of the measurement transmitters used in the objective function were obtained from Shell. The weighting factors can be used to place emphasis on certain measured variables for a variety of reasons. Weighting of the objective function was implemented in both simulators, however it was not used to place emphasis on any variables in this study (i.e., all the weights were set to same value).

### 4.2 Sequential Modular Simulation

Development of the sequential modular data reconciliation simulation was performed using the MODELMANAGER graphical user interface [8, 9] to produce an ASPEN PLUS input file. Some direct editing of the input file was also required, particularly in developing the in-line FORTRAN blocks and the FORTRAN objective function. Details of the optimization algorithm used, objective function and manipulated variable selection are covered in the following subsections.

#### 4.2.1 Optimization Algorithm

The optimization algorithm used to converge the data reconciliation objective function was the SQP (sequential or successive quadratic programming) method [9]. This optimization algorithm follows a feasible path for this problem, converging the tear stream at every iteration of the optimization. The exact steps used by the ASPEN PLUS SQP algorithm are not detailed in
any of the manuals. The SQP optimization algorithm is probably based on
the general method summarised in Figure 4.3 [37].

The solution of the optimization problem is performed to an optimization
tolerance of $1 \times 10^{-1}$. That is, until the improvement of the objective
function on successive iterations is reduced below this tolerance. The con-
vergence of the process flowsheet and tear streams are performed using the
same tolerances and methods detailed in Section 3.3.4.

4.2.2 Objective Function

The objective function in ASPEN PLUS is supplied as FORTRAN 77 code.
The objective function given in Equation (4.1) was implemented by calcu-
lating the 28 least square error terms, $E_i$ corresponding to each measured
variable, first. An example error term calculation for the stabilizer feed flow,
F01, is given below:

$$F \quad EF01 = WF01 \times ((F01 - SF01)/VF01)^{**2}$$

where EF01 = least squares error term corresponding to F01;
WF01 = weighting factor associated with F01;
F01 = reconciled value;
SF01 = measured value of F01;
VF01 = the standard deviation associated with F01.

These error terms were then summed to give the data reconciliation objective
to be minimized.

The weighting factors, measured values and standard deviations are read
from the data files IWGHT.DAT, IMEAS.DAT and IVARNC.DAT respectively using an in-line FORTRAN block (see Appendix B for a detailed de-
scription of these data files). This in-line FORTRAN block is executed before
the data reconciliation optimization commences. The data read in from the
files are stored in FORTRAN "common" blocks for use during the calculation
Figure 4.3: Flow diagram summarising a general SQP optimization algorithm [37].
of the objective function. These common blocks need to be declared in both the ASPEN PLUS in-line FORTRAN block and the optimization block.

The reconciled variable values used in the data reconciliation objective function correspond to flowsheet variables in the process model. These ASPEN PLUS flowsheet variables are accessed in the objective function by being declared as FORTRAN variables.

4.2.3 Manipulated Variable Selection

Manipulated variables in ASPEN PLUS must correspond to specified variables in the process model, that is, manipulated variables cannot correspond to calculated (or result) variables. The manipulated variables used in the ASPEN PLUS data reconciliation optimization problem are given in Table 4.1.

The initial guess used for a manipulated variable is the corresponding input specification value. Upper and lower bounds are also required for manipulated variables. These bounds are specified using FORTRAN expressions. The bounds are set to the initial manipulated variable value plus or minus a range. These ranges are specified in the input data file IDFREE.DAT. and read into a FORTRAN common block before the data reconciliation commences. Since this data reconciliation is an unconstrained optimization, these manipulated variable bounds should not be reached during the data reconciliation optimization. The bounds are still required, however, as they are used by the optimization algorithm to help determine manipulated variable scaling and step sizes. Therefore the manipulated variables bounds must be wide enough not restrict the movement of the optimization algorithm. yet narrow enough to prevent too large a step being taken.

4.3 Equation-oriented Simulation

Development of the equation-oriented data reconciliation simulation was performed by editing an ASCII text keyword based SPEEDUP input file. Details of the optimization algorithm used, objective function and manipulated
Table 4.1: ASPEN PLUS data reconciliation manipulated variables.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>STAB feed stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>STAB feed stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C1 molar reflux ratio</td>
<td>lbmol/lbmol</td>
</tr>
<tr>
<td>C1 condenser molar vapour fraction</td>
<td>lbmol/lbmol</td>
</tr>
<tr>
<td>C1 reboiler mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C1 reboiler outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>E1 outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C2 liquid distillate mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2 reboiler mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2 reboiler outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C2 condenser sub-cooled temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C4 reboiler heat duty</td>
<td>MMBTU/hr</td>
</tr>
<tr>
<td>C5 reboiler heat duty</td>
<td>MMBTU/hr</td>
</tr>
<tr>
<td>C4 feed stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C5 feed stream mole flow</td>
<td>lbmol/hr</td>
</tr>
</tbody>
</table>
variable selection are covered in the following subsections.

### 4.3.1 Optimization Algorithm

The optimization algorithm used to converge the data reconciliation objective function was the SRQP (successive reduced quadratic programming) method \[13, 25\]. This method is used to converge the process flowsheet in addition to optimizing the data reconciliation objective function. SRQP is an infeasible path optimization method. This means that the optimizer does not necessarily converge the flowsheet, constraints or variable bounds at the end of each iteration. SRQP is particularly suited to the solution of sparse systems with large numbers of equality constraints, typically found in equation-oriented process flowsheets. The steps used by the SRQP optimization algorithm are summarized in Figure 4.4.

The solution of the optimization problem is performed to an optimization tolerance of \(1 \times 10^{-1}\), that is, until the improvement of the objective function on successive iterations is reduced below this tolerance. The convergence of the flowsheet is performed to a residual tolerance of \(1 \times 10^{-5}\), that is, until all the flowsheet equation residuals are less than this tolerance. The global convergence scheme chosen for the SRQP method was a line search method with a modified Lagrangian. All other SRQP options were set to their default values.

### 4.3.2 Objective Function

The objective function in SPEEDUP is specified in the global section of the input file using the same equation syntax used in SPEEDUP models. The objective function itself is the sum of the 28 least square error terms, \(E_i\), corresponding to each measured variable as given in Equation (4.1). These error terms are calculated as additional equality constraints in the Global section. An example error term calculation for the stabilizer feed temperature, T01, is given below:
Figure 4.4: Flow diagram summarising the SRQP optimization algorithm [25].
\[ \text{ET01} = \text{WT01} \times ((\text{MFEED.T_OUT} - \text{ST01}) / \text{VT01})^2; \]

where \( \text{ET01} \) = least squares error term corresponding to \( \text{T01} \):
\( \text{WT01} \) = weighting factor associated with \( \text{T01} \):
\( \text{MFEED.T.OUT} \) = reconciled value of \( \text{T01} \):
\( \text{ST01} \) = measured value of \( \text{T01} \):
\( \text{VT01} \) = the standard deviation associated with \( \text{T01} \).

The weighting factors, measured values and standard deviations are read from the data files IWGHT.DAT, IMEAS.DAT and IVARNC.DAT respectively using SPEEDUP’s external data interface (EDI) (see Appendix C for a detailed description of these data files). The EDI is used prior to the data reconciliation to assign variables with the values read in from external data files. The EDI is specified in two parts. The first is the external section of the SPEEDUP input file which specifies which SPEEDUP variables are to be read in or written out. The second is an EDI FORTRAN input file which is used to interface with the external data in this case to read from the data files.

The reconciled variable values used in the data reconciliation objective function correspond to flowsheet variables in the process model. These flowsheet variables are accessed directly by using their full SPEEDUP variable name.

### 4.3.3 Manipulated Variable Selection

Manipulated variables, or “free” variables, must correspond to variables already set in the operation section of the input file. The manipulated variables used in the SPEEDUP data reconciliation optimization problem are given in Table 4.2.

The initial guess used for a manipulated variable is the corresponding value set in the operation section for that variable. Upper and lower bounds are for manipulated variables are specified by adding bound specifications in the set subsection of the operation section. These bound specifications are
Table 4.2: SPEEDUP data reconciliation manipulated variables.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1 condenser heat duty</td>
<td>MMBTU/hr</td>
</tr>
<tr>
<td>DIST-C4 stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>STAB stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>STAB stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>E1 inlet mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C1 reboiler mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2 condenser heat duty</td>
<td>MMBTU/hr</td>
</tr>
<tr>
<td>C2 condenser subcooled temperature drop</td>
<td>°F</td>
</tr>
<tr>
<td>(bubble point less subcooled temperature)</td>
<td></td>
</tr>
<tr>
<td>E1 outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>SSFEED stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2 reboiler mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C4 feed stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C5 feed stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>HV-ISO stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>LT-DIST stream mole flow</td>
<td>lbmol/hr</td>
</tr>
</tbody>
</table>
set using the EDI before the data reconciliation commences. The bounds are equal to the initial guess for the manipulated variable plus or minus a range. These ranges are specified in the input data file IDFREE.DAT and are read in and added to or subtracted from the initial guesses using the EDI FORTRAN code. Since this data reconciliation is unconstrained, these manipulated variable bounds should not be reached during the data reconciliation optimization. The bounds are still required, however, as they are used by the optimization algorithm to help determine manipulated variable scaling and step sizes.

4.4 Discussion

The following subsections discuss various problems encountered using both the sequential modular and equation-oriented simulators for data reconciliation. A summary comparing various quantitative aspects of the data reconciliation development and performance are presented in Table 4.3.

4.4.1 Sequential Modular Simulation

The building and debugging of the data reconciliation objective function in ASPEN PLUS was relatively easy. Two problems arose when trying to debug the transfer of data between simulation blocks using the FORTRAN common blocks. The first was caused by the differences between input and result variables in ASPEN PLUS. Input variables are used to specify the problem and provide initial estimates. However, they are not updated with their final values at the end of a simulation; the final values are stored in a result variable instead. The only exceptions are the optimization manipulated variables which have their final values stored in the input variable. It is very easy to confuse the two types of variables when developing the simulation, thereby passing incorrect data between blocks. Secondly, there is no simple way to check the intermediate values of the data being transferred between blocks. The easiest way to check these variables was to temporarily add FORTRAN
Table 4.3: Comparison of both process simulators for data reconciliation.

<table>
<thead>
<tr>
<th></th>
<th>Sequential Modular Simulator</th>
<th>Equation-oriented Simulator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Development Time (hours)</td>
<td>133.5</td>
<td>395.5</td>
</tr>
<tr>
<td>Input file size (bytes)</td>
<td>63.514</td>
<td>275.288</td>
</tr>
<tr>
<td>(without preset variables)</td>
<td>(60.714)</td>
<td>(61.114)</td>
</tr>
<tr>
<td>Number of manipulated variables</td>
<td>15</td>
<td>15</td>
</tr>
<tr>
<td>Number of reconciled variables</td>
<td>28</td>
<td>28</td>
</tr>
<tr>
<td>CPU time (mins)*</td>
<td>380.52</td>
<td>106.21</td>
</tr>
<tr>
<td>Optimization iterations</td>
<td>15</td>
<td>28</td>
</tr>
<tr>
<td>Flowsheet passes or function evaluations</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(tear stream iterations)</td>
<td>424</td>
<td>50</td>
</tr>
<tr>
<td>(derivative evaluations)</td>
<td>(5.660)</td>
<td></td>
</tr>
<tr>
<td>Initial objective function value</td>
<td>255.7225</td>
<td>255.72</td>
</tr>
<tr>
<td>Final objective function value</td>
<td>41.1884</td>
<td>55.20</td>
</tr>
</tbody>
</table>

*aCPU time is measured for calculations only on an IBM RS 6000 Model 530H computer.
code which writes variable values to a file to check that the correct values were being passed between blocks. This was time consuming method of checking the data.

Since the variables to be manipulated during the optimization must be chosen from input (or set) variables, the choice of manipulated variables is severely restricted. This is because only certain combinations of variables can be used to specify a given process model in a sequential modular simulation. In addition, even though a given combination of variables are allowed to be specified, convergence of that process model may still be impossible. Initially, the condenser duties for both columns C1 and C2 and the bottoms molar flow rates were used as manipulated variables. Unfortunately convergence of both columns C1 and C2 were not possible using this combination of input variables, even during steady state process model only simulations.

The manipulated variable bounds were initially chosen by guessing how much each variable would be varied during the data reconciliation. These guesses were then adjusted until eventually the variable bounds were wide enough to be inactive throughout the optimization. It was found that if these bounds were too wide, the optimizer would take a large step on the first iteration which sometimes caused the optimization algorithm or flowsheet convergence to fail, thereby terminating the simulation.

The following tuning parameters were used to promote convergence of the SQP optimization algorithm:

- **EST-STEP=**YES. An estimation step is performed before the first iteration to determine the initial step lengths to be taken. This helped prevent large steps being taken on the first iteration of the optimization.

- **DERIV-SWITCH=**YES. When convergence failure occurs, the numerical derivative method is changed from forward difference to central difference. This helped produce better numerical derivative information for the optimizer to use, thereby promoting convergence.
The speed of the optimizer was affected mostly by the tear stream convergence on the splitter column. Since this convergence block was required to converge for each flowsheet evaluation, this resulted in a total of 5,660 passes through the process units C2C4C5, C2SPL1 and F2. Therefore, an average of 13 tear stream iterations were required for each flowsheet pass. To try and reduce the number of tear stream iterations, the SQP optimization algorithm was also used as an infeasible path method. That is, the algorithm was used to solve the tear streams as well, but not necessarily on each flowsheet pass. An extra optimization algorithm tuning parameter, \texttt{MAXLSPASS}, was used to specify the maximum number of tear stream iterations allowed on each flowsheet pass. Unfortunately the number required was the same as using SQP as a feasible path method to achieve convergence on the final iteration. Therefore, it was decided use SQP as a feasible path optimizer as there was no performance penalty and tear stream convergence was improved.

### 4.4.2 Equation-oriented Simulation

Building and debugging of the data reconciliation objective function in \texttt{SPEEDUP} was relatively easy. Transferring data to and from the optimization block (global section) is very simple and easy to check. Variables from other flowsheet blocks are specified directly by typing their full name in the form \texttt{unitname.variablename}.

Extreme difficulty was encountered in choosing the manipulated (or free) variables for this flowsheet. Equation-oriented simulators allow any combination of variables to specify the flowsheet, provided they match the degrees of freedom available. However, this does not mean that the flowsheet can necessarily be converged using these variables. \texttt{SPEEDUP} performs checks to see that each equation block is not under or over specified, but does not check for the independence of the manipulated variables. Initially, the same manipulated variables used in the \texttt{ASPIN PLUS} data reconciliation were chosen for the \texttt{SPEEDUP} simulation, however, the flowsheet failed to converge. The manipulated variables used to specify the condensers and reboilers
for C1 and C2 were then changed to achieve flowsheet convergence. However, the optimizer was unable to find a solution and failed for several different reasons including inconsistent constraints, slow convergence and property errors. Slight changes in presets or tuning parameters would cause completely different errors. Eventually it was discovered after analysis of the mass and energy balances around individual process units, that the manipulated variables chosen were completely specifying the mass balance around the stabilizer column and the energy balance around the splitter column. SPEEDUP cannot, however, detect this problem and tries to solve this simulation thereby causing the inconsistent error messages observed. With even larger process flowsheets, this problem could become extremely difficult to detect.

Several other problems were also observed while trying to promote convergence of the data reconciliation problem. The optimization algorithm, SRQP, provides very poor information on its progress when solving. Several print levels are provided which give either too little information, or more information than can reasonably be handled. This makes it very hard to determine if the optimizer has hit variables bounds other than those on the manipulated variables. Also, the SPEEDUP/PROPERTIES PLUS interface is unable to track at which point in the flowsheet that a property errors occur. An error message such as “error in flash” is produced with no indication of which of the 63 flashes in this flowsheet caused the problem. Finally, looking at intermediate values for an infeasible path optimizer solving an equation-oriented simulation flowsheet provides very little useful information. This is because the optimization algorithm does not converge the flowsheet at each iteration, therefore individual variables may have values outside their bounds and may not fulfil mass and energy balances when the optimizer fails. It is sometimes useful to look at equation residuals at the end of an iteration to see which equations are contributing the most error to the solution of the flowsheet. These residuals may indicate problems with either that equation or one of the variables used in that equation.
The manipulated variable bounds were initially chosen by guessing how much each variable would be varied during the data reconciliation. These guesses were then adjusted until eventually they were wide enough to be inactive throughout the optimization. The manipulated variables bounds were found to be critical in preventing the optimization algorithm from taking extremely large steps on the first few iterations. Taking large optimization steps with this process flowsheet tends to cause extremely large flowsheet convergence residual errors which may prevent convergence of the optimizer. In extreme cases, physical property errors occur which generally causes a severe error crashing the SPEEDUP simulation.

Several optimization algorithms were available in SPEEDUP. The standard optimizer, FEASOPT, was unable to even initialize the optimization problem within 8 hours of CPU time. SRQP can be used with three slightly different convergence strategies. The default method uses a line search method with an absolute penalty function to promote convergence. This method tended to take extremely conservative steps and consistently failed due to “slow convergence”. The other two methods both use a modified Lagrangian function as the global convergence scheme. The augmented modified Lagrangian function was not required for the data reconciliation optimization problem since no additional inequality constraints were used in the problem.

Tuning of the SRQP optimization algorithm was difficult due to lack of tuning parameters available to modify the behaviour of the optimizer. The only numerical tuning parameters available are the optimization tolerance and the flowsheet residual convergence tolerance. There was no parameter to control the number of iterations taken before the optimization error “slow convergence” is given. There was also no way to directly restrict the manipulated variable step sizes taken to prevent the algorithm from occasionally taking large steps. Scaling of both manipulated variables and process flowsheet variables is not available with SRQP. These would both help convergence of both the flowsheet and optimizer. It is expected that these will
be added in a future release of SPEEDUP.

Some tuning of the optimization problem was possible by varying the data reconciliation weighting factors. The weighting factors were still all equal, but were varied together between 1 and 2 to scale the whole objective function. By varying these weights, it was possible to get convergence for nearly every problem attempted. However, the weights required for convergence were often different for different starting points, and there was no automatic method for choosing these weighting factors. Therefore, since these weights need to be determined manually by the user for each problem attempted, this SPEEDUP simulation is not practically suited for use in a real time optimization system.

4.4.3 Checking for Model Differences

Table 4.4 shows the differences between the ASPEN PLUS and SPEEDUP process models. The results in this table were produced by performing a steady state simulation in ASPEN PLUS using the results obtained at the end of the SPEEDUP data reconciliation. The largest discrepancy found between the two process models for any stream property was a 0.42% difference for the standard volume flow of the Heavy Iso stream. For this operating point, SPEEDUP gave a data reconciliation objective function value of 55.20. ASPEN PLUS calculated the data reconciliation objective function to be 56.04 for the same operating point, a discrepancy of 1.52%. Therefore it can be concluded that the differences between the two process models are extremely small.

Unfortunately ASPEN PLUS does not include any options to view the reduced gradients from the process model during the optimization. This would allow the comparison of the gradients produced by both ASPEN PLUS and SPEEDUP to see if the difference in results were caused by the optimization algorithm or inaccuracies in derivatives from the process models.
Table 4.4: Discrepancies between ASPEN PLUS and SPEEDUP process models at the SPEEDUP data reconciliation optimum.

<table>
<thead>
<tr>
<th>Stream Name</th>
<th>Molar Flow</th>
<th>Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vapour</td>
<td>0.01%</td>
<td>0.00%</td>
</tr>
<tr>
<td>C₄-distillate</td>
<td>0.01%</td>
<td>0.00%</td>
</tr>
<tr>
<td>Splitter Feed</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>Light Iso</td>
<td>0.01%</td>
<td>0.00%</td>
</tr>
<tr>
<td>Heavy Iso</td>
<td>0.03%</td>
<td>0.01%</td>
</tr>
<tr>
<td>Light Distillate</td>
<td>0.01%</td>
<td>0.00%</td>
</tr>
<tr>
<td>SS Feed</td>
<td>0.00%</td>
<td>0.01%</td>
</tr>
</tbody>
</table>
Chapter 5

Economic Optimization Development

5.1 Introduction

5.1.1 Objectives

The objective of the economic optimization is to optimize the process set points to maximize the profitability of the process subject to operating constraints. The adjustments made to the process set points from one cycle of the real time optimizer should be restricted to prevent large changes to the process operating conditions being passed to the plant’s process control system. The economic optimization is to be performed using the process model developed in Chapter 3. Figure 5.1 highlights the part of the real time optimizer to be developed in this chapter.

5.1.2 Economic Objective Function

The economic optimization of the stabilizer-splitter process is a nonlinear, steady state, constrained optimization problem. The profit based objective function consists of the sum of the product values less the feed and utility
Figure 5.1: Real time optimizer process flow diagram with the economic optimization highlighted.

costs as shown in Equation (5.1).

\[
\max_x \left[ \sum_{i=1}^{6} P_i - C_{\text{feed}} - C_{\text{utilities}} \right] \\
\text{subject to } g(\mathbf{x}) \geq 0 \\
\quad h(\mathbf{x}) = 0
\]

(5.1)

where \( P_i \) = product stream values (\$/hr);
\( C_{\text{feed}} \) = feed stream cost (\$/hr);
\( C_{\text{utilities}} \) = total utility costs (\$/hr);
\( g(\mathbf{x}) \) = the set of process inequality constraints;
\( h(\mathbf{x}) \) = the set of equality constraints represented by the process model.

The six product values are calculated by the following equation:

\[
P_i = D_i v_i \quad i = 1, \ldots, 6
\]

(5.2)
where \( D_i \) = the product streams unit prices ($/m^3$); for the base case, these unit prices are given in Table 5.1 except for the Light Iso product stream which is more complex and is given by Equation (5.3):
\[
\nu_i = \text{the standard volume flow rate of the product stream (m}^3/\text{hr}).
\]
The unit cost for the Light Iso product stream also includes a quality premium based on the Reid vapour pressure of the stream. The following equation shows how this quality premium is added to the Light Iso unit price, \( d_L \), from Table 5.1:
\[
D_L = d_L + q_L(P_L - P_{\text{spec}})
\]  
(5.3)
where \( D_L \) = Light Iso product stream unit price including the Reid vapour pressure quality premium ($/m^3$);
\( q_L \) = Reid vapour pressure quality premium ($/m^3/kPa$);
\( P_L \) = Light Iso product stream Reid vapour pressure (kPa);
\( P_{\text{spec}} \) = Reid vapour pressure specification (kPa).

For the base case, the quality premium, \( q_L \), used was -0.18 $/m^3/kPa$, and the Reid vapour pressure specification, \( P_{\text{spec}} \), was 97.0 kPa.

The feed cost is calculated similarly to the product values using the following equation:
\[
C_{\text{feed}} = D_{\text{feed}} \nu_{\text{feed}}
\]  
(5.4)
where \( D_{\text{feed}} \) = the stabilizer feed stream unit price ($/m^3$); for the base case, this unit price is given in Table 5.1:
\( \nu_{\text{feed}} \) = the standard volume flow rate of the stabilizer feed stream (m$^3$/hr).

Finally, the utility cost of the furnace heating oil for the reboilers on both columns C1 and C2 is calculated from Equation (5.5). This method uses the API liquid fuel equivalent (LFE) volume estimated from the reboiler heat duty to determine the utility costs [1].
\[
C_{\text{utilities}} = \sum_{i=1}^{2} [D_F O C_a c_b (1/\eta_i) Q_i]
\]  
(5.5)
Table 5.1: Stream and utility unit prices.

<table>
<thead>
<tr>
<th>Name</th>
<th>Price</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vapour product stream</td>
<td>0.15</td>
<td>$/m^3</td>
</tr>
<tr>
<td>C₄-Distillate product stream</td>
<td>100.07</td>
<td>$/m^3</td>
</tr>
<tr>
<td>Light Iso product stream</td>
<td>182.69</td>
<td>$/m^3</td>
</tr>
<tr>
<td>Heavy Iso product stream</td>
<td>193.89</td>
<td>$/m^3</td>
</tr>
<tr>
<td>Light Distillate product stream</td>
<td>180.52</td>
<td>$/m^3</td>
</tr>
<tr>
<td>C₂ bottoms product stream</td>
<td>158.34</td>
<td>$/m^3</td>
</tr>
<tr>
<td>Stabilizer feed stream cost</td>
<td>158.34</td>
<td>$/m^3</td>
</tr>
<tr>
<td>Furnace heating oil cost a</td>
<td>82.14</td>
<td>$/LFEm³</td>
</tr>
</tbody>
</table>

*a unit price is given in dollars per Liquid Fuel Equivalent standard volume flow

where \( D_{FO} \) = the furnace heating oil unit price ($/LFEm³); for the base case. this unit price is given in Table 5.1:

\( c_a = \) volume conversion from barrels to cubic metres (0.1589873 m³/bbl);

\( c_b = \) conversion from heat duty to liquid fuel equivalent volume (0.158730158 MMBTU/LFEbbl);

\( \eta_i = \) furnace efficiency for columns C1 and C2 respectively (assumed to be 70%);

\( Q_i = \) furnace heat duty for columns C1 and C2 respectively (MMBTU/hr).

5.1.3 Process Inequality Constraints

In addition to the equality constraints represented by the process model, 25 process inequality constraints were required. These inequality constraints prevent the economic optimization from moving outside plant safety limits, product quality specifications or other operating limits. The inequality constraints required for the stabilizer-splitter process flowsheet are summarised
in Table 5.2.

5.1.4 Set Point Movement Restriction

Bounds restricting the movement of the manipulated variables during the economic optimization are used to prevent large movements in the process set points being returned to the plant after a cycle of the real time optimizer. Large movements in the process set points may upset the plant, affecting the true plant profits or destabilizing the plant's operating conditions. Therefore restriction of the manipulated variable movements is required.

The manipulated variable bounds were chosen from plant operation experience on how large a change can be made to each set point in the plant. For the stabilizer-splitter economic optimization, the manipulated variables were allowed to move by up to ±5.0% of their original values, except temperatures which may move by up to ±5.0°C from their original values during one cycle of the real time optimizer. Therefore, for all manipulated variables except temperatures, the size of the "window" created by the bounds can vary between cycles of the real time optimizer (i.e., 0.05x₀ ≠ 0.05x₁ as shown in Figure 5.2). Figure 5.2 illustrates how these manipulated variable bounds are implemented using an example optimization problem with 2 manipulated variables.

5.2 Sequential Modular Simulation

The sequential modular economic optimization simulation was developed using the MODELMANAGER graphical user interface [8, 9] to produce an ASPEN PLUS input file. Some direct editing of the input file was also required, particularly in developing the in-line FORTRAN blocks, and the FORTRAN objective function.

The SQP optimization algorithm was used to solve this optimization problem. The implementation of the SQP method was similar to that used for the data reconciliation problem; see Section 4.2.1 for more details. Details of
Table 5.2: Economic optimization inequality constraints.

<table>
<thead>
<tr>
<th>Lower Bound</th>
<th>Variable</th>
<th>Upper Bound</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.005</td>
<td>C₄-Distillate stream C₅ mole fraction</td>
<td>0.150</td>
<td>lbmol/lbmol</td>
</tr>
<tr>
<td></td>
<td>Light Iso stream Reid vapour pressure</td>
<td>14.0</td>
<td>psi</td>
</tr>
<tr>
<td>110.0</td>
<td>Light Iso stream bubble point temperature</td>
<td></td>
<td>°F</td>
</tr>
<tr>
<td>176.0</td>
<td>Heavy Iso 10% volume distilled true boiling point temperature</td>
<td>266.0</td>
<td>°F</td>
</tr>
<tr>
<td>284.0</td>
<td>Heavy Iso 90% volume distilled true boiling point temperature</td>
<td>464.0</td>
<td>°F</td>
</tr>
<tr>
<td>302.0</td>
<td>Light Distillate 10% volume distilled true boiling point temperature</td>
<td>554.0</td>
<td>°F</td>
</tr>
<tr>
<td>302.0</td>
<td>Light Distillate 90% volume distilled true boiling point temperature</td>
<td>554.0</td>
<td>°F</td>
</tr>
<tr>
<td>1000</td>
<td>C1 column reflux standard liquid volume flow</td>
<td>9000</td>
<td>bbl/day</td>
</tr>
<tr>
<td></td>
<td>C2 column reflux standard liquid volume flow</td>
<td>25,000</td>
<td>bbl/day</td>
</tr>
<tr>
<td></td>
<td>C4 column feed standard liquid volume flow</td>
<td>10,604</td>
<td>bbl/day</td>
</tr>
<tr>
<td></td>
<td>C5 column feed standard liquid volume flow</td>
<td>6000</td>
<td>bbl/day</td>
</tr>
<tr>
<td>125.0</td>
<td>C1 column tray 3 temperature</td>
<td>220.0</td>
<td>°F</td>
</tr>
<tr>
<td>530.0</td>
<td>C1 column reboiler outlet temperature</td>
<td>675.0</td>
<td>°F</td>
</tr>
<tr>
<td>120.0</td>
<td>C2 column tray 2 temperature</td>
<td>250.0</td>
<td>°F</td>
</tr>
<tr>
<td>550.0</td>
<td>C2 column reboiler outlet temperature</td>
<td>700.0</td>
<td>°F</td>
</tr>
</tbody>
</table>
Figure 5.2: Example optimization illustrating the use of manipulated variable bounds. This graph shows how the manipulated variables on cycle 1 of the optimizer are restricted to the dashed box around \((x_0, y_0)\). Cycle 2 of the optimizer starts from the optimum of cycle 1 and is restricted to the second dashed box around \((x_1, y_1)\).
the objective function, inequality constraints and manipulated variables are covered in the following subsections.

5.2.1 Objective Function

The profit objective function in ASPEN PLUS is supplied as FORTRAN 77 code. The objective function is calculated in the following order:

1. Calculate the Light Iso unit price including the Reid vapour pressure quality premium from Equation (5.3):

2. Calculate the six product values individually using Equation (5.2), then sum them to give the total product value:

3. Calculate the feed cost from Equation (5.4):

4. Calculate the two furnace utility costs individually using Equation (5.5):

5. Finally, subtract the feed cost and the two furnace utility costs from the total product value to give the profit to be maximized.

Where necessary, unit conversions were added to the above equations to convert variables from the imperial units used in the process flowsheet to the metric units used in the objective function. The current value of the stream flow rate and reboiler heat duty variables used in the above equations were accessed directly from the process flowsheet. These ASPEN PLUS flowsheet variables are defined as FORTRAN variables prior to execution of the of the objective function code.

The Reid vapour pressure premium ($q_L$) and specification ($P_{spec}$), unit prices given in Table 5.1 and the furnace efficiencies ($\eta_i$) are all read in from the data file IOBJFN.DAT using an in-line FORTRAN block (see Appendix B for a detailed description of this data file). This in-line FORTRAN block is executed before the economic optimization commences. The data read in from the file are stored in FORTRAN “common” blocks for use during the calculation of the objective function.
5.2.2 Process Inequality Constraints

The 25 inequality constraints listed in Table 5.2 were implemented using 25 constraint blocks in ASPEN PLUS. Each constraint block is also listed in the optimization block in order to apply the constraint to that optimization problem. Each constraint requires a specification involving ASPEN PLUS flowsheet variables defined as FORTRAN variables, and FORTRAN common block variables. A tolerance specification for each constraint is also required. The constraint is said to be “active” if the constrained variables are within this tolerance, “inactive” if the variables are inside the constraint and “violated” if the variables are outside the constraint.

The constraint values given in Table 5.2 are read in from the data file ICNSTR.DAT using an in-line FORTRAN block (see Appendix B for a detailed description of this data file). The data read in from the file are stored in FORTRAN “common” blocks for use during the calculation of the constraints.

5.2.3 Manipulated Variable Selection and Bounding

The manipulated variables used in the ASPEN PLUS economic optimization are the same as those used in the data reconciliation, except the stabilizer feed stream flow rate and temperature. The stabilizer feed stream conditions cannot be affected by the stabilizer-splitter process, and therefore cannot be manipulated during the economic optimization. The manipulated variables used are summarised in Table 5.3. The initial guesses used for the manipulated variables are the corresponding process flowsheet input specification values.

The condenser heat duties for columns C1 and C2 cannot be varied automatically by the process control system in this plant. Unfortunately, these heat duties are result variables in the process model and therefore cannot be fixed easily. Therefore, two equality constraint blocks were added to prevent movement of the condenser heat duties during the economic optimization.
Table 5.3: ASPEN PLUS economic optimization manipulated variables.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1 molar reflux ratio</td>
<td>lbmol/lbmol</td>
</tr>
<tr>
<td>C1 condenser molar vapour fraction</td>
<td>lbmol/lbmol</td>
</tr>
<tr>
<td>C1 reboiler mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C1 reboiler outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>E1 outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C2 liquid distillate mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2 reboiler mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2 reboiler outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C2 condenser sub-cooled temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C4 reboiler heat duty</td>
<td>MMBTU/hr</td>
</tr>
<tr>
<td>C5 reboiler heat duty</td>
<td>MMBTU/hr</td>
</tr>
<tr>
<td>C4 feed stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C5 feed stream mole flow</td>
<td>lbmol/hr</td>
</tr>
</tbody>
</table>

These constraint blocks work by storing the initial value of the condenser heat duty to a FORTRAN common block variable before the optimization commences. The constraint is then specified by requiring the condenser heat duty to be equal to its initial value stored in the common block variable, to within the specified tolerance of 0.1 MMBTU/hr.

The upper and lower bounds on the manipulated variables are used to restrict the movement of the optimizer to prevent large changes in the set points being returned to the plant’s process control system (see Section 5.1.4 for more detail). These manipulated bounds are specified for all manipulated variables except temperatures similarly to the following example ASPEN PLUS input code:

```
LIMITS "C2MD-(C2MD*PC2MD)" "C2MD+(C2MD*PC2MD)"
```

where C2MD = initial manipulated variable value (for this example, the Light Iso stream molar flow rate);
PC2MD = the fraction of the initial manipulated value value that this variable may be varied. For this problem, PC2MD is equal to 0.05 for all manipulated variables except temperatures.

For temperature manipulated variables, the manipulated variable bounds are specified in the same manner as the following ASPEN PLUS input code:

```plaintext
LIMITS "C1RBT - PC1RBT" "C1RBT + PC1RBT"
```

where C1RBT = initial manipulated variable value (for this example, the C1 reboiler outlet temperature);
PC1RBT = the number of degrees Fahrenheit this manipulated variable may be varied. For this problem, PC1RBT is equal to 5°F for all manipulated temperature variables.

The variables specifying the ranges in which the manipulated variables may move (for the above example codes, PC2MD and PC1RBT) are read in from the data file IOFREE.DAT using an in-line FORTRAN block (see Appendix B for a detailed description of this data file). The data read in from this file are stored in FORTRAN “common” blocks for use during the calculation of the manipulated variable bounds.

### 5.3 Equation-oriented Simulation

Development of the equation oriented economic optimization was performed by editing the ASCII text keyword based SPEEDUP input file. Details of the objective function, inequality constraints and manipulated variables are covered in the following subsections.

#### 5.3.1 Optimization Algorithm

The SRQP optimization algorithm was used to solve the SPEEDUP economic optimization problem. The implementation of the SRQP method was similar
to that used for the data reconciliation problem, except that the global convergence scheme chosen was a line search method with a modified augmented Lagrangian. The modified augmented Lagrangian was used because of the inequality constraints present in this optimization problem. See Section 4.3.1 for more details on how the SRQP algorithm was implemented.

5.3.2 Objective Function

The objective function was specified in the global section of the SPEEDUP input file using the same equation syntax used in SPEEDUP models. The objective function to be maximized is the profit calculated by subtracting the feed cost and the two furnace utility costs from the total product value. This profit objective is also multiplied by a weighting factor which can be varied to help promote convergence (see Section 5.4.2 for more detail). The following equations are included as equality constraints in the global section of the input file to be solved simultaneously with the rest of the process flowsheet:

- Calculate the Light Iso unit price including the Reid vapour pressure quality premium from Equation (5.3);
- Calculate the six product values individually using Equation (5.2), then sum them to give the total product value;
- Calculate the feed cost from Equation (5.4);
- Calculate the two furnace utility costs individually using Equation (5.5):

Where necessary, unit conversions were added to the above equations to convert variables from the imperial units used in the process models to the metric units used in the objective function. The current value of the stream flow rate and reboiler heat duty variables used in the above equations were accessed directly from the process flowsheet by using their full SPEEDUP variable name.
The Reid vapour pressure premium \((q_L)\) and specification \((P_{\text{spec}})\), unit prices given in Table 5.1, furnace efficiencies \((\eta_i)\) and the objective function weighting factor are all read in from the data file IOBJFN.DAT using SPEEDUP's external data interface (EDI) (see Appendix C for a detailed description of this data file). The EDI is used prior to the optimization to assign SPEEDUP variables with variables read in from external data files.

### 5.3.3 Process Inequality Constraints

The 25 inequality constraints listed in Table 5.2 were implemented in the global constraint subsection of the SPEEDUP input file. Each inequality constraint is also specified as a variable bound for the corresponding constrained variable through the EDI. This method of duplicating constraints in both the global section and as a variable bounds is recommended when using SRQP. This is because SRQP can handle simple variable bounds directly without the use of slack variables [13]. These simple bounds will always be satisfied by the SRQP method, unlike the inequality constraints.

The constraint values given in Table 5.2 are read in from the data file ICNSTR.DAT using SPEEDUP's EDI (see Appendix C for a detailed description of this data file).

### 5.3.4 Manipulated Variable Selection and Bounding

The manipulated variables used in the SPEEDUP economic optimization are the same as those used in the data reconciliation, except the stabilizer feed stream flow rate and temperature, and the condenser heat duties. The stabilizer feed stream conditions cannot be affected by the stabilizer-splitter process, and therefore cannot be manipulated during the economic optimization. Likewise, the condenser heat duties for the columns C1 and C2 cannot be adjusted automatically by the process control system in this plant and are therefore not manipulated during the economic optimization. The manipulated variables used are summarised in Table 5.4. The initial guesses
Table 5.4: SPEEDUP economic optimization manipulated variables.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>DIST-C4 stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>E1 inlet mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C1 reboiler mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2 condenser subcooled temperature drop (bubble point less subcooled temperature)</td>
<td>°F</td>
</tr>
<tr>
<td>E1 outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>SSFEED stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2 reboiler mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C4 feed stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C5 feed stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>HV-ISO stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>LT-DIST stream mole flow</td>
<td>lbmol/hr</td>
</tr>
</tbody>
</table>

used for the manipulated variables are the corresponding input specification values.

The upper and lower bounds on the manipulated, or free, variables are used to restrict the movement of the optimizer to prevent large set point changes as detailed in Section 5.1.4. From testing of this optimization problem in SPEEDUP, it was found that the SRQP optimization algorithm was unable to find an optimum if it lay on a manipulated variable bound. Therefore the manipulated variable bounds were applied indirectly as bounds and inequality constraints on flowsheet variables equal to the manipulated variables. For example, the column C1 bottoms mole flow, C1BT29.L.OUT1 is a manipulated variable. The heat exchanger E1 inlet mole flow, E1.F_IN should also be at the same value as the bottoms mole flow, therefore both bounds and global inequality constraints are placed on this variable instead. Similar equivalent variables were found for all of the manipulated variables in this optimization.
The upper and lower bounds, and inequality constraints on the variables equivalent to the manipulated variables were implemented in the optimization simulation as follows:

- For all variable types except temperature, the upper and lower bounds and inequality constraints are calculated from:

\[
\begin{align*}
y^{UB}_i &= x^{(0)}_i + q_i x^{(0)}_i \\
y^{LB}_i &= x^{(0)}_i - q_i x^{(0)}_i
\end{align*}
\]  

(5.6)

where \( y^{UB}_i \) = upper bound for the variable equivalent to the manipulated variable;
\( y^{LB}_i \) = lower bound for the variable equivalent to the manipulated variable;
\( x^{(0)}_i \) = initial manipulated variable value;
\( q_i \) = the fraction of the initial manipulated variable value that this variable may be varied. For this problem, all \( q_i \) are equal to 0.05.

- For temperature variables, the upper and lower bounds and inequality constraints are calculated from:

\[
\begin{align*}
y^{UB}_i &= x^{(0)}_i + r_i \\
y^{LB}_i &= x^{(0)}_i - r_i
\end{align*}
\]  

(5.7)

where \( r_i \) = the number of degrees Fahrenheit this manipulated variable may be varied. For this problem, all \( r_i \) are equal to 5°F.

The variables specifying the ranges in which the manipulated variables may move (the values \( q_i \) and \( r_i \) in Equations (5.6) and (5.7)) are read in from the data file IOFREE.DAT using SPEEDUP’s EDI (see Appendix C for a detailed description of this data file). The values of the bounds \( y^{UB}_i \) and \( y^{LB}_i \) are calculated in the EDI FORTRAN code and then assigned directly to the variable’s upper and lower bounds, and also to SPEEDUP global variables for use in the inequality constraints.
The manipulated variables also require upper and lower bounds for use by the optimization algorithm to determine initial step sizes. These bounds, however, should not be reached during the optimization simulation. Therefore, these bounds are set outside the bounds placed on the variables equivalent to the manipulated variables. This is achieved by the following method:

- For all variable types except temperature, the upper and lower manipulated variable bounds are calculated from:

\[ x_i^{UB} = x_i^{(0)} + 1.5 q_i x_i^{(0)} \]
\[ x_i^{LB} = x_i^{(0)} - 1.5 q_i x_i^{(0)} \]  

(5.8)

where \( x_i^{UB} \) = upper bound for the manipulated variable:
\( x_i^{LB} \) = lower bound for the manipulated variable.

- For temperature variables, the upper and lower bounds and inequality constraints are calculated from:

\[ x_i^{UB} = x_i^{(0)} + 1.5 r_i \]
\[ x_i^{LB} = x_i^{(0)} - 1.5 r_i \]  

(5.9)

The values of the bounds \( x_i^{UB} \) and \( x_i^{LB} \) are also calculated in the EDI FORTRAN code and then assigned directly to the manipulated variable's upper and lower bounds.

5.4 Discussion

The following subsections discuss various problems encountered using both the sequential modular and equation-oriented simulators for economic optimization. A summary comparing various quantitative aspects of the economic optimization development and performance are presented in Table 5.5.
Table 5.5: Comparison of both process simulators for economic optimization.

<table>
<thead>
<tr>
<th></th>
<th>Sequential Modular Simulator</th>
<th>Equation-oriented Simulator</th>
</tr>
</thead>
<tbody>
<tr>
<td>Development Time (hours)</td>
<td>73.5</td>
<td>134.5</td>
</tr>
<tr>
<td>Input file size (bytes)</td>
<td>40,746</td>
<td>291,130</td>
</tr>
<tr>
<td>(without preset variables)</td>
<td>(37,616)</td>
<td>(71,374)</td>
</tr>
<tr>
<td>Number of manipulated variables</td>
<td>13</td>
<td>11</td>
</tr>
<tr>
<td>Number of inequality constraints</td>
<td>25</td>
<td>47</td>
</tr>
<tr>
<td>Number of additional equality constraints</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>CPU time (mins)(^a)</td>
<td>119.78</td>
<td>104.89</td>
</tr>
<tr>
<td>Optimization iterations</td>
<td>6</td>
<td>28</td>
</tr>
<tr>
<td>Flowsheet passes or function evaluations</td>
<td>139</td>
<td>55</td>
</tr>
<tr>
<td>(tear stream iterations)</td>
<td>(1,519)</td>
<td></td>
</tr>
<tr>
<td>(derivative evaluations)</td>
<td>(29)</td>
<td></td>
</tr>
<tr>
<td>Initial objective function value ($/hr)</td>
<td>-159.7225</td>
<td>-159.73</td>
</tr>
<tr>
<td>Final objective function value ($/hr)</td>
<td>91.1353</td>
<td>416.00</td>
</tr>
<tr>
<td>Number of constraints active at solution</td>
<td>1(^b)</td>
<td>1(^c)</td>
</tr>
</tbody>
</table>

\(^a\)CPU time is measured for calculations only on an IBM RS 6000 Model 530H computer.
\(^b\)Light Iso stream Reid vapour pressure upper bound constraint active.
\(^c\)C\(_4\)-Distillate stream C\(_3\) component mole fraction lower bound constraint active.
5.4.1 Sequential Modular Simulation

The building and debugging of the economic optimization simulation was relatively simple. A problem arose when trying to find a method of preventing the column C1 and C2 condenser heat duties from being varied during the economic optimization. Ideally, the condenser heat duties would have been specified variables in process flowsheet preventing them from changing throughout the simulation. However, flowsheet convergence was unable to be obtained when the condenser heat duties were used as specified variables. Therefore, two equality constraints were added to ensure that the condenser heat duties remained at their initial value. It was found that unless this constraint was 'converged' on the first iteration of the optimizer, it was extremely unlikely that the SQP optimization algorithm would be able to satisfy the constraint before the end of the simulation. The solution to this was to ensure that the initial values of the condenser heat duties were passed to the optimization simulation from the results of the previous data reconciliation simulation. This ensured that both of the equality constraints were converged on the first iteration of the SQP algorithm, and usually remained converged throughout the optimization.

The only other problems with the ASPEN PLUS economic optimization were found when trying to debug errors in passing information between simulation blocks using FORTRAN common blocks. This was the same problem encountered with the data reconciliation simulation development, and was solved in the same way using temporary FORTRAN code to print out the values of the variables being passed between simulation blocks (see Section 4.4.1 for more detail).

One extra SQP optimization algorithm tuning parameter was used in addition to those described in Section 4.4.1 for the data reconciliation simulation. This parameter was CONST-ITER which was set to 10 iterations. This parameter specifies the number of additional iterations that the SQP optimization algorithm should take after the optimization convergence test has been satisfied to satisfy any violated constraints. This parameter was
increased to 10 iterations to help improve the optimizer's ability to converge any violated constraints.

Most convergence problems encountered when testing this optimization simulation were caused by violated constraints. It was found that if the simulation began with significantly violated inequality constraints that the SQP optimization algorithm appeared to have some difficulty in satisfying these constraints during the course of the optimization. The errors returned by the SQP optimization algorithm were either "Up hill search direction predicted" or "Line search failed on the final iteration". This was especially noticeable on violations of the constraints involving "property set" variables: Reid vapour pressure, 10% and 90% volume distilled true boiling point temperatures, and bubble point temperature. Property set variables are measurements defined by the user to be calculated for flowsheet streams other than the standard flow, composition and thermodynamic data produced by ASPEN PLUS. Increasing the parameter CONST-ITER helped, but not in all cases.

As found with the data reconciliation optimization in ASPEN PLUS, computational speed of the optimizer was affected mostly by the tear stream convergence on the splitter column. A total of 1519 passes through the process units C2C4C5, C2SPL1 and F2 were required for the 139 flowsheet evaluations required during the optimization. Therefore an average of 11 tear stream iterations were required for each flowsheet pass requiring a significant amount of computational time.

5.4.2 Equation-oriented Simulation

Development of the objective function and inequality constraints was relatively straightforward for the SPEEDUP economic optimization. The manipulated variables were chosen to be the same as the data reconciliation optimization except for the stabilizer feed stream mole flow and temperature, and the column C1 and C2 condenser heat duties. This prevented the convergence problems due to poor choice of manipulated variables as seen in
the data reconciliation optimization development. Also, since the column C1 and C2 condenser heat duties were already specified variables, there was no need for equality constraints to prevent the economic optimizer from varying these variables as with ASPEN PLUS.

The main problem encountered in debugging the SPEEDUP economic optimization was restricting the movement of the manipulated variables. Initially, the manipulated variable bounds were applied directly to the manipulated variables. This resulted in repeatable errors from the SRQP optimization algorithm caused by "inconsistent constraints" when the optimum was found to lie on a manipulated variable bound. Since the manipulated variable bounds are being used deliberately to limit the movement of the economic optimization on each cycle of the real time optimizer, several manipulated variable bounds will often be active at the optimum. To alleviate this problem, indirect manipulated variable bounds were added to prevent the true manipulated variable bounds from being reached as described in Section 5.3.4. These indirect bounds were implemented as both bounds and global inequality constraints on the variables equivalent to the manipulated variables. The reason for both bounds and inequality constraints is because the variable bounds can be handled directly by the SRQP optimization algorithm, and presence of the inequality constraints provide Lagrangian and other information at the end of the optimization. This is the same reason for duplicating the process inequality constraints in both the global constraint subsection and also as variables bounds. No reason has been found for why the SRQP optimization algorithm consistently fails when the optimum lies on a manipulated variable bound, however the above work around does appear to fix this problem.

Tuning of the SRQP optimization algorithm was again found to be difficult for the same reasons found in the data reconciliation optimization, mostly due to a lack of tuning parameters with which to modify the algorithms behaviour. The global convergence scheme chosen was the augmented modified Lagrangian function due to the presence of inequality constraints.
It was found that the line search method with an absolute penalty function tended to take very small step sizes and consistently failed due to "slow convergence".

The profit objective function was multiplied by a weighting factor to provide a method for tuning the optimization. This weighting factor was varied between 1 and 2 to promote convergence of the economic optimization. Generally the weighting factor was found to lie between 1.2 and 1.5. This method worked for most of the problems attempted, but often required retuning of the weighting factor even for slight changes in starting point. Convergence failures for problems with poorly tuned weighting factors were reported by the SRQP optimization algorithm to be caused by either "slow convergence" or "inconsistent constraints". No consistent pattern or reason for these convergence failures could be found. A possible reason may be the unscaled manipulated and process flowsheet variables in this problem. Also the criteria for "slow convergence" appears to be too strict and often occurs when the optimizer seems close to an answer. Unfortunately, there is no way to tune the SRQP algorithm's criteria for slow convergence to prevent this error.

From Table 5.5, it can be seen that SPEEDUP achieved a significantly better profit objective function value for this one run of the economic optimization. This higher objective function profit may have been caused by a combination of SPEEDUP's infeasible path SRQP optimization method and more accurate derivative information available from the process flowsheet models. See Section 6.6.2 for a more detailed comparison of the ASPEN PLUS and SPEEDUP economic optimization results.

5.4.3 Checking for Model Differences

Table 5.6 shows the differences between the ASPEN PLUS and SPEEDUP process models. The results in this table were produced by performing a steady state simulation in ASPEN PLUS using the results obtained at the end of the SPEEDUP economic optimization. The largest discrepancy found between the two process models for any stream property was a 0.93%
Table 5.6: Discrepancies between ASPEN PLUS and SPEEDUP process models at the SPEEDUP economic optimization optimum.

<table>
<thead>
<tr>
<th>Stream Name</th>
<th>Molar Flow</th>
<th>Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vapour</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>C4-distillate</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>Splitter Feed</td>
<td>0.01%</td>
<td>0.00%</td>
</tr>
<tr>
<td>Light Iso</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>Heavy Iso</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>Light Distillate</td>
<td>0.02%</td>
<td>0.00%</td>
</tr>
<tr>
<td>SS Feed</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
</tbody>
</table>

difference for the Heavy Iso stream 10% volume distilled true boiling point temperature. For this operating point, SPEEDUP gave a profit objective function value of $416.00/hr. ASPEN PLUS calculated the profit to be $411.23/hr for the same operating point, a discrepancy of 1.15%. Therefore it can be concluded that the differences between the two process models are extremely small.

Unfortunately ASPEN PLUS does not include any options to view the reduced gradients from the process model during the optimization. This would allow the comparison of the gradients produced by both ASPEN PLUS and SPEEDUP to see if the difference in results were caused by the optimization algorithm or inaccuracies in derivatives from the process models.
Chapter 6

Real Time Optimizer Linking and Results

6.1 Real Time Optimizer Linking

The data reconciliation and economic optimization simulations developed in the previous two chapters need to be linked together to form the real time optimizer. The linking of the optimizer involves writing a program to call the data reconciliation and economic optimization simulations when required, transfer data between the simulations and the plant, store the results produced and detect any errors encountered during the real time optimization. Figure 6.1 highlights the part of the real time optimizer to be developed in this section.

The data to be transferred within the real time optimization system is similar for both real time optimizers. Figure 6.2 illustrates the data files which need to be transferred between the data reconciliation and economic optimization simulations, and also between the real time optimizer and the plant’s process control system. The real time optimizer cycle begins with the data reconciliation module reading in the measurement data from the plant’s process control system. For these simulations, the process data is supplied either from process data provided by Shell Canada, or from a steady state
process simulation acting as the plant. The Shell process data are averaged over one hour of measurements from the plant and are used for the first cycle of most of the following real time optimizer runs. All subsequent cycles use data provided from the steady state simulation either with or without random noise added (see Section 6.2 for details of the noise added).

The data reconciliation simulation reads in the measurement data variances and data reconciliation weights from data files. Before the data reconciliation commences, the final simulation settings from the previous economic optimization simulation are read in from a file. These simulation settings are used to provide the best known starting point for the data reconciliation. When the data reconciliation is completed, the reconciled variables and other results files are produced by the simulation. The simulation settings at the end point of this simulation are also transmitted to the economic optimization simulation to provide the starting point.

The economic optimization simulation then reads in the economic data
Figure 6.2: Real time optimizer data transfer.
and inequality constraint values from data files. At the end of the optimization, the new optimized set points for the process are sent to the plant's process control system for implementation in the plant. Also, the simulation settings from the end point of the optimization are stored in a data file for use by the data reconciliation simulation during the next cycle of the real time optimizer.

As previously mentioned, most testing of the real time optimizer is performed using measurement data from a steady state ASPEN PLUS simulation of the stabilizer-splitter process. This simulation is used to simulate the set points received from the economic optimization and output a new set of measurement data for the next cycle. Random noise is added to the process data using a small FORTRAN program which calls a NAG FORTRAN Library Routine [84] for generating random numbers. The input code for both the plant simulation and the FORTRAN program to add noise are included in Appendix F.

### 6.1.1 Sequential Modular Simulator

Figure B.2 in Appendix B shows a flow chart of the sequential modular simulator implementation of the real time optimizer cycle illustrated in Figure 6.2. A Unix C-Shell script is used to control the real time optimizer by starting the simulations when required, moving the data files between simulations, storing the results and checking for errors. The data reconciliation and economic optimization simulations were combined into a single input file and sequenced using an ASPEN PLUS sequence block. This allows the economic optimization to start using the end point of the data reconciliation without the need to write out to a data file. Passing the results of the economic optimization back to the data reconciliation for the next cycle was more difficult. Every specified and estimated variable needs to written out and read in through a user specified FORTRAN block. This involved a lot of code and was difficult to debug.

Before running the real time optimizer, a setup program needs to be ex-
executed which translates and compiles the simulations. Appendix B provides the documentation for setting up and running the ASPEN PLUS based real time optimizer. The input code used for the sequential modular real time optimizer is included in Appendix D.

6.1.2 Equation-oriented Simulator

Figure C.2 in Appendix C shows a flow chart of the equation-oriented simulator implementation of the real time optimizer cycle illustrated in Figure 6.2. Similar to the sequential modular simulator, a Unix C-Shell script is used to control the real time optimizer by starting the simulations when required, moving the data files between simulations, storing the results and checking for errors. SPEEDUP has no sequencing feature, so the data reconciliation and economic optimization have to be run as separate simulations in different directories. Therefore the results of the data reconciliation have to written to file and passed on to the economic optimization simulation. However, this was accomplished simply by issuing a single command which saves the results of previous run to file. These results are then read back in and are then used to preset a simulation using SPEEDUP's "Use" environment. To run SPEEDUP simulations in batch mode, a text file storing the commands for the SPEEDUP Executive is specified in the command line when running the simulation.

Before running the real time optimizer, a setup program needs to be executed which translates and compiles the simulations, and runs the PROPERTIES PLUS input files. Appendix C provides the documentation for setting up and running the SPEEDUP based real time optimizer. The input code used for the equation-oriented real time optimizer is included in Appendix E.

6.2 Real Time Optimizer Comparison

The first run comparing the sequential modular and equation-oriented real time optimizers used the base case economic data presented in Table 5.1. The
two optimizers were run for as many cycles as possible using this economic data with no random noise added to the process measurements. That is, the economic optimization on each cycle was started with the results of the previous economic optimization. The term "cycle" of a real time optimizer will be used in this thesis to refer to one complete run through the flow chart given in Figure 6.1. That is, the measured data is read in from the plant. data reconciliation is performed on this data, then the process is optimized before the set points are passed back to the plant.

Figure 6.3 graphs the progress of the economic objective function on each cycle for both of the real time optimizers. The expected global optimum profit of $751.95/hr shown in Figure 6.3 was the highest obtained profit over several runs for this problem when all restrictions on the movement of the manipulated variables were removed (the process inequality constraints were still applied). Since the actual shape of the shape of the objective function is extremely complex, and also because of any process modelling errors, this optimum cannot be guaranteed to be the true global optimum for this process.

SPEEDUP failed after fewer cycles, unable to converge the economic optimization on sixth cycle, however, it achieved a higher profit objective than the ASPEN PLUS real time optimizer, nearly reaching the expected global optimum profit. Twelve different weighting factors were tried manually in the economic objective function, all of which ended with the same "slow convergence" error given by the SRQP optimization algorithm. It is possible that a weighting factor exists which can converge this problem, however it was extremely difficult to determine the value of the weighting value manually for this particular optimization.

ASPEN PLUS failed on the eleventh cycle due to a violated inequality constraint which the SQP algorithm could not satisfy. The violated constraint was the upper limit on the Light Distillate stream 90% volume distilled true boiling point temperature. The error given by the optimization algorithm was "line search failed on final iteration; solution may not be op-
Figure 6.3: Graph comparing base case with no measurement noise profits (economic objective function) for both real time optimizers. The expected global optimum profit for this optimization is shown as a dashed line.
timal”.

The active inequality constraint at the end of the first cycle was the Light Iso stream Reid vapour pressure upper bound for both real time optimizers. For all subsequent cycles of the ASPEN PLUS real time optimizer, the active constraint was the upper bound on the Light Distillate stream 90% volume distilled true boiling point temperature. The upper bound constraint on the Light Iso stream Reid vapour pressure was also active at the end of cycles 2, 6, 7 and 10. For all cycles, except the first, of the SPEEDUP real time optimizer, the active inequality constraints were lower bound on the C₄-Distillate stream C₅ mole fraction and the upper bound on the Light Distillate stream 90% volume distilled true boiling point temperature. Figures 6.4 and 6.5 show the set point changes made at the end of each cycle by both of the real time optimizers. For more information on the performance of the two real time optimizers, see Table A.3 and Table A.4 in Appendix A.

A second run comparing the two types of real time optimizer was performed on the base case economic data with noise added to the plant measurements. Again, the two optimizers were run for as many cycles as possible using the economic data presented in Table 5.1. The random noise was added to the process measurements calculated by the plant simulation was normally distributed with a standard deviation equal to 5% of the measured value.

A graph comparing the profit objective function values achieved by the two real time optimizers is given in Figure 6.6. As can be seen from this graph, both optimizers managed to complete only a few real time optimization cycles. Again, the expected global optimum of $751.95/hr is shown in Figure 6.6.

The SPEEDUP real time optimizer failed on the third cycle due to severe property errors which could not be corrected, however, it still attained a higher profit than the ASPEN PLUS optimizer. The property error occurred during a flash calculation by PROPERTIES PLUS when the bubble point for a mixture could not be found. Unfortunately there is no way to determine which flash in the flowsheet was consistently causing this error during
Figure 6.4: Graphs of the set point changes made during the base case runs with no measurement noise (1 of 2).
Figure 6.5: Graphs of the set point changes made during the base case runs with no measurement noise (2 of 2).
Figure 6.6: Graph comparing base case profits (economic objective function) with measurement noise for both real time optimizers. The expected global optimum profit for this optimization is shown as a dashed line.
the economic optimization on the third cycle of the real time optimizer. It should be noted that SPEEDUP required the objective function weights for both data reconciliation and economic optimization objective functions to be changed on both cycles completed. Changing the economic objective function weight for the third cycle of the real time optimizer had no effect on the property errors generated.

The ASPEN PLUS real time optimizer failed on the fifth cycle due to a violated inequality constraint which the SQP optimization algorithm could not satisfy. The violated bound was the upper limit on the Light Distillate stream 90% volume distilled true boiling point temperature. The error given by the optimization algorithm was “line search failed on final iteration: solution may not be optimal”.

The active inequality constraint at the end of the first cycle was the Light Iso stream Reid vapour pressure upper bound for both real time optimizers. For all subsequent cycles of the ASPEN PLUS real time optimizer, the active constraint was the upper bound on the Light Distillate stream 90% volume distilled true boiling point temperature. At the end of the second cycle of the SPEEDUP real time optimizer, the active inequality constraints were lower bound on the C4-Distillate stream C5 mole fraction and the upper bound on the Light Distillate stream 90% volume distilled true boiling point temperature. For more information on the performance of the two real time optimizers, see Table A.1 and Table A.2 in Appendix A.

6.3 Economic Model Changes

Three areas of the economic model were studied:

1. Changes to the two key product stream prices, Heavy Iso and Light Distillate.

2. Sensitivity analysis of the economic objective function.
3. The effect of changes in the economic parameters part way through a real time optimizer run. This was tested by changing the product prices from typical winter operating prices to typical summer operating prices. Please note that these runs were tested using ASPEN PLUS version 9.3 instead of version 9.2 as all other runs used. For more details on the different versions of ASPEN PLUS, see Section 6.5.

The results of these studies are presented in the following subsections. Only the ASPEN PLUS real time optimizer was used in the following studies due to the problems encountered tuning the SPEEDUP real time optimizer for each cycle.

6.3.1 Product Price Changes

Four real time optimizer runs were performed to study the effect of Heavy Iso and Light Distillate product stream price changes. High and low values were chosen for each of these product prices to see what effect they have on the operation of the real time optimizer. The high and low prices were $193.89/m^3 and $173.89/m^3 for the Heavy Iso product stream and $200.52/m^3 and $180.52/m^3 for the Light Distillate product stream respectively. The run with the Heavy Iso and Light Distillate stream prices at $193.89/m^3 and $180.52/m^3 respectively corresponds to the base case run in Section 6.2. Random measurement noise was added to the data produced by the "plant" simulation for all four of the following real time optimizer runs.

A graph comparing the objective function profits at the end of each cycle for each of the four real time optimizer runs is presented in Figure 6.7. It should be noted that the negative profits shown in Figure 6.7 mean that the stabilizer-splitter process is being run at a loss, however, this does not necessarily reflect a loss for the refinery as a whole. This is because the feed flow rate to this process is being determined by an upstream process and is not being varied by the real time optimizer. Since the feed to the stabilizer-splitter process cannot be used as a product, it must be split into products
Figure 6.7: Graph comparing profits (economic objective function) for different Heavy Iso and Light Distillate prices using the ASPEN PLUS real time optimizer.

Even if that incurs a loss for this process. In this case the real time optimizer is trying to minimize the loss incurred by the stabilizer-splitter process.

The real time optimizer runs shown in Figure 6.7 were attempted for four cycles each, however, the case where the Heavy Iso and Light Distillate prices were $173.89/m³ and $200.52/m³ respectively, convergence of the economic optimization on the fourth cycle was not possible. This convergence failure was for the same reason as the previous ASPEN PLUS real time optimizer failures, that is, the SQP optimization algorithm was unable to satisfy the upper bound inequality constraint on the Light Distillate stream 90% volume distilled true boiling point temperature. The error given by the optimization
algorithm was "no feasible point found to quadratic subproblem".

The active inequality constraints at the end of each real time optimizer cycle were the same as the base case run except for the case where both Heavy Iso and Light Distillate stream prices were at their high values. For all cases, the active inequality constraint after the first cycle was the Light Iso stream Reid vapour pressure upper bound, and at the end of the other cycles, the upper bound on the Light Distillate stream 90% volume distilled true boiling point temperature was active. For the case where the Heavy Iso and Light Distillate prices were $193.39/m^3 and $200.52/m^3 respectively, at the end of the fourth cycle, the lower bound on the Heavy Iso stream 10% volume distilled true boiling point temperature was also active. Figures 6.8 and 6.9 show the changes in set points made at the end of each cycle of the four real time optimization runs completed. For more information on the performance of real time optimizer on each of the four cases studied, see Tables A.1, A.5, A.6 and A.7 in Appendix A.

6.3.2 Economic Objective Function Sensitivity Analysis

To perform the economic objective function sensitivity analysis, the economic optimization simulation developed in Chapter 5 was modified to allow free movement of the manipulated variables. That is, the bounds used to constric the manipulated variable movements on each real time optimizer cycle were widened to allow the economic optimization to proceed directly to the optimum subject to the inequality constraints. The product stream prices, feed stream cost and utility fuel oil costs were then varied by ±5% from their original values (the original prices and costs are given in Table 5.1). The results of this study were produced by Fenton [39] and are summarised in Table 6.1. Each of the 14 runs detailed in Table 6.1 began from the simulation settings of an optimized base case run. The initial profit before and after optimization with the new product price or cost is given, along with
Figure 6.8: Graphs of the set point changes made during the runs with different Heavy Iso and Light Distillate prices using the ASPEN PLUS real time optimizer (1 of 2).
Figure 6.9: Graphs of the set point changes made during the runs with different Heavy Iso and Light Distillate prices using the ASPEN PLUS real time optimizer (2 of 2).
the penalty for not re-optimizing after this price or cost change occurred.

6.3.3 Changes in Economics During Real Time Optimization Runs

Four real time optimizer runs were performed using the ASPEN PLUS version 9.3 real time optimizer instead of version 9.2 (see Section 6.5 for more details on the changes between versions). Two of the runs used winter economic conditions throughout, that is, the prices were $173.89/m³ and $200.52/m³ for Heavy Iso and Light Distillate streams respectively and a Light Iso product Reid vapour pressure upper limit was set to 14 psi. The other two runs were performed with product prices changing part way through the run to summer prices from the winter conditions given above. The summer conditions used were $193.89/m³ and $180.52/m³ for Heavy Iso and Light Distillate streams respectively and a Light Iso product Reid vapour pressure upper limit of 10.5 psi. The price changes were chosen to reflect the change between typical summer and winter economic conditions, that is, in winter heating oil is generally in higher demand, while in summer, gasoline is in higher demand.

Graphs comparing the profit objective functions at each cycle for the winter case and winter to summer price change runs, with and without measurement noise, are presented in Figure 6.10. The ASPEN PLUS version 9.3 real time optimizer failed on the fifth cycle of the winter case run with random measurement noise due to two violated constraints. For the winter to summer run with measurement noise, the real time optimizer failed on the sixth cycle, also due to two violated inequality constraints. In both cases, the constraints violated were the upper bound on the stabilizer column C1 reflux flow and the upper bound on the Light Distillate stream 90% volume distilled true boiling point temperature. The error returned by the SQP optimization algorithm for the winter case was “no feasible point found to quadratic subproblem”, and for the winter to summer run the error returned
Table 6.1: ASPEN PLUS economic objective function sensitivity study results [39].

<table>
<thead>
<tr>
<th>Run</th>
<th>Profit before optimization ($/year)</th>
<th>Profit after optimization ($/year)</th>
<th>Penalty for not optimizing ($/year)</th>
<th>Penalty (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base case</td>
<td>4,901,000</td>
<td>4,901,100</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Low Vapour price</td>
<td>4,901,000</td>
<td>5,530,800</td>
<td>628,700</td>
<td>12.8</td>
</tr>
<tr>
<td>High Vapour price</td>
<td>4,901,200</td>
<td>5,137,500</td>
<td>236,300</td>
<td>4.8</td>
</tr>
<tr>
<td>Low C₄-Distillate price</td>
<td>4,375,200</td>
<td>4,477,400</td>
<td>102,200</td>
<td>2.3</td>
</tr>
<tr>
<td>High C₄-Distillate price</td>
<td>5,427,100</td>
<td>5,574,900</td>
<td>147,800</td>
<td>2.7</td>
</tr>
<tr>
<td>Low Light Iso price</td>
<td>4,227,300</td>
<td>4,663,500</td>
<td>436,200</td>
<td>10.3</td>
</tr>
<tr>
<td>High Light Iso price</td>
<td>5,575,000</td>
<td>7,548,700</td>
<td>1,973,700</td>
<td>35.4</td>
</tr>
<tr>
<td>Low Heavy Iso price</td>
<td>3,025,800</td>
<td>4,004,100</td>
<td>978,300</td>
<td>32.3</td>
</tr>
<tr>
<td>High Heavy Iso price</td>
<td>7,450,300</td>
<td>9,717,200</td>
<td>2,266,900</td>
<td>30.4</td>
</tr>
<tr>
<td>Low Light Distillate price</td>
<td>4,152,400</td>
<td>4,656,700</td>
<td>511,000</td>
<td>12.3</td>
</tr>
<tr>
<td>High Light Distillate price</td>
<td>5,649,900</td>
<td>8,066,800</td>
<td>2,416,900</td>
<td>42.8</td>
</tr>
<tr>
<td>Low Stabilizer feed cost</td>
<td>9,110,600</td>
<td>9,269,600</td>
<td>159,000</td>
<td>1.7</td>
</tr>
<tr>
<td>High Stabilizer feed cost</td>
<td>691,600</td>
<td>1,832,800</td>
<td>1,141,200</td>
<td>165.0</td>
</tr>
<tr>
<td>Low fuel oil cost</td>
<td>4,947,900</td>
<td>7,257,000</td>
<td>2,309,100</td>
<td>46.7</td>
</tr>
<tr>
<td>High fuel oil cost</td>
<td>4,854,400</td>
<td>6,380,200</td>
<td>1,525,800</td>
<td>31.4</td>
</tr>
</tbody>
</table>
was "line search failed on final iteration; solution may not be optimal".

The winter case and the winter to summer run with no measurement noise were both completed without errors for all 10 cycles of the real time optimizer attempted. However, the winter to summer run with no measurement noise did have violated constraints at the end of both cycles 4 and 5, the two cycles completed after the change to summer conditions. The constraints violated at the end of the fourth cycle were the Light Iso Reid vapour pressure and the Light Distillate stream 90\% volume distilled true boiling point temperature upper bounds. At the end of the fifth cycle, just the Light Iso Reid vapour pressure constraint was violated.

The active inequality constraints for most of the winter run with random measurement noise were the C₄-Distillate stream C₅ mole fraction lower bound and the Light Distillate stream 90\% volume distilled true boiling point temperature upper bound. For the winter run with no measurement noise, the active inequality constraints were the Light Iso stream Reid Vapour pressure for the first few cycles. For the latter cycles, the active constraints were both the upper and lower bounds on the Light Distillate stream 90\% volume distilled true boiling point temperature. For more information on the performance of real time optimizer on the winter case runs, see Tables A.8 and A.9 in Appendix A.

For the winter to summer run with noise added to the measurement data, the active constraints for most of the summer cycles was the upper limits on the Light Distillate stream 90\% volume distilled true boiling point temperature and the Light Iso stream Reid vapour pressure. The Light Distillate stream 90\% volume distilled true boiling point temperature was at its upper limit for all of the summer cycles of the winter to summer run without measurement noise. For the first 4 summer cycles, the Light Iso stream Reid vapour pressure was also at its upper limit. For more information on the performance of real time optimizer on the two winter to summer runs, see Tables A.10 and A.11 in Appendix A.
Figure 6.10: Graphs comparing profits (economic objective function) for winter case and winter to summer price change with and without noise using the ASPEN PLUS version 9.3 real time optimizer.
Figure 6.11: Graphs of the set point changes made during the winter case and winter to summer price change with no measurement noise runs using the ASPEN PLUS version 9.3 real time optimizer (1 of 2).
Figure 6.12: Graphs of the set point changes made during the winter case and winter to summer price change with no measurement noise runs using the ASPEN PLUS version 9.3 real time optimizer (2 of 2).
6.4 Process Disturbances

To test the effect of process disturbances on the performance of the real
time optimizer, the example of a restriction on the cooling capacity of the
condensers on columns C1 and C2 was chosen. This was implemented by
adjusting the measured condenser temperatures returned from the “plant”
simulation. For the cases tested, the condenser temperatures were forced
to be 100°F, approximately 10°F higher than normal. This test was used
to simulate an increase in ambient temperature and humidity around the
plant, thereby increasing the temperature of the cooling water used in the
condensers on columns C1 and C2.

Graphs comparing the profit objective functions at each cycle for the
base case and condenser temperature disturbance runs, with and without
measurement noise, are presented in Figure 6.13. Both runs, with and without
measurement noise, were run for as many cycles as possible. For the the
condenser disturbance run with measurement noise, the SQP optimization
algorithm failed due to violated inequality constraints on the fifth cycle. The
constraints violated were the upper limits on the C1 reflux flow and the Light
Distillate stream 90% volume distilled true boiling point temperature. The
error given by the optimization algorithm was “line search failed on final
iteration: solution may not be optimal”.

Similarly, the run with no measurement noise failed on the sixth cycle
of the real time optimizer due to violated inequality constraints and a con-
vergence failure within tear stream block on the stripper column. The con-
straints violated in this case were the upper limits on the Light Iso stream
Reid vapour pressure and the C4-Distillate stream C5 mole fraction. The
tear stream convergence failure appeared to be caused by problems with the
convergence of the PETROFRAC flowsheet block, C2C4C5, during some of
the tear stream iterations. This prevented the convergence of the tear stream
block within the required 30 tear stream iterations. The error given by the
optimization algorithm was “no feasible point found to quadratic subprob-
lem”.

Figure 6.13: Graphs comparing profits (economic objective function) for base case and condenser disturbance runs with and without noise using the ASPEN PLUS real time optimizer.
The active inequality constraints during the condenser disturbance run with measurement noise were then same as for the base case run (see Section 6.2). For the condenser disturbance run without measurement noise, the active inequality constraints for cycles 2, 3 and 5 were the upper limits on the Light Iso stream Reid vapour pressure, the C4-Distillate stream C5 mole fraction and the Light Distillate stream 90% volume distilled true boiling point temperature. At the end of cycle 4, both the Reid Vapour pressure and C5 mole fraction constraints were active. Figures 6.14 and 6.15 compare the changes in set points made at the end of each cycle for the base case and condenser disturbance runs without measurement noise added to the process data. For more information on the performance of real time optimizer on the two condenser disturbance runs, see Tables A.12 and A.13 in Appendix A.

6.5 ASPEN PLUS Software Upgrade

Soon after the previous real time optimizer runs were completed, the ASPEN PLUS process simulation package was upgraded from version 9.2 to 9.3. To test the effect of this upgrade, the real time optimizer was run without any modification using the new version of ASPEN PLUS on the base case. It was found that the optimizer failed on the second iteration due to process flowsheet convergence failures in both column C1 (modelled using RADFRAC) and columns C2, C4 and C5 (modelled using PETROFRAC). From the ASPEN PLUS version 9.3 manual [15], it was found that modifications had been been made to the RADFRAC and PETROFRAC unit operation models, and the SQP optimization algorithm.

During testing of the real time optimization problem, it was found that RADFRAC was now allows the use of different initialization methods for the column. It was found that setting the option INIT-OPTION=CRUDE in the RADFRAC model prevented the convergence errors encountered previously. No other changes were made to the real time optimizer code.

The graph in Figure 6.16 compares the profits returned from the economic
Figure 6.14: Graphs of the set point changes made during the base case and condenser disturbance with no measurement noise runs using the ASPEN PLUS real time optimizer (1 of 2).
Figure 6.15: Graphs of the set point changes made during the base case and condenser disturbance with no measurement noise runs using the ASPEN PLUS real time optimizer (2 of 2).
Figure 6.16: Graph comparing base case profits (economic objective function) with measurement noise for ASPEN PLUS versions 9.2 and 9.3.

Optimization for the two versions of ASPEN PLUS for the base case with measurement noise added to the plant data. The ASPEN PLUS version 9.3 real time optimization failed on the fourth cycle due to a violated inequality constraint which the SQP optimization algorithm could not satisfy. The violated constraint was the upper limit on the Light Distillate stream 90% volume distilled true boiling point temperature. The error given by the optimization algorithm was “line search failed on final iteration; solution may not be optimal”. For more information on the performance of the ASPEN PLUS version 9.3 real time optimizer, see Table A.14 in Appendix A.
6.6 Discussion

6.6.1 Real Time Optimizer Linking

Formation of the complete real time optimizer was relatively simple for both the sequential modular and equation-oriented process simulators. The linking of the real time optimizer took 37.5 hours of development time for ASPEN PLUS and 46 hours for SPEEDUP. Including the times for developing the process model, data reconciliation and economic optimization, the total real time optimizer development times were 436.5 hours for ASPEN PLUS and 886 hours for SPEEDUP.

The ability to perform sequencing of the data reconciliation and economic optimization simulations in ASPEN PLUS greatly simplified the linking of the real time optimizer. This allowed the whole real time optimization to be performed with a single ASPEN PLUS input file using one process flowsheet with two optimization blocks sequenced to run consecutively. SPEEDUP does not have a sequencing feature, therefore the data reconciliation and economic optimization simulations had to be performed using separate input files, and were sequenced externally using the Unix C-Shell controlling the real time optimizer.

SPEEDUP's ability to save the present operating point of a simulation and to re-read this operating point back into the simulation at any time simplified the transfer of data between simulations. In ASPEN PLUS, the transfer of the simulations settings at the end point of the economic optimization to the data reconciliation for the beginning of the next cycle had to coded manually using a user defined FORTRAN block. This was time consuming and required debugging of the FORTRAN code.

6.6.2 Real Time Optimizer Comparison

Both the sequential modular and equation-oriented process simulator based real time optimizers were able to be compared on only two problems due
to difficulties tuning the objective function weights in SPEEDUP. The two problems tested were the base case, using the economic data given in Table 5.1, and the base case with no measurement noise added to the data produced from the "plant" simulation.

Figure 6.3 shows that both the SPEEDUP and ASPEN PLUS real time optimizers were reasonably close to the expected global optimum when they failed for the case where no random noise was added to the measured data (SPEEDUP finished $53.30/hr and ASPEN PLUS $97.14/hr lower than the expected global optimum). However in Figure 6.6, for the runs where random noise was added to the process measurements, both optimizers were unable to get close to the expected global optimum (SPEEDUP finished $372.43/hr and ASPEN PLUS $504.92/hr lower than the expected global optimum). The global optimum shown in Figures 6.3 and 6.6 cannot be guaranteed to be the true economic global optimum for this process due to the highly complex and nonlinear nature of the objective function, and also because of any process modelling errors that may exist.

The graphs in Figures 6.3 and 6.6 show that SPEEDUP was able to achieve significantly higher profits than ASPEN PLUS, even though less optimizer cycles were able to be completed. The most likely reasons for the more aggressive economic optimization performed by SPEEDUP is due in part to the more accurate derivative information used by the optimization algorithm from the process model, and the use of an infeasible path optimization algorithm. Equation-oriented process models are able to produce analytical derivative information, where possible, instead of the numerical derivative information calculated from a sequential modular process flowsheet. This not only reduces the computational time required for an optimization, it also provides more accurate information for the optimization algorithm to estimate step lengths and search directions. The infeasible path SRQP optimization algorithm does not require the process flowsheet to be converged at every iteration and permits violation of constraints and variable bounds on the way to the optimum. ASPEN PLUS's SQP optimization algorithm can
only violate the inequality and equality constraints specified in the input file constraint blocks at each iteration. This ability to violate constraints allows the optimizer the possibility of finding a better optimum by stepping outside constraints temporarily on the way to the optimum.

Also, SPEEDUP used significantly less computational time to complete each real time optimization cycle requiring an average of 232.14 CPU minutes for the base case and 93.70 CPU minutes for the base case with no measurement noise. ASPEN PLUS required an average of 479.11 CPU minutes for the base case and 116.10 CPU minutes for the base case with no measurement noise to complete a real time optimizer cycle. The main reason for this difference in computational times is the iterative method used by the sequential modular simulator to solve tear stream blocks. See Section 4.4.1 for a more thorough discussion of how tear stream convergence affects the computational time taken by ASPEN PLUS.

As already discussed in Sections 4.4.2 and 5.4.2, many problems were encountered tuning the SPEEDUP real time optimizer by adjusting weighting factors in the objective function to promote convergence of the SRQP optimization algorithm. Unfortunately, the SRQP algorithm does not allow the user to modify any parameters that affect the algorithm’s criteria for “slow convergence”, the most common error message returned when the optimization fails to converge. Another factor that may contribute to the convergence difficulties in SPEEDUP optimization problems is poor flowsheet and manipulated variable scaling with the process models used. At this time, automatic flowsheet scaling using user defined scaling parameters is only available for steady state and dynamic simulations. Flowsheet scaling for optimization problems will be added in a future version of SPEEDUP according to the program documentation [11, 12]. Flowsheet scaling was observed to have significant benefits in promoting flowsheet convergence during the steady state development of the process model (see Section 3.5.3).

Another problem encountered with the equation-oriented simulation based real time optimizer was the failure of the economic optimization due to prop-
ertty errors during the third cycle of the base case run. This error in an undetermined flash calculation occurred consistently on the second iteration of the economic optimization on the third cycle of the real time optimizer. This error did not prevent the simulation from continuing, but did cause the constraint violations to be approximately 3 orders of magnitude larger than normal during this optimization. This resulted in the SRQP optimization algorithm failing due to "inconsistent constraints" on every attempt to solve this problem. Some method of tracking which flash and/or model equations caused this property error is required to allow the user a chance to place bounds on the offending variable to restrict its movement within reasonable limits.

Several problems were also encountered with the sequential modular simulation based real time optimizer. The most common problem was the inability of the SQP optimization algorithm to satisfy violated constraints after converging the economic objective function. This usually occurred when two or more constraints became active during the economic optimization. The two inequality constraints which commonly caused the failure of the ASPEN PLUS real time optimizer by being violated were the upper limit on the Light Distillate stream 90% volume distilled true boiling point temperature, and the upper limit on the C4-Distillate stream C5 mole fraction. By looking at the optimization history, it appears that once a constraint is violated, the SQP optimization algorithm makes very little effort to satisfy the constraint until the end of the optimization. At this stage, the constraint has usually been violated to such an extent, that the optimizer is unable to satisfy the constraint on subsequent iterations. It is likely that this problem is caused by the lack of accurate derivative information available to the SQP optimization algorithm from the sequential modular process flowsheet.

Occasionally, failures in the tear stream convergence were noticed during flowsheet passes of the ASPEN PLUS process flowsheet. These failures generally did not cause any problems other than adding extra computation time to the optimization convergence, and possibly returning inaccurate numerical
derivative information to the SQP optimization algorithm. Flowsheet convergence was only found to be a problem in one run of the ASPEN PLUS real time optimizer. It occurred on the sixth cycle of the condenser disturbance with no measurement noise run (see Section 6.4). However, since this process flowsheet contains relatively few recycle loops, convergence of the flowsheet recycle loops is a concern when using sequential modular process simulators in real time optimization on more complicated industrial processes.

From the graphs in Figures 6.4 and 6.5 comparing the set point changes made by both real time optimizers on the base case without measurement noise, it can be seen that the SPEEDUP tended to make fairly large changes to the composition related set points. In particular, the largest changes occurred on the C₄-Distillate stream C₅ mole fraction and the Heavy Iso stream 10% volume distilled true boiling point temperature. Decreasing the C₄-Distillate stream C₅ mole fraction as low as possible increases the profit by forcing these C₅ components into the higher priced Light Iso product stream, provided the constraints on the bubble point in the condenser on column C2 and the Light Iso stream Reid vapour pressure can be maintained. ASPEN PLUS is slower to accomplish this reduction in C₅ components in the C₄-Distillate product stream. In turn, the Heavy Iso product stream 10% volume distilled true boiling point temperature is increased to provide some heavier components in the Light Iso stream to reduce the Reid vapour pressure. Reducing the Reid vapour pressure increases the Light Iso stream price because of the quality specification associated with the Light Iso Reid vapour pressure as given in Equation (5.3). It is likely that the SPEEDUP real time optimizer made these changes in set points more quickly than ASPEN PLUS because of SPEEDUP’s infeasible path optimization method, and also due to the more accurate derivative information provided by the process flowsheet in an equation-oriented simulation. Both real time optimizers quickly increased the Light Distillate stream 90% volume distilled true boiling point temperature the upper limit, to allow as many heavy components as possible into the Light Distillate product stream rather than to the splitter bottoms
stream for further cracking. It is likely that this constraint will always be active during this economic optimization for this reason.

Figures 6.4 and 6.5 also show that at the end of the first cycle, there were already significant differences in the $C_4$-Distillate stream $C_5$ mole fraction between the two real time optimizers. Some of this difference can be attributed to the more aggressive optimization performed by SPEEDUP's SRQP optimization algorithm. However, this large difference may have also been caused in part by differences in the results from the data reconciliation of the measured data performed by both of the real time optimizers. Slight differences between the process models used in the two process simulation packages may also contribute to this difference.

6.6.3 Economic Model Changes

The first economic runs performed tested the effect of changes in the Heavy Iso and Light Distillate product stream prices. These runs were chosen to test the performance of the ASPEN PLUS real time optimizer under different economic conditions where the expected performance of the optimizer was known from Shell Canada's experience. In particular, the base case run where the price of the Heavy Iso stream was $193.89/m^3 and the Light Distillate stream was $180.52/m^3, and the run where the price of the Heavy Iso stream was $173.89/m^3 and the Light Distillate stream was $200.52/m^3, correspond to typical summer and winter economic operating conditions respectively (however, the summer or base case has the same Light Iso Reid vapour pressure upper limit of 14 psi as used under normal winter operation). The graphs of the objective function profit at the end of each real time optimizer cycle given in Figure 6.7 show similar shaped curves for all of the runs with different stream prices.

Differences in the performance of the real time optimizer in the runs with different Heavy Iso and Light Distillate stream prices can be seen on the graphs of the set point changes made in Figures 6.8 and 6.9. Not surprisingly, the runs where the Heavy Iso and Light Distillate stream prices were both
at their highest values or at their lowest values produced very similar set point changes as the difference between the two stream prices was the same for both runs. The largest difference in set point changes made were for the base case (summer) run and the winter run. For the base case run, the emphasis for the economic optimization is to produce as much Heavy Iso product as possible, because this stream has the highest associated price. To achieve this, the optimization forces the set points on the Heavy Iso stream 90% volume distilled and the Light Distillate stream 10% volume distilled true boiling point temperatures as high as possible to encourage the production of as much Heavy Iso as possible. Also the flow to the column C₅ sidestripper, where the Light Distillate product draw is taken, is reduced as much as possible within the process constraints.

Similarly for the winter run, the emphasis for the economic optimizer is to produce as much Light Distillate product as possible. To achieve this, the optimization forces the set points on the Heavy Iso stream 90% volume distilled and the Light Distillate stream 10% volume distilled true boiling point temperatures as low as possible to encourage the production of as much Light Distillate as possible. These results are similar to those observed with Shell Canada's real time optimizer.

The results of the sensitivity study on the economic objective function performed by Fenton [39] in Table 6.1 seem to show some inconsistent data. The optimizations performed with the modified economic data were all initialized with the results of the optimized base case run. However, it is likely that the optimized base case was not solved to the global optimum profit, and that the optimizer on this run finished at a local optimum of the profit objective function. This is especially evident from the high and low fuel oil costs where the optimizer was able to increase the starting profit by 31% and 47% respectively. This seems to represent a large change in optima for just a ±5% change in the reboiler furnace heating oil cost. Unfortunately, there is no way to guarantee that an optimization has reached the global optimum of a given objective function, therefore is is always possible that the profit
returned from the real time optimization is actually a local optimum.

This economic sensitivity study does, however, show how continuous optimization of the process can help increase the profit made by the process. In every run tested in this study, the economic optimization was able to find a better operating point. Therefore, even though the optimum found cannot be guaranteed to be the global optimum for the process, it can be seen that continuously optimizing the plant does produce higher profits than not optimizing after changes in economic parameters.

The effect of changing the economics from typical winter to typical summer operating conditions part way through the optimizer run can clearly be seen in Figure 6.10. For these runs, the Light Iso Reid vapour pressure upper limit was also changed for summer to 10.5 psi from the limit of 14 psi used during winter operation. Changing the economics at the beginning of cycle 3 for the run with measurement noise and cycle 4 for the run with no measurement noise caused the profits to remain almost constant for three cycles as the real time optimizer changed optimization strategies. The optimizer was then able to make gains in profit for the run with no measurement noise at almost the same rate as the winter case. This was an expected result, as the optimizer had been trying to maximize the production of Heavy Iso up to the change in economic conditions, and had to switch to maximizing production of the Light Distillate product stream. This can be seen in the graphs comparing the set point changes made at the end of each cycle for the runs with no measurement noise added, given in Figures 6.11 and 6.12. For the winter case, the real time optimizer lowered the Heavy Iso product stream 90% volume distilled and the Light Distillate stream 10% volume distilled true boiling point temperatures as much as possible on each cycle, to allow as many components as possible to be included in the Light Distillate product. For the summer cycles of the winter to summer run, the real time optimizer swapped to a strategy of increasing the Heavy Iso product stream 90% volume distilled and the Light Distillate stream 10% volume distilled true boiling point temperature to maximize the amount of Heavy Iso being
produced for gasoline products.

The change in the Light Iso Reid vapour pressure upper constraint from 14 psi to 10.5 psi had an obvious effect on the operation of the condenser on the C1 stabilizer column. From Figure 6.11, it can be seen that the amount of C5 components retained in the C4-Distillate stream increased noticeably. This is to reduce the number of lighter components in the Light Iso product, thereby lowering the Reid vapour pressure of this stream to comply with the lowered Reid vapour pressure constraint.

6.6.4 Process Disturbances

The disturbance created by the increased condenser temperatures in both columns C1 and C2 reduced the profit attained by the real time optimizer significantly, as can be seen in Figure 6.13. Both of the condenser disturbance runs with and without measurement noise produced similar results, with profit objective function unable to be pushed higher than approximately $180/hour. For the first two cycles of both condenser disturbance runs, the profits obtained were almost identical to the base case runs at which point the optimizers were unable to make any further significant gains in profit.

Comparing the set point changes made during the base case and condenser disturbance runs with no measurement noise in Figures 6.14 and 6.15, it can be seen that the major difference was in the handling of the C4-Distillate C5 mole fraction set point. This set point was forced to its upper bound within 2 cycles of the real time optimizer to reduce the amount of light components reaching the splitter column. This was the expected reaction to a loss in cooling in the condensers, therefore causing a reduction in the ability to condense lighter components at the top of both columns. This resulted in increased Vapour product stream flow and a corresponding decrease in C4-Distillate product stream flow compared with the base case run.

Originally this run was planned have the process disturbance added at the ASPEN PLUS base case optimum solution. However, due to the problems the
SQP optimization algorithm had in satisfying active inequality constraints once the process disturbance was added, this was not possible. Therefore, it was decided to have the process disturbance added right from the start of the run. Unfortunately this meant that no runs were possible to test the performance of the real time optimizers once it had attained a near optimal operation of the plant.

### 6.6.5 ASPEN PLUS Software Upgrade

From the results shown in Figure 6.16, it can be seen that even small changes to process models and optimization algorithms can have a significant effect on the performance of a real time optimizer. The optimization algorithm in ASPEN PLUS version 9.3 was able to obtain a slightly higher profit (approximately $40/hr more) in fewer real time optimizer cycles. This profit was still approximately $100/hr less than the profit achieved by SPEEDUP on the base case, and used more real time optimizer cycles and computation time. The ASPEN PLUS version 9.3 real time optimizer still failed due to violated inequality constraints in a similar manner to the version 9.2 real time optimizer.

The problems encountered in trying to achieve convergence of the real time optimizer with the new version of ASPEN PLUS show how care must be taken when upgrading process simulation packages. Testing, debugging and retuning of the real time optimizer needs to be performed to verify that the real time optimization application is still producing valid results.
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Chapter 7

Conclusions

The conclusions from this research are covered in the next three sections. Conclusions from the development of the real time optimizers using both sequential modular and equation-oriented process simulation packages are covered in Section 7.1 below. Comparison of the two types of process simulation packages used with respect to their performance in real time optimization applications are covered in Section 7.2. In Section 7.3, conclusions specific to the stabilizer-splitter process studied are made. Finally, in Section 7.4, some suggestions for future work following on from this research are made.

7.1 Real Time Optimizer Development

Overall, it can be concluded that sequential modular process simulation packages are easier to use when developing real time optimization applications. However, equation-oriented simulators are more flexible for manipulated variable choice and recycle loop convergence. Development of the same real time optimizer using SPEEDUP, an equation-oriented process simulator, took approximately twice as long as the development using ASPEN PLUS, a sequential modular process simulator.

The main reason for this development time difference was due to the lack of useful, or meaningful, error messages produced by an equation-oriented
simulator when either the process flowsheet or optimization algorithm fails to converge. Debugging convergence problems is a slow process of eliminating all possible sources of error over many runs of the simulation, since different errors often result in the same error message from the convergence algorithm. This lack of useful information is caused in part by the simultaneous solution of equation-oriented process flowsheet equations and also the infeasible path convergence algorithms used. Since an equation-oriented simulator solves the process flowsheet as a large set of simultaneous equations, it is difficult to track errors to a particular equation or variable.

A few mathematical tools are available in SPEEDUP to help determine the cause of a convergence failure. One method of tracking these errors is to monitor the largest equation residuals during the solution of the flowsheet to track down problem equations and/or variables. Another method is to track the variables which changed by the largest amount between iterations of the flowsheet convergence algorithm. These equations and/or variables can then be checked by hand to see if the problem is caused by incorrect modelling equations, poor starting point values, incorrect variable bounds, or is caused by errors in other variables or equations. However, the large number of equations and variables involved, 6066 equations and unknown variables for the stabilizer-splitter process flowsheet, make this a time consuming task. The infeasible path algorithms used to solve the process flowsheet and optimization problems also make it difficult to detect errors because intermediate variable values do not necessarily satisfy constraints and bounds. This can result in some strange intermediate variable values which have no physical meaning, for example, negative component compositions. Therefore looking at the actual intermediate value of variables provides very little information with respect to convergence failures.

Sequential modular process flowsheet errors can always be tracked to a particular unit operation, and often a reasonably accurate error message is produced. This makes debugging of flowsheet convergence problems relatively simple. Optimization algorithm convergence failures are somewhat
more difficult to debug, however more useful information is available for finding the cause of the error than in an equation-oriented simulator. Since the flowsheet solution is always feasible at the end of an iteration, variable values can be used to help find the cause of the convergence failure.

Sequential modular process simulators usually also have the advantage of a graphical user interface. However, graphical user interfaces are presently being developed for several equation-oriented packages including SPEEDUP and MASSBAL. A graphical user interface is useful for preventing syntax errors in the input file, quickly building process flowsheets and ensuring that the correct number of variables have been specified before running a simulation. However most of the time in developing a real time optimizer is spent fixing convergence errors and ensuring that the process flowsheet is adequately modelling the plant. For these tasks, a graphical user interface does not offer many advantages over direct editing of the input code.

An equation-oriented process simulator has two main advantages over a sequential modular process simulator when developing a real time optimizer. The first advantage is how equation-oriented process simulators handle the convergence of recycle loops and tear streams. A recycle loop in an equation-oriented simulator is handled by inserting a tear block which equates the inlet and outlet streams plus a slack variable which is set to zero. The tear stream is then converged at the same time as all the other flowsheet equations. In a sequential modular simulator, a recycle loop results in the creation of a tear stream convergence loop which iterates through all the blocks in the recycle loop until convergence of the torn stream is obtained. This tear stream convergence method is computationally time consuming and also less robust, particularly for large recycle loops. For complex process flowsheets with more recycle than the stabilizer-splitter flowsheet studied, convergence of tear streams in a sequential modular simulator would be extremely difficult to guarantee over the range that the real time optimizer is required to operate.

The second main advantage of using equation-oriented process simulators to develop a real time optimizer is their flexibility in choosing specified or
manipulated variables. A sequential modular simulator restricts the user to specifying the inputs available for that process model. If any other variables need to specified, a design specification is required which is solved using an iterative procedure to converge the specification. In an equation-oriented simulator, any combination of variables (input or output variables) can be chosen directly as the specified or manipulated variables, provided they fulfill the degrees of freedom required, and do not over or under specify equations or block after decomposition has been performed. This does not mean that any combination of variables will necessarily converge the flowsheet, but it does offer more flexibility than a sequential modular flowsheet.

This flexibility in the choice of manipulated variables does cause some other problems. During the development of the SPEEDUP real time optimizer, problems were encountered when the manipulated variables chosen fully specified the mass balance around column C1 and the energy balance around column C2. Since this problem was not detected during analysis of the flowsheet by SPEEDUP, solution of the flowsheet was performed which resulted in many different error messages such as "inconsistent constraints", "slow convergence" and various property errors. This problem was only detected after extensive analysis of the process flowsheet by hand. For larger flowsheets, this problem would be difficult and time consuming to find and correct.

Several process simulator specific problems were found with both ASPEN PLUS and SPEEDUP. Errors in the transfer of data between blocks in ASPEN PLUS using FORTRAN common blocks were difficult to debug since there is no automatic method for checking the variable values being transferred. Also ASPEN PLUS has no simple mechanism for saving the results of a simulation, and then using these results to initialize another simulation as with SPEEDUP. Several useful features not available in SPEEDUP at present are the addition of variable scaling for optimization simulations, sequencing of global optimization blocks similar to ASPEN PLUS's convergence block sequencing, and improved error tracking for property errors indicating in
which unit the error occurred.

When developing the real time optimizers using both types of process simulator, it was found that the properties used had a large effect on the accuracy of the process models. In particular, it was found with the stabilizer-splitter process that the cross over from conventional components to pseudocomponents was critical when modelling the operation of the condensers in both columns C1 and C2. When analysing the assay data provided, it was found that PROPERTIES PLUS assumed the stream was a typical refinery stream, and therefore used typical specific gravity, boiling point and molecular weight curves when estimating the pseudocomponent properties. However, hydrocracked refinery streams exhibit different typical stream properties, particularly for the light and heavy pseudocomponents, which had to be corrected. This problem highlights how errors can be caused by not checking the underlying assumptions used in the property calculation routines.

7.2 Real Time Optimizer Comparison

From testing of both the equation-oriented and sequential modular process simulator based real time optimizers, it can be concluded that the equation oriented real time optimizer was a far more powerful optimizer. This was due to the benefits of open form equation solution methods allowing for very robust and quick tear stream convergence, infeasible path optimization methods not requiring the solution of the flowsheet on each iteration and the availability of more accurate analytical derivative information from the process model equations. The closed form equation based models, with only one recycle loop in the flowsheet, took approximately between 2 and 4 times longer to complete a cycle of the same optimization and data reconciliation problems as the open form equation based models. A more complicated flowsheet with more recycle would add even more to the convergence time for a sequential modular simulator, in addition to the problems with convergence robustness for closed form tear stream solution.
A process simulator specific conclusion that should be noted is that neither the ASPEN PLUS nor the SPEEDUP process simulator based real time optimizers were robust enough for an industrial application in their present form. SPEEDUP, however, was able to find better profits with less optimizer cycles and computational time than ASPEN PLUS on all runs tested. The following conclusions are based on the results from the testing of the two real time optimizers. Where appropriate, more general conclusions will also be pointed out.

Two problems were encountered when testing the ASPEN PLUS real time optimizer. The first was the poor handling of violated inequality constraints by the SQP optimization algorithm used in ASPEN PLUS. This was the most common reason for failure of the real time optimizer and almost always occurred when two inequality constraints had been active on the previous cycle of the optimizer. The economic optimizer would then violate one or both of these constraints searching for an improved profit objective function. However, it was unable to satisfy these constraints again once a new optimum had been found. The most commonly violated constraints were the upper limits on the column C1 reflux flow rate and the Light Distillate stream 90% volume distilled true boiling point temperature. The most likely cause for this problem is the SQP optimization algorithm implemented in ASPEN PLUS. With more refinement of the algorithm, it is possible this problem may be alleviated. Another contributing cause for this is the less accurate derivative information available for the optimization algorithm from the numerical derivatives calculated using the sequential modular process flowsheet models. Adding to some of the poor derivative information, some flowsheet passes used to determine derivative values failed to converge due to tear stream or process model convergence failures. The less accurate derivative information is typical of all sequential modular flowsheet simulators due to the closed form of the modelling equations.

The second problem encountered using ASPEN PLUS was the occasional failure to converge the tear stream block. This failure usually did not di-
rectly cause failure of the real time optimizer, but did add significantly the computational time taken during optimization. It also possibly contributed to inaccurate information being passed to the SQP optimization algorithm. For complex flowsheets with more recycle loops than the stabilizer splitter process, tear stream convergence failures would make optimization of the process very difficult to achieve over all process operating conditions. Problems converging tear streams quickly and robustly is typical of all closed form equation solution methods because of the iterative nature of their solution.

The main problem with the SPEEDUP real time optimizer was the lack of tuning parameters available for the SQP optimization algorithm. Almost all convergence failures encountered when running the SPEEDUP real time optimizer produced the error message "slow convergence", however there was no method for changing the criteria used to determine slow convergence. On many occasions, it appeared that the optimizer was very close to the optimum when the "slow convergence" error occurred. For this reason, weighting factors had to be used in the objective functions for the data reconciliation and economic optimization to promote convergence of the optimization algorithm. These weighting factors could not be automatically determined during the real time optimization and required the user to find their value which allowed convergence. This is not practical for implementation in a real time optimizer. Another factor which may have caused these convergence problems was scaling of the process flowsheet and manipulated variables. This result is a process simulator specific problem, as many other optimization algorithms are available which may be more suitable for solving this problem. Unfortunately, no other optimization algorithms were available for testing with SPEEDUP for this study.

Another problem encountered with SPEEDUP was the occurrence of property errors, particularly during flash calculations. SPEEDUP does not provide any method of tracking which process model flash procedure was being calculated at the time. This would allow bounds restricting movement of some variables to be set, preventing the optimizer from moving into regions
where property calculations may fail. Again, this is likely to be a process simulator specific result due to problems either in the properties or convergence algorithms used.

SPEEDUP consistently found better profit objective function values, usually by $200/hr or more, at each cycle of the real time optimizer than ASPEN PLUS. For the base case runs with no measurement noise (see Figure 6.3), both ASPEN PLUS and SPEEDUP came very close to achieving the expected global optimum before the real time optimizers failed. However, SPEEDUP used half as many cycles to achieve this increase in profit. The reason for this could be seen from SPEEDUP's more aggressive set point changes made at the end of each real time optimizer cycle. The most likely reasons for the better performance of the SPEEDUP real time optimizer are more accurate analytical derivative information available from the equation-oriented process flowsheet and the infeasible path optimization algorithm used.

The SPEEDUP real time optimizer was also computationally more efficient than ASPEN PLUS, taking approximately half as long to complete each cycle of the real time optimizer. The difference in computation times was mostly due to the extra time taken by ASPEN PLUS to converge the tear stream on each flowsheet pass, and the time taken to calculate the numerical derivatives for the optimization algorithm. It is likely that for complex flowsheets with more recycle loops, that a sequential modular process simulator would become even slower relative to an equation-oriented simulator. This was an expected result for an open equation model based optimization.

It is likely that if the above problems with the SPEEDUP equation-oriented process simulation package can be addressed, then SPEEDUP could become a very useful tool for developing and performing real time optimization. Despite the added difficulty in developing and converging an equation-oriented process flowsheet model, the added flexibility in terms of variable specification, robust and rapid tear stream convergence, and more powerful optimization algorithms make the equation-oriented process simulator a more
attractive tool for real time optimization. It is unlikely that the problems with the ASPEN PLUS process simulator's ability to converge flowsheet recycle loops quickly and robustly can solved easily using the sequential modular architecture. Some simultaneous-modular methods have been incorporated into ASPEN PLUS to speed convergence of tear streams, however it is unlikely that these will achieve the level of performance required for complex flowsheets used in real time optimization. For less complex flowsheets with little or no recycle, a sequential modular simulator provides a very simple method to develop a real time optimization application, provided the SQP optimization algorithm's convergence with respect to violated constraints can be improved.

A final conclusion regarding upgrading versions of the process simulation software should be noted. When ASPEN PLUS was upgraded from version 9.2 to 9.3, the real time optimizer failed to converge without adjustments to the process simulation code. Considering that version 9.3 was only a minor software upgrade, this shows that care must be taken when upgrading to ensure that the real time optimizer is still producing valid results. Even small changes to the process models and the optimization algorithm can have an impact on the performance of the optimization. This conclusion should apply equally to both sequential modular and equation-oriented simulator based real time optimizers. Upgrading to version 9.3 of ASPEN PLUS did cause the real time optimizer to be slightly more robust, however constraint handling and tear stream convergence problems were still observed similar to those seen with version 9.2.

7.3 Process Specific Conclusions

The development of real time optimizers with both ASPEN PLUS and SPEED-UP fulfilled the objective of developing a "test bed" for real time optimization to allow further research to be conducted. It should be noted that the process studied in this thesis is somewhat less complex than those typically used
with industrial real time optimizers. The process chosen was smaller than normal to allow the solution of a real time optimizer cycle to be completed within a reasonable period of time with the computing resources available. Therefore it could be argued that the objective of real time optimization on this process as implemented could also be achieved using a combination of advanced control and process insight. This is because only two major operating strategies were observed in the testing of this process, that is, a summer and a winter operating strategy based on the economic conditions. To implement some form of model based local optimizer would be the correct decision in an industrial situation if this was the whole process to optimized. However, for the purposes of researching real time optimization this process produces valid results.

The stabilizer-splitter process at Shell Canada's Sarnia refinery is included in a real time optimizer which also optimizes the operation of the catalytic cracking units. This addition of several extra unit operations to the real time optimizer introduces many different operating strategies and trade-offs that can be made between process units. These trade-offs between the operation of several units and changes in operating conditions are where the payback from installing a real time optimization application can be made. Also, with more unit operations included in a real time optimizer, less conflict is possible between the operating strategies used in different parts of the plant.

All of the following conclusions were based on testing of the ASPEN PLUS real time optimizer under varying economic conditions and process disturbances.

Several real time optimizer runs were carried out to check the performance of the real time optimizer under typical summer and winter economic operating conditions. It was concluded that the real time optimizer performed as expected by trying to maximize production of the Heavy Iso gasoline product stream during typical summer economic conditions, and maximizing Light Distillate heating oil product stream under typical winter economics. Two
runs were also performed where the economic conditions were changed from winter to summer part way through the real time optimizer run. These runs produced similar set point changes and results after the change in economics as the previous real time optimizer run completely with typical winter economic conditions.

From the results of the winter only and the winter to summer runs presented in Section 6.3.3. the two operating strategies that could be implemented using advanced control for optimizing only the stabilizer-splitter process would be:

1. For summer economics and process constraints, the objective would be to increase the Heavy Iso and Light Distillate 90% volume distilled true boiling point temperatures as close to their constraints as possible while maintaining the Light Iso stream Reid vapour pressure at its upper limit.

2. For winter economics and process constraints, the operating objective is to increase the Light Distillate 90% volume distilled true boiling point temperature and decrease the Light Distillate 10% volume distilled true boiling point temperature as close to their constraints as possible. The C₄-Distillate stream C₅ mole fraction should also be reduced as much as possible while the Light Iso stream Reid vapour pressure at its upper limit.

A sensitivity study performed by individually varying the economic objective function prices by ±5% concluded that continually optimizing the plant does produce higher profits than not optimizing after economic changes. In every case tested, the real time optimizer was able to find a better operating point after a change in economic parameters. However, this study also showed that there is no way to guarantee that the optimization has found a global optimum profit objective function which made the results of this study difficult to analyse.
Finally, a process disturbance in the condenser cooling water temperature was simulated by increasing the condenser temperatures returned in the measured data to the real time optimizer. The real time optimizer performed as expected to the reduction in the available cooling in the condensers which significantly reduced the profit attained by the economic optimization.

### 7.4 Recommendations for Future Research

Researching real time optimization is difficult due to the large amount of time required to develop, debug and test the real time optimizer code. The development of an industrial real time optimization application from this research allows many areas of real time optimization to be studied in the future. Several possible areas of future research are outlined below.

A new version of SPEEDUP, version 6.0, is expected before the end of 1997 [16] which may address some of the shortcomings found when using SPEEDUP for real time optimization. With the addition of flowsheet scaling, SRQP optimization interface enhancements and optimization manipulated variable scaling, it should be possible to fix the “slow convergence” problems encountered with the SPEEDUP real time optimizer. Further testing of the equation-oriented real time optimizer will then be possible, thereby providing more comparison runs with the sequential modular simulator based real time optimizer.

Shell Canada has modified the stabilizer-splitter plant over the last year adding a draw from column C2 which is fed back to column C1, thereby creating a flowsheet recycle loop. By making this process modification to both the ASPEN PLUS and SPEEDUP based real time optimizers, this would show the effect of adding a recycle loop to the flowsheet on both sequential modular and equation-oriented solution methods. This study could also be used to show how easily the process model in the two types of process simulators can be modified and maintained.

The simulation model used as the “plant” in this study should be im-
proved to allow more effective analysis of the real time optimization applications. Modelling of the process control used in the stabilizer-splitter process using a dynamic simulation would allow several studies to be researched:

- the effect of real time optimization set point changes on the stability and performance of the plant's process control.

- the cost of disturbing the plant by making continuous process control set point changes compared to the profit gained by moving the plant's operating point.
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Bibliography


NOTE TO USERS

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Appendix A

Real Time Optimizer Run Data

This appendix contains tables summarising the real time optimizer runs for both ASPEN PLUS and SPEEDUP. The results presented in these tables are analysed in Chapter 6. Unless otherwise stated, all ASPEN PLUS real time optimizer runs were performed using version 9.2.
Table A.1: Base case ASPEN PLUS real time optimizer run.

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<tr>
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<tbody>
<tr>
<td><strong>Economic Optimization:</strong></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Profit ($/hr)</td>
<td>-9.84</td>
<td>169.55</td>
<td>215.21</td>
<td>247.03</td>
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<tr>
<td>Optimization iterations</td>
<td>10</td>
<td>4</td>
<td>12</td>
<td>10</td>
</tr>
<tr>
<td>Total product values ($/hr)</td>
<td>23035.02</td>
<td>23188.05</td>
<td>23273.30</td>
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</tr>
<tr>
<td>Total feed cost ($/hr)</td>
<td>22928.41</td>
<td>22907.03</td>
<td>22940.42</td>
<td>22897.70</td>
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<tr>
<td>Total utility costs ($/hr)</td>
<td>116.45</td>
<td>111.48</td>
<td>117.67</td>
<td>121.27</td>
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</tbody>
</table>

| **Economic Optimization Set Points:** |      |      |      |      |
| C1 reflux flow (bbl/day)           | 6913.71 | 7447.16 | 8040.20 | 8631.66 |
| C1 tray 3 temperature (°F)         | 181.26  | 173.25  | 166.41  | 161.44  |
| DIST-C4 C5 mole fraction           | 0.11882 | 0.06883 | 0.03562 | 0.01633 |
| C1 reboiler temperature (°F)       | 595.10  | 602.16  | 609.97  | 612.36  |
| C2 reflux flow (bbl/day)           | 13951.69 | 13682.32 | 13610.05 | 13556.18 |
| C4 feed flow (bbl/day)             | 5998.29  | 6279.27  | 6396.15  | 6638.08  |
| C5 feed flow (bbl/day)             | 3334.48  | 3452.69  | 3341.47  | 3219.25  |
| C2 reboiler temperature (°F)       | 595.10  | 602.16  | 609.97  | 612.36  |
| HV-ISO 10% TBP temperature (°F)    | 197.38  | 199.39  | 194.49  | 198.87  |
| HV-ISO 90% TBP temperature (°F)    | 351.62  | 364.27  | 371.09  | 377.21  |
| LT-DIST 10% TBP temperature (°F)   | 338.26  | 357.10  | 364.90  | 370.57  |
| LT-DIST 90% TBP temperature (°F)   | 496.25  | 553.97  | 554.04  | 553.90  |

| **Economic Optimization Inequality Constraints:** |      |      |      |      |
| C1 reflux flow (bbl/day)           | 6913.71 | 7447.16 | 8040.20 | 8631.66 |
| C2 reflux flow (bbl/day)           | 13951.69 | 13682.32 | 13610.05 | 13556.18 |
| C4 feed flow (bbl/day)             | 5998.29  | 6279.27  | 6396.15  | 6638.08  |
| C5 feed flow (bbl/day)             | 3334.48  | 3452.69  | 3341.47  | 3219.25  |
| C1 tray 3 temperature (°F)         | 181.26  | 173.25  | 166.41  | 161.44  |
| C1 reboiler temperature (°F)       | 595.10  | 602.16  | 609.97  | 612.36  |
| C2 tray 2 temperature (°F)         | 153.02  | 154.64  | 155.96  | 157.11  |
| C2 reboiler temperature (°F)       | 651.22  | 642.93  | 636.87  | 630.89  |
| DIST-C4 C5 mole fraction           | 0.11882 | 0.06883 | 0.03562 | 0.01633 |
| LT-ISO Reid vapour pressure (psi)  | 14.000a | 12.395  | 11.613  | 11.410  |
| LT-ISO bubble point temperature (°F) | 115.05 | 121.52 | 124.89 | 125.88 |
| HV-ISO 10% TBP temperature (°F)    | 197.38  | 199.39  | 194.49  | 198.87  |
| HV-ISO 90% TBP temperature (°F)    | 351.62  | 364.27  | 371.09  | 377.21  |
| LT-DIST 10% TBP temperature (°F)   | 338.26  | 357.10  | 364.90  | 370.57  |
| LT-DIST 90% TBP temperature (°F)   | 496.25  | 553.97a | 554.04a | 553.90a |

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<td>Vapour Product (bbl/day)</td>
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<td>913.00</td>
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<td>Light Iso Product (bbl/day)</td>
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<td>Splitter (C2) Reboiler (MMBTU/hr)</td>
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Table A.2: Base case SPEEDUP real time optimizer run.

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<td>7143.64</td>
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<td>0.00500</td>
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<td>C1 reboiler temperature (°F)</td>
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<td>582.34</td>
</tr>
<tr>
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<td>12389.58</td>
<td>11410.13</td>
</tr>
<tr>
<td>C4 feed flow (bbl/day)</td>
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<td>233.85</td>
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<td>HV-ISO 90% TBP temperature (°F)</td>
<td>362.14</td>
<td>384.48</td>
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<tr>
<td>LT-DIST 10% TBP temperature (°F)</td>
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<td>LT-DIST 90% TBP temperature (°F)</td>
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<td>554.00</td>
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<td>C2 reflux flow (bbl/day)</td>
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<td>C4 feed flow (bbl/day)</td>
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<td>5600.68</td>
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<td>C5 feed flow (bbl/day)</td>
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<td>3663.28</td>
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<td>C1 tray 3 temperature (°F)</td>
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<td>155.47</td>
</tr>
<tr>
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<td>582.34</td>
</tr>
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<td>HV-ISO 90% TBP temperature (°F)</td>
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<td>Vapour Product (bbl/day)</td>
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<td>Light Iso Product (bbl/day)</td>
<td>185.05</td>
<td>192.66</td>
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<td>Heavy Iso Product (bbl/day)</td>
<td>493.36</td>
<td>582.19</td>
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<td>Light Distillate Product (bbl/day)</td>
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<td>Splitter Bottoms Product (bbl/day)</td>
<td>437.75</td>
<td>484.33</td>
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<td><strong>Reboiler Heat Duties After Economic Optimization:</strong></td>
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<tr>
<td>Splitter (C2) Reboiler (MMBTU/hr)</td>
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<tr>
<td><strong>Economic Optimization Marginal Stream Values:</strong></td>
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<tr>
<td>Light Iso Marginal Stream Value ($/m³)</td>
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Table A.3: Base case with no measurement noise ASPEN PLUS real time optimizer run.

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<td></td>
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</tr>
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<td>7</td>
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<tr>
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<tr>
<td>Total utility costs ($/hr)</td>
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**Economic Optimization Set Points:**

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<tbody>
<tr>
<td>C1 reflux flow (bbl/day)</td>
<td>6913.71</td>
<td>6814.09</td>
<td>6695.27</td>
<td>6603.68</td>
</tr>
<tr>
<td>C1 tray 3 temperature (°F)</td>
<td>181.26</td>
<td>180.16</td>
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<td>179.97</td>
</tr>
<tr>
<td>DIST-C4 C₅ mole fraction</td>
<td>0.11882</td>
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<tr>
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<td>13610.48</td>
<td>13642.27</td>
</tr>
<tr>
<td>C4 feed flow (bbl/day)</td>
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<td>6253.26</td>
<td>6396.92</td>
<td>6454.85</td>
</tr>
<tr>
<td>C5 feed flow (bbl/day)</td>
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**Economic Optimization Inequality Constraints:**

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<tr>
<td>C1 reboiler temperature (°F)</td>
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<td>11291.19</td>
<td>11212.03</td>
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| **Reboiler Heat Duties After Economic Optimization:** |       |       |       |       |
| Stabilizer (C1) Reboiler (MMBTU/hr)        | 21.2420 | 20.9219 | 20.9620 | 20.6658 |
| Splitter (C2) Reboiler (MMBTU/hr)          | 18.0814 | 17.0053 | 17.5860 | 17.7914 |

| **Economic Optimization Marginal Stream Values:** |       |       |       |       |
| Light Iso Marginal Stream Value ($/m³)       | 182.78  | 182.77 | 183.50 | 182.80 |

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<td>Profit ($/hr)</td>
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<td>Total product values ($/hr)</td>
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<td>Total utility costs ($/hr)</td>
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<td>111.15</td>
<td>112.34</td>
<td>115.98</td>
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| **Economic Optimization Set Points:** |       |       |       |       |
| C1 reflux flow (bbl/day) | 6504.24 | 6428.55 | 6359.33 | 6278.80 |
| C1 tray 3 temperature (°F) | 179.75 | 178.34 | 176.79 | 176.23 |
| DIST-C4 C5 mole fraction | 0.10933 | 0.10103 | 0.09249 | 0.08949 |
| C1 reboiler temperature (°F) | 592.24 | 592.71 | 587.74 | 583.68 |
| C2 reflux flow (bbl/day) | 13567.97 | 13358.32 | 13087.92 | 12841.07 |
| C4 feed flow (bbl/day) | 6526.93 | 6253.07 | 6095.12 | 6105.22 |
| C5 feed flow (bbl/day) | 3349.02 | 3503.47 | 3684.20 | 3528.07 |
| C2 reboiler temperature (°F) | 592.24 | 592.71 | 587.74 | 583.68 |
| HV-ISO 10% TBP temperature (°F) | 204.03 | 206.50 | 208.80 | 213.20 |
| HV-ISO 90% TBP temperature (°F) | 387.67 | 383.33 | 381.43 | 389.02 |
| LT-DIST 10% TBP temperature (°F) | 375.11 | 368.37 | 362.46 | 366.61 |
| LT-DIST 90% TBP temperature (°F) | 557.76 | 554.01 | 554.01 | 554.04 |

| **Economic Optimization Inequality Constraints:** |       |       |       |       |
| C1 reflux flow (bbl/day) | 6504.24 | 6428.55 | 6359.33 | 6278.80 |
| C2 reflux flow (bbl/day) | 13567.97 | 13358.32 | 13087.92 | 12841.07 |
| C4 feed flow (bbl/day) | 6526.93 | 6253.07 | 6095.12 | 6105.22 |
| C5 feed flow (bbl/day) | 3349.02 | 3503.47 | 3684.20 | 3528.07 |
| C1 tray 3 temperature (°F) | 179.75 | 178.34 | 176.79 | 176.23 |
| C1 reboiler temperature (°F) | 592.24 | 592.71 | 587.74 | 583.68 |
| C2 tray 2 temperature (°F) | 157.18 | 159.11 | 162.46 | 166.43 |
| C2 reboiler temperature (°F) | 670.79 | 674.19 | 679.19 | 684.17 |
| DIST-C4 C5 mole fraction | 0.10933 | 0.10103 | 0.09249 | 0.08949 |
| LT-ISO Reid vapour pressure (psi) | 13.946* | 13.997* | 14.000* | 13.790 |
| LT-ISO bubble point temperature (°F) | 115.66 | 115.52 | 115.60 | 116.61 |
| HV-ISO 10% TBP temperature (°F) | 204.03 | 206.50 | 208.80 | 213.20 |
| HV-ISO 90% TBP temperature (°F) | 387.67 | 383.33 | 381.43 | 389.02 |
| LT-DIST 10% TBP temperature (°F) | 375.11 | 368.37 | 362.46 | 366.61 |
| LT-DIST 90% TBP temperature (°F) | 557.76* | 554.01* | 554.01* | 554.04* |

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<td>Vapour Product (bbl/day)</td>
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<td>Splitter Bottoms Product (bbl/day)</td>
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<td>10967.38</td>
<td>10778.12</td>
<td>10680.81</td>
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</table>

| **Reboiler Heat Duties After Economic Optimization:** |       |       |       |       |
| Stabilizer (C1) Reboiler (MMBTU/hr) | 20.5113 | 20.1392 | 19.7603 | 19.5556 |
| Splitter (C2) Reboiler (MMBTU/hr) | 17.6509 | 17.3952 | 18.1745 | 19.6115 |

| **Economic Optimization Marginal Stream Values:** |       |       |       |       |
| Light Iso Marginal Stream Value ($/m³) | 182.84 | 182.78 | 182.78 | 183.04 |

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Table A.3 continued from the previous page

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<td>Total utility costs ($/hr)</td>
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| **Economic Optimization Set Points:** |       |       |
| C1 reflux flow (bbl/day) | 6235.53 | 6190.11 |
| C1 tray 3 temperature (°F) | 173.54 | 172.83 |
| DIST-C4 C5 mole fraction | 0.07630 | 0.07304 |
| C1 reboiler temperature (°F) | 581.63 | 578.51 |
| C2 reflux flow (bbl/day) | 12598.46 | 12496.08 |
| C4 feed flow (bbl/day) | 6053.62 | 6208.55 |
| C5 feed flow (bbl/day) | 3693.02 | 3536.63 |
| C2 reboiler temperature (°F) | 581.63 | 578.51 |
| HV-ISO 10% TBP temperature (°F) | 215.82 | 219.00 |
| HV-ISO 90% TBP temperature (°F) | 387.90 | 395.04 |
| LT-DIST 10% TBP temperature (°F) | 365.03 | 374.28 |
| LT-DIST 90% TBP temperature (°F) | 554.00 | 553.99 |

| **Economic Optimization Inequality Constraints:** |       |       |
| C1 reflux flow (bbl/day) | 6235.53 | 6190.11 |
| C2 reflux flow (bbl/day) | 12598.46 | 12496.08 |
| C4 feed flow (bbl/day) | 6053.62 | 6208.55 |
| C5 feed flow (bbl/day) | 3693.02 | 3536.63 |
| C1 tray 3 temperature (°F) | 173.54 | 172.83 |
| C1 reboiler temperature (°F) | 581.63 | 578.51 |
| C2 tray 2 temperature (°F) | 168.44 | 169.63 |
| C2 reboiler temperature (°F) | 689.17 | 694.17 |
| DIST-C4 C5 mole fraction | 0.07630 | 0.07304 |
| LT-ISO Reid vapour pressure (psi) | 13.985<sup>a</sup> | 14.005<sup>a</sup> |
| LT-ISO bubble point temperature (°F) | 115.79 | 115.72 |
| HV-ISO 10% TBP temperature (°F) | 215.82 | 219.00 |
| HV-ISO 90% TBP temperature (°F) | 387.90 | 395.04 |
| LT-DIST 10% TBP temperature (°F) | 365.03 | 374.28 |
| LT-DIST 90% TBP temperature (°F) | 554.00<sup>a</sup> | 553.99<sup>a</sup> |

<sup>a</sup>constraint upper bound active

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<td><strong>Product Standard Volume Flows After Economic Optimization:</strong></td>
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<td>Vapour Product (bbl/day)</td>
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<td>C₄-Distillate Product (bbl/day)</td>
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Table A.4: Base case with no measurement noise SPEEDUP real time optimizer run.

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<td>HV-ISO 90% TBP temperature (°F)</td>
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<td>173.45</td>
</tr>
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<td>Light Iso Product (bbl/day)</td>
<td>185.05</td>
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<tr>
<td>Heavy Iso Product (bbl/day)</td>
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<td>Splitter Bottoms Product (bbl/day)</td>
<td>437.75</td>
<td>449.78</td>
<td>476.21</td>
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</table>

| **Reboiler Heat Duties After Economic Optimization:** |         |         |
| Stabilizer (C1) Reboiler (MMBTU/hr) | 18.3094 | 18.2981 | 18.5659 |
| Splitter (C2) Reboiler (MMBTU/hr) | 20.5302 | 18.1831 | 19.7151 |

| **Economic Optimization Marginal Stream Values:** |         |         |
| Light Iso Marginal Stream Value ($/m³) | 182.78  | 185.16  | 185.53  |

continued on the next page...
### Economic Optimization:

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<td>Profit ($/hr)</td>
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### Economic Optimization Set Points:

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<td>6586.74</td>
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<td>C1 tray 3 temperature (°F)</td>
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<td>0.00500</td>
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<tr>
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<td>569.12</td>
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<tr>
<td>C2 reflux flow (bbl/day)</td>
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<td>11945.53</td>
</tr>
<tr>
<td>C4 feed flow (bbl/day)</td>
<td>5181.86</td>
<td>4979.68</td>
</tr>
<tr>
<td>C5 feed flow (bbl/day)</td>
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<td>3213.04</td>
</tr>
<tr>
<td>C2 reboiler temperature (°F)</td>
<td>570.19</td>
<td>569.12</td>
</tr>
<tr>
<td>HV-ISO 10% TBP temperature (°F)</td>
<td>235.72</td>
<td>234.06</td>
</tr>
<tr>
<td>HV-ISO 90% TBP temperature (°F)</td>
<td>400.70</td>
<td>410.38</td>
</tr>
<tr>
<td>LT-DIST 10% TBP temperature (°F)</td>
<td>380.79</td>
<td>382.21</td>
</tr>
<tr>
<td>LT-DIST 90% TBP temperature (°F)</td>
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<td>554.00</td>
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### Economic Optimization Inequality Constraints:

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<td>6586.74</td>
</tr>
<tr>
<td>C2 reflux flow (bbl/day)</td>
<td>11549.58</td>
<td>11945.53</td>
</tr>
<tr>
<td>C4 feed flow (bbl/day)</td>
<td>5181.86</td>
<td>4979.68</td>
</tr>
<tr>
<td>C5 feed flow (bbl/day)</td>
<td>3325.22</td>
<td>3213.04</td>
</tr>
<tr>
<td>C1 tray 3 temperature (°F)</td>
<td>153.61</td>
<td>153.19</td>
</tr>
<tr>
<td>C1 reboiler temperature (°F)</td>
<td>570.19</td>
<td>569.12</td>
</tr>
<tr>
<td>C2 tray 2 temperature (°F)</td>
<td>186.46</td>
<td>183.83</td>
</tr>
<tr>
<td>C2 reboiler temperature (°F)</td>
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<td>700.00</td>
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<tr>
<td>DIST-C4 C₅ mole fraction</td>
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<td>0.00500⁺</td>
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<tr>
<td>LT-ISO Reid vapour pressure (psi)</td>
<td>11.536</td>
<td>11.919</td>
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<tr>
<td>LT-ISO bubble point temperature (°F)</td>
<td>127.18</td>
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<tr>
<td>HV-ISO 10% TBP temperature (°F)</td>
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<td>234.06</td>
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<tr>
<td>HV-ISO 90% TBP temperature (°F)</td>
<td>400.70</td>
<td>410.38</td>
</tr>
<tr>
<td>LT-DIST 10% TBP temperature (°F)</td>
<td>380.79</td>
<td>382.21</td>
</tr>
<tr>
<td>LT-DIST 90% TBP temperature (°F)</td>
<td>554.00⁺</td>
<td>554.00⁺</td>
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<td>Vapour Product (bbl/day)</td>
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<td>4783.01</td>
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<tr>
<td>C₄-Distillate Product (bbl/day)</td>
<td>164.20</td>
<td>154.29</td>
</tr>
<tr>
<td>Light Iso Product (bbl/day)</td>
<td>219.20</td>
<td>229.33</td>
</tr>
<tr>
<td>Heavy Iso Product (bbl/day)</td>
<td>596.79</td>
<td>579.04</td>
</tr>
<tr>
<td>Light Distillate Product (bbl/day)</td>
<td>983.67</td>
<td>1035.38</td>
</tr>
<tr>
<td>Splitter Bottoms Product (bbl/day)</td>
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<td>531.99</td>
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<td><strong>Reboiler Heat Duties After Economic Optimization:</strong></td>
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<tr>
<td>Stabilizer (C1) Reboiler (MMBTU/hr)</td>
<td>18.8524</td>
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<td>Splitter (C2) Reboiler (MMBTU/hr)</td>
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<td>Light Iso Marginal Stream Value ($/m³)</td>
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Table A.5: ASPEN PLUS real time optimizer run with Heavy Iso price at $173.89/m³.

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<td>C1 reflux flow (bbl/day)</td>
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<td>163.80</td>
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<td>DIST-C4 C₅ mole fraction</td>
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<td>0.06024</td>
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<td>606.28</td>
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<td>C2 reflux flow (bbl/day)</td>
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<td>LT-DIST 90% TBP temperature (°F)</td>
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<td>482.14</td>
<td>554.04</td>
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<td>171.59</td>
<td>163.80</td>
</tr>
<tr>
<td>C1 reboiler temperature (°F)</td>
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<td>606.28</td>
<td>612.59</td>
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<td>LT-ISO bubble point temperature (°F)</td>
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<td>198.34</td>
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<td>HV-ISO 90% TBP temperature (°F)</td>
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<td>Light Iso Product (bbl/day)</td>
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<td><strong>Reboiler Heat Duties After Economic Optimization:</strong></td>
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Table A.6: ASPEN PLUS real time optimizer run with Light Distillate price at $200.52/m³.

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<td>Profit ($/hr)</td>
<td>239.54</td>
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<td>567.85</td>
<td>545.78</td>
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<td>Total product values ($/hr)</td>
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<td>Total feed cost ($/hr)</td>
<td>22928.41</td>
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<tr>
<td>Total utility costs ($/hr)</td>
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<td>117.51</td>
<td>120.83</td>
<td>128.02</td>
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| **Economic Optimization Set Points:** |       |       |       |       |
| C1 reflux flow (bbl/day) | 6913.39 | 7439.98 | 8046.32 | 8650.61 |
| C1 tray 3 temperature (°F) | 181.28 | 172.98 | 166.60 | 159.42 |
| DIST-C4 C₅ mole fraction | 0.11899 | 0.06710 | 0.03623 | 0.01015 |
| C1 reboiler temperature (°F) | 595.14 | 605.12 | 607.09 | 609.89 |
| C2 reflux flow (bbl/day) | 13958.13 | 14185.04 | 13734.76 | 13136.78 |
| C4 feed flow (bbl/day) | 5585.31 | 6032.91 | 5765.59 | 5560.68 |
| C5 feed flow (bbl/day) | 3586.48 | 4177.17 | 4233.95 | 4115.21 |
| C2 reboiler temperature (°F) | 595.14 | 605.12 | 607.09 | 609.89 |
| HV-ISO 10% TBP temperature (°F) | 195.84 | 189.44 | 177.87 | 176.56 |
| HV-ISO 90% TBP temperature (°F) | 336.09 | 347.28 | 332.51 | 328.29 |
| LT-DIST 10% TBP temperature (°F) | 315.69 | 328.09 | 312.97 | 306.72 |
| LT-DIST 90% TBP temperature (°F) | 482.72 | 553.98 | 553.98 | 553.98 |

| **Economic Optimization Inequality Constraints:** |       |       |       |       |
| C1 reflux flow (bbl/day) | 6913.39 | 7439.98 | 8046.32 | 8650.61 |
| C2 reflux flow (bbl/day) | 13958.13 | 14185.04 | 13734.76 | 13136.78 |
| C4 feed flow (bbl/day) | 5585.31 | 6032.91 | 5765.59 | 5560.68 |
| C5 feed flow (bbl/day) | 3586.48 | 4177.17 | 4233.95 | 4115.21 |
| C1 tray 3 temperature (°F) | 181.28 | 172.98 | 166.60 | 159.42 |
| C1 reboiler temperature (°F) | 595.14 | 605.12 | 607.09 | 609.89 |
| C2 tray 2 temperature (°F) | 152.96 | 150.06 | 142.65 | 142.03 |
| C2 reboiler temperature (°F) | 651.22 | 649.17 | 631.71 | 621.86 |
| DIST-C₄ C₅ mole fraction | 0.11899 | 0.06710 | 0.03623 | 0.01015 |
| LT-ISO Reid vapour pressure (psi) | 14.000 | 12.645 | 13.236 | 13.304 |
| LT-ISO bubble point temperature (°F) | 115.05 | 119.87 | 116.46 | 115.99 |
| HV-ISO 10% TBP temperature (°F) | 195.84 | 189.44 | 177.87 | 176.56 |
| HV-ISO 90% TBP temperature (°F) | 336.09 | 347.28 | 332.51 | 328.29 |
| LT-DIST 10% TBP temperature (°F) | 315.69 | 328.09 | 312.97 | 306.72 |
| LT-DIST 90% TBP temperature (°F) | 482.72 | 553.98 | 553.98 | 553.98 |

*constraint upper bound active

*constraint lower bound active

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Table A.6 continued from the previous page

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<td></td>
<td></td>
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<tr>
<td>Vapour Product (bbl/day)</td>
<td>1025.12</td>
<td>1004.98</td>
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<td>940.21</td>
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<td>C₄-Distillate Product (bbl/day)</td>
<td>902.25</td>
<td>918.66</td>
<td>926.18</td>
<td>929.92</td>
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<tr>
<td>Light Iso Product (bbl/day)</td>
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<td>1453.38</td>
<td>1335.76</td>
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<td>Light Distillate Product (bbl/day)</td>
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<tr>
<td>Stabilizer (C1) Reboiler (MMBTU/hr)</td>
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<td>Splitter (C2) Reboiler (MMBTU/hr)</td>
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<tr>
<td>Light Iso Marginal Stream Value ($/m³)</td>
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<td>183.64</td>
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<td><strong>Data Reconciliation:</strong></td>
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<tr>
<td>Initial objective function value</td>
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Table A.7: ASPEN PLUS real time optimizer run with Heavy Iso price at $173.89/m³ and Light Distillate price at $200.52/m³.

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<td>Profit ($/hr)</td>
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<td>Total feed cost ($/hr)</td>
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<td>Total utility costs ($/hr)</td>
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<td>C1 tray 3 temperature (°F)</td>
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<td>DIST-C4 C₅ mole fraction</td>
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<tr>
<td>C1 reboiler temperature (°F)</td>
</tr>
<tr>
<td>C2 reflux flow (bbl/day)</td>
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<tr>
<td>C4 feed flow (bbl/day)</td>
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<tr>
<td>C5 feed flow (bbl/day)</td>
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<tr>
<td>C2 reboiler temperature (°F)</td>
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<tr>
<td>HV-ISO 10% TBP temperature (°F)</td>
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<tr>
<td>HV-ISO 90% TBP temperature (°F)</td>
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<tr>
<td>LT-DIST 10% TBP temperature (°F)</td>
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<td>LT-DIST 90% TBP temperature (°F)</td>
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<td>C2 reflux flow (bbl/day)</td>
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<td>C4 feed flow (bbl/day)</td>
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<td>C5 feed flow (bbl/day)</td>
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<tr>
<td>C1 tray 3 temperature (°F)</td>
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<tr>
<td>C1 reboiler temperature (°F)</td>
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<tr>
<td>C2 tray 2 temperature (°F)</td>
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<tr>
<td>C2 reboiler temperature (°F)</td>
</tr>
<tr>
<td>DIST-C4 C₅ mole fraction</td>
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<tr>
<td>LT-ISO Reid vapour pressure (psi)</td>
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<tr>
<td>LT-ISO bubble point temperature (°F)</td>
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<tr>
<td>HV-ISO 10% TBP temperature (°F)</td>
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<td>HV-ISO 90% TBP temperature (°F)</td>
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<td>LT-DIST 90% TBP temperature (°F)</td>
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*constraint upper bound active

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<td><strong>Product Standard Volume Flows After Economic Optimization:</strong></td>
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<td></td>
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<tr>
<td>Vapour Product (bbl/day)</td>
<td>1025.12</td>
<td>1024.17</td>
<td>994.90</td>
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<tr>
<td>C4-Distillate Product (bbl/day)</td>
<td>902.25</td>
<td>937.02</td>
<td>931.90</td>
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<tr>
<td>Light Iso Product (bbl/day)</td>
<td>1559.68</td>
<td>1639.70</td>
<td>1686.47</td>
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<td>Heavy Iso Product (bbl/day)</td>
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<td>3778.85</td>
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<tr>
<td>Light Distillate Product (bbl/day)</td>
<td>2331.66</td>
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<td>3567.86</td>
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<td>Splitter Bottoms Product (bbl/day)</td>
<td>12325.98</td>
<td>11340.73</td>
<td>11532.20</td>
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<td><strong>Reboiler Heat Duties After Economic Optimization:</strong></td>
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<td>Stabilizer (C1) Reboiler (MMBTU/hr)</td>
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<td>21.2672</td>
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<td>Light Iso Marginal Stream Value ($/m^3)</td>
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Table A.8: Winter ASPEN PLUS v9.3 real time optimizer run.

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<td></td>
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<tr>
<td>Profit ($/hr)</td>
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<td>137.13</td>
<td>294.02</td>
<td>404.23</td>
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<td>Optimization iterations</td>
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<td>5</td>
<td>11</td>
<td>10</td>
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<td>Total product values ($/hr)</td>
<td>22958.75</td>
<td>23285.14</td>
<td>23365.12</td>
<td>23426.27</td>
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<td>Total feed cost ($/hr)</td>
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<td>23028.10</td>
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<td>22885.32</td>
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<td>Total utility costs ($/hr)</td>
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<td>119.91</td>
<td>129.24</td>
<td>136.72</td>
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</table>

| **Economic Optimization Set Points:** |     |     |     |     |
| C1 reflux flow (bbl/day)          | 7012.25 | 7569.65 | 8154.29 | 8705.16 |
| C1 tray 3 temperature (°F)        | 172.17 | 161.52 | 157.22 | 157.73 |
| DIST-C4 C5 mole fraction          | 0.06538 | 0.02080 | 0.00500 | 0.00513 |
| C1 reboiler temperature (°F)      | 587.59 | 597.02 | 600.06 | 601.49 |
| C2 reflux flow (bbl/day)          | 14212.28 | 14207.00 | 14166.87 | 14157.81 |
| C4 feed flow (bbl/day)            | 5647.83 | 5951.76 | 5831.13 | 5815.26 |
| C5 feed flow (bbl/day)            | 3586.57 | 4149.26 | 4488.58 | 4793.16 |
| C2 reboiler temperature (°F)      | 587.59 | 597.02 | 600.06 | 601.49 |
| HV-ISO 10% TBP temperature (°F)   | 195.23 | 199.55 | 191.67 | 196.92 |
| HV-ISO 90% TBP temperature (°F)   | 335.84 | 348.39 | 349.79 | 348.03 |
| LT-DIST 10% TBP temperature (°F)  | 312.59 | 323.86 | 320.67 | 314.69 |
| LT-DIST 90% TBP temperature (°F)  | 481.35 | 549.80 | 553.93 | 553.96 |

| **Economic Optimization Inequality Constraints:** |     |     |     |     |
| C1 reflux flow (bbl/day)          | 7012.25 | 7569.65 | 8154.29 | 8705.16 |
| C2 reflux flow (bbl/day)          | 14212.28 | 14207.00 | 14166.87 | 14157.81 |
| C4 feed flow (bbl/day)            | 5647.83 | 5951.76 | 5831.13 | 5815.26 |
| C5 feed flow (bbl/day)            | 3586.57 | 4149.26 | 4488.58 | 4793.16 |
| C1 tray 3 temperature (°F)        | 172.17 | 161.52 | 157.22 | 157.73 |
| C1 reboiler temperature (°F)      | 587.59 | 597.02 | 600.06 | 601.49 |
| C2 tray 2 temperature (°F)        | 151.82 | 154.51 | 156.85 | 159.65 |
| C2 reboiler temperature (°F)      | 652.65 | 651.52 | 660.78 | 665.42 |
| DIST-C4 C5 mole fraction          | 0.06538 | 0.02080 | 0.00500 | 0.00513 |
| LT-ISO Reid vapour pressure (psi) | 14.009a | 12.185 | 11.563 | 11.117 |
| LT-ISO bubble point temperature (°F) | 116.54 | 124.36 | 127.57 | 129.87 |
| HV-ISO 10% TBP temperature (°F)   | 195.23 | 199.55 | 191.67 | 196.92 |
| HV-ISO 90% TBP temperature (°F)   | 335.84 | 348.39 | 349.79 | 348.03 |
| LT-DIST 10% TBP temperature (°F)  | 312.59 | 323.86 | 320.67 | 314.69 |
| LT-DIST 90% TBP temperature (°F)  | 481.35 | 549.80 | 553.93 | 553.96 |

*a* constraint lower bound active

*a* constraint upper bound active
Table A.8 continued from the previous page

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<tbody>
<tr>
<td>Product Standard Volume Flows After Economic Optimization:</td>
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<td></td>
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<tr>
<td>Vapour Product (bbl/day)</td>
<td>992.20</td>
<td>976.49</td>
<td>948.96</td>
<td>930.38</td>
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<tr>
<td>C₄-Distillate Product (bbl/day)</td>
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<td>895.74</td>
<td>910.08</td>
<td>927.94</td>
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<tr>
<td>Light Iso Product (bbl/day)</td>
<td>1623.75</td>
<td>1673.87</td>
<td>1749.32</td>
<td>1831.18</td>
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<tr>
<td>Heavy Iso Product (bbl/day)</td>
<td>3711.10</td>
<td>3800.22</td>
<td>3663.05</td>
<td>3410.52</td>
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<td>Light Distillate Product (bbl/day)</td>
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<td>Splitter Bottoms Product (bbl/day)</td>
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<td>Reboiler Heat Duties After Economic Optimization:</td>
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<td>Stabilizer (C1) Reboiler (MMBTU/hr)</td>
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<td>30.1392</td>
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<td>18.8338</td>
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Table A.9: Winter with no measurement noise ASPEN PLUS v9.3 real time optimizer run.

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<td>Profit ($/hr)</td>
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<td>5</td>
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<td>Total product values ($/hr)</td>
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<td>Total utility costs ($/hr)</td>
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<td>114.44</td>
<td>116.27</td>
<td>113.04</td>
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</table>

**Economic Optimization Set Points:**

| C1 reflux flow (bbl/day) | 7012.25 | 6951.80 | 6926.19 | 6845.08 |
| C1 tray 3 temperature (°F) | 172.17 | 169.36 | 165.32 | 163.36 |
| DIST-C4 C5 mole fraction | 0.06538 | 0.05396 | 0.03911 | 0.03305 |
| C1 reboiler temperature (°F) | 587.39 | 588.18 | 583.72 | 584.78 |
| C2 reflux flow (bbl/day) | 14212.28 | 14084.92 | 13764.29 | 13715.39 |
| C4 feed flow (bbl/day) | 5647.83 | 5860.43 | 5594.30 | 5373.38 |
| C5 feed flow (bbl/day) | 3586.57 | 4043.16 | 4240.16 | 4429.91 |
| C2 reboiler temperature (°F) | 587.39 | 588.18 | 583.72 | 584.78 |
| HV-ISO 10% TBP temperature (°F) | 195.23 | 199.97 | 192.49 | 195.83 |
| HV-ISO 90% TBP temperature (°F) | 335.84 | 349.58 | 349.12 | 344.96 |
| LT-DIST 10% TBP temperature (°F) | 312.59 | 326.12 | 320.73 | 314.48 |
| LT-DIST 90% TBP temperature (°F) | 481.35 | 547.24 | 552.99 | 552.69 |

**Economic Optimization Inequality Constraints:**

| C1 reflux flow (bbl/day) | 7012.25 | 6951.80 | 6926.19 | 6845.08 |
| C2 reflux flow (bbl/day) | 14212.28 | 14084.92 | 13764.29 | 13715.39 |
| C4 feed flow (bbl/day) | 5647.83 | 5860.43 | 5594.30 | 5373.38 |
| C5 feed flow (bbl/day) | 3586.57 | 4043.16 | 4240.16 | 4429.91 |
| C1 tray 3 temperature (°F) | 172.17 | 169.36 | 165.32 | 163.36 |
| C1 reboiler temperature (°F) | 587.39 | 588.18 | 583.72 | 584.78 |
| C2 tray 2 temperature (°F) | 151.82 | 153.16 | 154.97 | 156.74 |
| C2 reboiler temperature (°F) | 652.65 | 657.52 | 662.68 | 659.93 |
| DIST-C4 C5 mole fraction | 0.06538 | 0.05396 | 0.03911 | 0.03305 |
| LT-ISO Reid vapour pressure (psi) | 14.000* | 13.994* | 14.000* | 13.964* |
| LT-ISO bubble point temperature (°F) | 116.54 | 116.59 | 116.59 | 116.77 |
| HV-ISO 10% TBP temperature (°F) | 195.23 | 199.97 | 192.49 | 195.83 |
| HV-ISO 90% TBP temperature (°F) | 335.84 | 349.58 | 349.12 | 344.96 |
| LT-DIST 10% TBP temperature (°F) | 312.59 | 326.12 | 320.73 | 314.48 |
| LT-DIST 90% TBP temperature (°F) | 481.35 | 547.24 | 552.99 | 552.69 |

*constraint upper bound active

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Table A.9 continued from the previous page

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<tr>
<td>Vapour Product (bbl/day)</td>
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<td>863.01</td>
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<td>Light Iso Product (bbl/day)</td>
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<td>Heavy Iso Product (bbl/day)</td>
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### Economic Optimization:

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<tbody>
<tr>
<td>Profit ($/hr)</td>
<td>449.50</td>
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<td>646.13</td>
<td>720.02</td>
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<td>Optimization iterations</td>
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<td>13</td>
<td>5</td>
<td>15</td>
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<td>Total product values ($/hr)</td>
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<td>23754.80</td>
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<td>Total feed cost ($/hr)</td>
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<td>Total utility costs ($/hr)</td>
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### Economic Optimization Set Points:

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<tbody>
<tr>
<td>C1 reflux flow (bbl/day)</td>
<td>6759.18</td>
<td>6645.49</td>
<td>6638.26</td>
<td>6537.43</td>
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<tr>
<td>C1 tray 3 temperature (°F)</td>
<td>160.31</td>
<td>161.51</td>
<td>154.13</td>
<td>153.76</td>
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<tr>
<td>DIST-C4 C5 mole fraction</td>
<td>0.02418</td>
<td>0.02849</td>
<td>0.00885</td>
<td>0.00874</td>
</tr>
<tr>
<td>C1 reboiler temperature (°F)</td>
<td>584.02</td>
<td>581.32</td>
<td>576.67</td>
<td>572.41</td>
</tr>
<tr>
<td>C2 reflux flow (bbl/day)</td>
<td>13544.79</td>
<td>13276.08</td>
<td>13022.14</td>
<td>12685.23</td>
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<tr>
<td>C4 feed flow (bbl/day)</td>
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<td>5309.43</td>
<td>5035.32</td>
<td>5026.37</td>
</tr>
<tr>
<td>C5 feed flow (bbl/day)</td>
<td>4642.20</td>
<td>4887.17</td>
<td>5090.37</td>
<td>5223.63</td>
</tr>
<tr>
<td>C2 reboiler temperature (°F)</td>
<td>584.02</td>
<td>581.32</td>
<td>576.67</td>
<td>572.41</td>
</tr>
<tr>
<td>HV-ISO 10% TBP temperature (°F)</td>
<td>198.37</td>
<td>203.23</td>
<td>203.35</td>
<td>210.34</td>
</tr>
<tr>
<td>HV-ISO 90% TBP temperature (°F)</td>
<td>342.26</td>
<td>343.01</td>
<td>334.07</td>
<td>335.97</td>
</tr>
<tr>
<td>LT-DIST 10% TBP temperature (°F)</td>
<td>311.02</td>
<td>311.53</td>
<td>302.00</td>
<td>302.03</td>
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<tr>
<td>LT-DIST 90% TBP temperature (°F)</td>
<td>553.83</td>
<td>554.11</td>
<td>554.00</td>
<td>554.16</td>
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</table>

### Economic Optimization Inequality Constraints:

| C1 reflux flow (bbl/day) | 6759.18 | 6645.49 | 6638.26 | 6537.43 |
| C2 reflux flow (bbl/day) | 13544.79 | 13276.08 | 13022.14 | 12685.23 |
| C4 feed flow (bbl/day) | 5330.80 | 5309.43 | 5035.32 | 5026.37 |
| C5 feed flow (bbl/day) | 4642.20 | 4887.17 | 5090.37 | 5223.63 |
| C1 tray 3 temperature (°F) | 160.31 | 161.51 | 154.13 | 153.76 |
| C1 reboiler temperature (°F) | 584.02 | 581.32 | 576.67 | 572.41 |
| C2 tray 2 temperature (°F) | 159.81 | 165.57 | 166.69 | 171.45 |
| C2 reboiler temperature (°F) | 664.86 | 670.51 | 667.50 | 671.91 |
| DIST-C4 C5 mole fraction | 0.02418 | 0.02849 | 0.00885 | 0.00874 |
| LT-ISO bubble point temperature (°F) | 116.41 | 118.77 | 116.70 | 118.49 |
| HV-ISO 10% TBP temperature (°F) | 198.37 | 203.23 | 203.35 | 210.34 |
| HV-ISO 90% TBP temperature (°F) | 342.26 | 343.01 | 334.07 | 335.97 |
| LT-DIST 10% TBP temperature (°F) | 311.02 | 311.53 | 302.00 | 302.03 |
| LT-DIST 90% TBP temperature (°F) | 553.83 | 554.11 | 554.00 | 554.16 |

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*constraint lower bound active

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Table A.9 continued from the previous page

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<td><strong>Product Standard Volume Flows After Economic Optimization:</strong></td>
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<tr>
<td>Vapour Product (bbl/day)</td>
<td>759.06</td>
<td>713.78</td>
<td>654.86</td>
<td>612.84</td>
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<td>C₄-Distillate Product (bbl/day)</td>
<td>1013.00</td>
<td>1063.51</td>
<td>1068.88</td>
<td>1102.80</td>
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<td>Light Iso Product (bbl/day)</td>
<td>2007.02</td>
<td>2112.60</td>
<td>2215.71</td>
<td>2343.01</td>
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<td>Heavy Iso Product (bbl/day)</td>
<td>3269.41</td>
<td>3138.29</td>
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<td>Light Distillate Product (bbl/day)</td>
<td>3896.56</td>
<td>4083.66</td>
<td>4335.68</td>
<td>4447.03</td>
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<td>Splitter Bottoms Product (bbl/day)</td>
<td>10992.02</td>
<td>10822.20</td>
<td>10857.30</td>
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<td><strong>Reboiler Heat Duties After Economic Optimization:</strong></td>
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<td></td>
<td></td>
<td></td>
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<tr>
<td>Stabilizer (C1) Reboiler (MMBTU/hr)</td>
<td>20.3736</td>
<td>20.3296</td>
<td>19.7150</td>
<td>19.5143</td>
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<tr>
<td>Splitter (C2) Reboiler (MMBTU/hr)</td>
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<td>19.2232</td>
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<td>19.3937</td>
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<td>Light Iso Marginal Stream Value ($/m³)</td>
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### Economic Optimization:

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<td>Profit ($/hr)</td>
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<td>Total utility costs ($/hr)</td>
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### Economic Optimization Set Points:

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<tr>
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<td>6292.07</td>
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<tr>
<td>C1 tray 3 temperature (°F)</td>
<td>151.90</td>
<td>154.94</td>
</tr>
<tr>
<td>DIST-C4 C5 mole fraction</td>
<td>0.00535</td>
<td>0.01307</td>
</tr>
<tr>
<td>C1 reboiler temperature (°F)</td>
<td>571.09</td>
<td>576.04</td>
</tr>
<tr>
<td>C2 reflux flow (bbl/day)</td>
<td>12436.63</td>
<td>12223.36</td>
</tr>
<tr>
<td>C4 feed flow (bbl/day)</td>
<td>4816.08</td>
<td>4617.93</td>
</tr>
<tr>
<td>C5 feed flow (bbl/day)</td>
<td>5366.10</td>
<td>5549.39</td>
</tr>
<tr>
<td>C2 reboiler temperature (°F)</td>
<td>571.09</td>
<td>576.04</td>
</tr>
<tr>
<td>HV-ISO 10% TBP temperature (°F)</td>
<td>218.93</td>
<td>216.49</td>
</tr>
<tr>
<td>HV-ISO 90% TBP temperature (°F)</td>
<td>338.82</td>
<td>343.15</td>
</tr>
<tr>
<td>LT-DIST 10% TBP temperature (°F)</td>
<td>302.03</td>
<td>302.00</td>
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<td>LT-DIST 90% TBP temperature (°F)</td>
<td>554.05</td>
<td>553.99</td>
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### Economic Optimization Inequality Constraints:

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<td>C1 reflux flow (bbl/day)</td>
<td>6471.86</td>
<td>6292.07</td>
</tr>
<tr>
<td>C2 reflux flow (bbl/day)</td>
<td>12436.63</td>
<td>12223.36</td>
</tr>
<tr>
<td>C4 feed flow (bbl/day)</td>
<td>4816.08</td>
<td>4617.93</td>
</tr>
<tr>
<td>C5 feed flow (bbl/day)</td>
<td>5366.10</td>
<td>5549.39</td>
</tr>
<tr>
<td>C1 tray 3 temperature (°F)</td>
<td>151.90</td>
<td>154.94</td>
</tr>
<tr>
<td>C1 reboiler temperature (°F)</td>
<td>571.09</td>
<td>576.04</td>
</tr>
<tr>
<td>C2 tray 2 temperature (°F)</td>
<td>174.67</td>
<td>179.88</td>
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<td>C2 reboiler temperature (°F)</td>
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<td>DIST-C4 C5 mole fraction</td>
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<td>0.01307</td>
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<td>LT-ISO Reid vapour pressure (psi)</td>
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<td>LT-ISO bubble point temperature (°F)</td>
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<td>HV-ISO 10% TBP temperature (°F)</td>
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<td>216.49</td>
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<tr>
<td>HV-ISO 90% TBP temperature (°F)</td>
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<td>343.15</td>
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<tr>
<td>LT-DIST 10% TBP temperature (°F)</td>
<td>302.03</td>
<td>302.00</td>
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<td>LT-DIST 90% TBP temperature (°F)</td>
<td>554.05</td>
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<tbody>
<tr>
<td><strong>Product Standard Volume Flows After Economic Optimization:</strong></td>
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<tr>
<td>Vapour Product (bbl/day)</td>
<td>573.19</td>
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<td>$C_4$-Distillate Product (bbl/day)</td>
<td>1123.05</td>
<td>1176.63</td>
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<td>Light Iso Product (bbl/day)</td>
<td>2470.17</td>
<td>2601.60</td>
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<tr>
<td>Heavy Iso Product (bbl/day)</td>
<td>2547.30</td>
<td>2385.88</td>
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<tr>
<td>Light Distillate Product (bbl/day)</td>
<td>4636.35</td>
<td>4879.34</td>
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<td>Splitter Bottoms Product (bbl/day)</td>
<td>10565.05</td>
<td>10342.68</td>
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<td><strong>Reboiler Heat Duties After Economic Optimization:</strong></td>
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<td>Stabilizer (C1) Reboiler (MMBTU/hr)</td>
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<td>Splitter (C2) Reboiler (MMBTU/hr)</td>
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<td>20.3809</td>
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<td><strong>Economic Optimization Marginal Stream Values:</strong></td>
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<td>Light Iso Marginal Stream Value ($/m^3$)</td>
<td>183.35</td>
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Table A.10: Winter to summer ASPEN PLUS v9.3 real time optimizer run.

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<th>Cycle</th>
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<th>Summer Prices</th>
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<tbody>
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<td>2</td>
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<tr>
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<td>Total feed cost ($/hr)</td>
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<td>Total utility costs ($/hr)</td>
<td>120.21</td>
<td>119.91</td>
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<tr>
<td>Economic Optimization Set Points:</td>
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<td></td>
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<tr>
<td>C1 reflux flow (bbl/day)</td>
<td>7012.25</td>
<td>7569.65</td>
</tr>
<tr>
<td>C1 tray 3 temperature (°F)</td>
<td>172.17</td>
<td>161.52</td>
</tr>
<tr>
<td>DIST-C4 C5 mole fraction</td>
<td>0.06538</td>
<td>0.02080</td>
</tr>
<tr>
<td>C1 reboiler temperature (°F)</td>
<td>587.59</td>
<td>597.02</td>
</tr>
<tr>
<td>C2 reflux flow (bbl/day)</td>
<td>14212.28</td>
<td>14207.00</td>
</tr>
<tr>
<td>C4 feed flow (bbl/day)</td>
<td>5647.83</td>
<td>5951.76</td>
</tr>
<tr>
<td>C5 feed flow (bbl/day)</td>
<td>3586.57</td>
<td>4149.26</td>
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<tr>
<td>C2 reboiler temperature (°F)</td>
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<td>597.02</td>
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<tr>
<td>HV-ISO 10% TBP temperature (°F)</td>
<td>195.23</td>
<td>199.55</td>
</tr>
<tr>
<td>HV-ISO 90% TBP temperature (°F)</td>
<td>335.84</td>
<td>348.39</td>
</tr>
<tr>
<td>LT-DIST 10% TBP temperature (°F)</td>
<td>312.59</td>
<td>323.86</td>
</tr>
<tr>
<td>LT-DIST 90% TBP temperature (°F)</td>
<td>481.35</td>
<td>549.80</td>
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<td>Economic Optimization Inequality Constraints:</td>
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<td>C1 reflux flow (bbl/day)</td>
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<td>7569.65</td>
</tr>
<tr>
<td>C2 reflux flow (bbl/day)</td>
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<td>14207.00</td>
</tr>
<tr>
<td>C4 feed flow (bbl/day)</td>
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<td>5951.76</td>
</tr>
<tr>
<td>C5 feed flow (bbl/day)</td>
<td>3586.57</td>
<td>4149.26</td>
</tr>
<tr>
<td>C1 tray 3 temperature (°F)</td>
<td>172.17</td>
<td>161.52</td>
</tr>
<tr>
<td>C1 reboiler temperature (°F)</td>
<td>587.59</td>
<td>597.02</td>
</tr>
<tr>
<td>C2 tray 2 temperature (°F)</td>
<td>151.82</td>
<td>154.51</td>
</tr>
<tr>
<td>C2 reboiler temperature (°F)</td>
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<td>651.52</td>
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<tr>
<td>DIST-C4 C5 mole fraction</td>
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<td>LT-ISO bubble point temperature (°F)</td>
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<td>HV-ISO 10% TBP temperature (°F)</td>
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<td>HV-ISO 90% TBP temperature (°F)</td>
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<td>348.39</td>
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<tr>
<td>LT-DIST 10% TBP temperature (°F)</td>
<td>312.59</td>
<td>323.86</td>
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<tr>
<td>LT-DIST 90% TBP temperature (°F)</td>
<td>481.35</td>
<td>549.80</td>
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</tr>
<tr>
<td><strong>Product Standard Volume Flows After Economic Optimization:</strong></td>
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</tr>
<tr>
<td>Vapour Product (bbl/day)</td>
<td>992.20</td>
<td>976.49</td>
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<td>C₄-Distillate Product (bbl/day)</td>
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<td>Light Iso Product (bbl/day)</td>
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<td>Heavy Iso Product (bbl/day)</td>
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<td>Light Distillate Product (bbl/day)</td>
<td>2442.23</td>
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<td>Splitter Bottoms Product (bbl/day)</td>
<td>12290.37</td>
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<tr>
<td><strong>Reboiler Heat Duties After Economic Optimization:</strong></td>
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<tr>
<td>Stabilizer (C1) Reboiler (MMBTU/hr)</td>
<td>21.7598</td>
<td>24.6837</td>
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<td>Splitter (C2) Reboiler (MMBTU/hr)</td>
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<tr>
<td>Light Iso Marginal Stream Value ($/m³)</td>
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<td><strong>Data Reconciliation:</strong></td>
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**Economic Optimization:**

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<tr>
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<td>Total feed cost ($/hr)</td>
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<td>Total utility costs ($/hr)</td>
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**Economic Optimization Set Points:**

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<tr>
<td>C1 reflux flow (bbl/day)</td>
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<td>C1 tray 3 temperature (°F)</td>
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<tr>
<td>DIST-C4 C₅ mole fraction</td>
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</tr>
<tr>
<td>C1 reboiler temperature (°F)</td>
<td>328.63</td>
</tr>
<tr>
<td>C2 reboiler temperature (°F)</td>
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<tr>
<td>HV-ISO 10% TBP temperature (°F)</td>
<td>133.53</td>
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<td>HV-ISO 90% TBP temperature (°F)</td>
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<tr>
<td>LT-DIST 10% TBP temperature (°F)</td>
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<td>LT-DIST 90% TBP temperature (°F)</td>
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<tr>
<td>LT-DIST 90% TBP temperature (°F)</td>
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**Economic Optimization Inequality Constraints:**

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<td>5982.55</td>
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<td>4304.87</td>
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<tr>
<td>DIST-C4 C₅ mole fraction</td>
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<tr>
<td>LT-ISO Reid vapour pressure (psi)</td>
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<tr>
<td>LT-ISO bubble point temperature (°F)</td>
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<td>LT-DIST 10% TBP temperature (°F)</td>
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<td>LT-DIST 90% TBP temperature (°F)</td>
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*a*constraint upper bound active

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<td>Vapour Product (bbl/day)</td>
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<tr>
<td>C4-Distillate Product (bbl/day)</td>
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<tr>
<td>Light Iso Product (bbl/day)</td>
<td>1658.41</td>
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<tr>
<td>Heavy Iso Product (bbl/day)</td>
<td>3822.38</td>
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<tr>
<td>Light Distillate Product (bbl/day)</td>
<td>3663.98</td>
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<tr>
<td>Splitter Bottoms Product (bbl/day)</td>
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<tr>
<td><strong>Reboiler Heat Duties After Economic Optimization:</strong></td>
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<tr>
<td>Stabilizer (C1) Reboiler (MMBTU/hr)</td>
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<td>Splitter (C2) Reboiler (MMBTU/hr)</td>
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<td><strong>Economic Optimization Marginal Stream Values:</strong></td>
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<td>Light Iso Marginal Stream Value ($/m³)</td>
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<td>Final objective function value</td>
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Table A.11: Winter to summer with no measurement noise ASPEN PLUS v9.3 real time optimizer run.

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<th>Winter Prices</th>
<th>Summer Prices</th>
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<td>Cycle</td>
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<td>2</td>
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<tr>
<td>Economic Optimization</td>
<td></td>
<td></td>
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<tr>
<td>Profit ($/hr)</td>
<td>-170.90</td>
<td>118.37</td>
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<tr>
<td>Optimization iterations</td>
<td>4</td>
<td>5</td>
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<tr>
<td>Total product values ($/hr)</td>
<td>22958.75</td>
<td>23216.48</td>
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<tr>
<td>Total feed cost ($/hr)</td>
<td>23000.43</td>
<td>22983.67</td>
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<tr>
<td>Total utility costs ($/hr)</td>
<td>120.21</td>
<td>114.44</td>
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</table>

Economic Optimization Set Points:

| C1 reflux flow (bbl/day) | 7012.25 | 6951.80 | 6926.19 | 6919.29 |
| C1 tray 3 temperature (°F) | 172.17  | 169.36  | 165.32  | 173.16  |
| DIST-C4 C5 mole fraction  | 0.06538 | 0.05396 | 0.03911 | 0.06974 |
| C1 reboiler temperature (°F) | 587.59  | 588.18  | 583.72  | 588.41  |
| C2 reflux flow (bbl/day) | 14212.28 | 14084.92 | 13764.29 | 13600.06 |
| C4 feed flow (bbl/day) | 5647.83 | 5860.43 | 5594.30 | 5675.63 |
| C5 feed flow (bbl/day) | 3586.57 | 4043.16 | 4240.16 | 4133.95 |
| C2 reboiler temperature (°F) | 587.59  | 588.18  | 583.72  | 588.41  |
| HV-ISO 10% TBP temperature (°F) | 195.23  | 199.97  | 192.49  | 204.85  |
| HV-ISO 90% TBP temperature (°F) | 335.84  | 349.58  | 349.12  | 358.03  |
| LT-DIST 10% TBP temperature (°F) | 312.59  | 326.12  | 320.73  | 332.32  |
| LT-DIST 90% TBP temperature (°F) | 481.35  | 547.24  | 552.99  | 557.70  |

Economic Optimization Inequality Constraints:

| C1 reflux flow (bbl/day) | 7012.25 | 6951.80 | 6926.19 | 6919.29 |
| C2 reflux flow (bbl/day) | 14212.28 | 14084.92 | 13764.29 | 13600.06 |
| C4 feed flow (bbl/day) | 5647.83 | 5860.43 | 5594.30 | 5675.63 |
| C5 feed flow (bbl/day) | 3586.57 | 4043.16 | 4240.16 | 4133.95 |
| C1 tray 3 temperature (°F) | 172.17  | 169.36  | 165.32  | 173.16  |
| C1 reboiler temperature (°F) | 587.59  | 588.18  | 583.72  | 588.41  |
| C2 tray 2 temperature (°F) | 151.82  | 153.16  | 154.97  | 164.89  |
| C2 reboiler temperature (°F) | 652.65  | 657.52  | 662.68  | 668.04  |
| DIST-C4 C5 mole fraction  | 0.06538 | 0.05396 | 0.03911 | 0.06974 |
| LT-ISO Reid vapour pressure (psi) | 14.000^a | 13.994^a | 14.000^a | 12.185^b |
| LT-ISO bubble point temperature (°F) | 116.54  | 116.59  | 116.59  | 124.93  |
| HV-ISO 10% TBP temperature (°F) | 195.23  | 199.97  | 192.49  | 204.85  |
| HV-ISO 90% TBP temperature (°F) | 335.84  | 349.58  | 349.12  | 358.03  |
| LT-DIST 10% TBP temperature (°F) | 312.59  | 326.12  | 320.73  | 332.32  |
| LT-DIST 90% TBP temperature (°F) | 481.35  | 547.24  | 552.99  | 557.70  |

^aconstraint upper bound active
^bconstraint upper bound violated

continued on the next page...
... Table A.11 continued from the previous page

<table>
<thead>
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<th>Cycle</th>
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<th>Summer Prices</th>
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<tbody>
<tr>
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<tr>
<td>Product Standard Volume Flows After Economic Optimization:</td>
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<tr>
<td>Vapour Product (bbl/day)</td>
<td>992.20</td>
<td>931.06</td>
</tr>
<tr>
<td>C4-Distillate Product (bbl/day)</td>
<td>876.60</td>
<td>914.42</td>
</tr>
<tr>
<td>Light Iso Product (bbl/day)</td>
<td>1623.75</td>
<td>1699.51</td>
</tr>
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<td>Heavy Iso Product (bbl/day)</td>
<td>3711.10</td>
<td>3862.46</td>
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<tr>
<td>Light Distillate Product (bbl/day)</td>
<td>2442.23</td>
<td>3180.03</td>
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<tr>
<td>Splitter Bottoms Product (bbl/day)</td>
<td>12290.37</td>
<td>11324.16</td>
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<td>Reboiler Heat Duties After Economic Optimization:</td>
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<tr>
<td>Stabilizer (C1) Reboiler (MMBTU/hr)</td>
<td>21.7598</td>
<td>21.5004</td>
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<td>Splitter (C2) Reboiler (MMBTU/hr)</td>
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<td>17.1447</td>
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<td>Economic Optimization Marginal Stream Values:</td>
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<tr>
<td>Light Iso Marginal Stream Value ($/m^3)</td>
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<tbody>
<tr>
<td>Summer Prices</td>
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</table>

**Economic Optimization:**
- Profit ($/hr)  
  253.60  
  335.06  
  399.57  
  476.62
- Optimization iterations  
  11  
  6  
  9  
  12
- Total product values ($/hr)  
  23354.58  
  23441.45  
  23504.31  
  23602.23
- Total feed cost ($/hr)  
  22977.60  
  22983.47  
  22980.93  
  22997.50
- Total utility costs ($/hr)  
  123.38  
  122.92  
  123.81  
  128.11

**Economic Optimization Set Points:**
- C1 reflux flow (bbl/day)  
  6828.33  
  6733.51  
  6629.28  
  6539.20
- C1 tray 3 temperature (°F)  
  180.41  
  178.63  
  177.62  
  177.22
- DIST-C4 C5 mole fraction  
  0.10436  
  0.09520  
  0.09027  
  0.08817
- C1 reboiler temperature (°F)  
  593.35  
  588.67  
  589.16  
  585.82
- C2 reflux flow (bbl/day)  
  13268.17  
  13022.09  
  12832.62  
  12662.60
- C4 feed flow (bbl/day)  
  5734.76  
  5724.41  
  5531.47  
  5799.03
- C5 feed flow (bbl/day)  
  4060.18  
  3913.34  
  4084.16  
  3939.03
- C2 reboiler temperature (°F)  
  593.55  
  588.67  
  589.16  
  585.82
- HV-ISO 10% TBP temperature (°F)  
  215.65  
  221.73  
  228.51  
  223.07
- HV-ISO 90% TBP temperature (°F)  
  366.13  
  374.91  
  376.10  
  387.78
- LT-DIST 10% TBP temperature (°F)  
  337.53  
  342.12  
  340.75  
  349.64
- LT-DIST 90% TBP temperature (°F)  
  554.13  
  554.64  
  553.86  
  553.98

**Economic Optimization Inequality Constraints:**
- C1 reflux flow (bbl/day)  
  6828.33  
  6733.51  
  6629.28  
  6539.20
- C2 reflux flow (bbl/day)  
  13268.17  
  13022.09  
  12832.62  
  12662.60
- C4 feed flow (bbl/day)  
  5734.76  
  5724.41  
  5531.47  
  5799.03
- C5 feed flow (bbl/day)  
  4060.18  
  3913.34  
  4084.16  
  3939.03
- C1 tray 3 temperature (°F)  
  180.41  
  178.63  
  177.62  
  177.22
- C1 reboiler temperature (°F)  
  593.35  
  588.67  
  589.16  
  585.82
- C2 tray 2 temperature (°F)  
  175.62  
  178.01  
  180.87  
  183.70
- C2 reboiler temperature (°F)  
  673.19  
  677.92  
  682.46  
  688.11
- DIST-C4 C5 mole fraction  
  0.10436  
  0.09520  
  0.09027  
  0.08817
- LT-ISO Reid vapour pressure (psi)  
  10.500  
  10.588  
  10.495  
  10.331
- LT-ISO bubble point temperature (°F)  
  133.85  
  133.49  
  134.15  
  135.21
- HV-ISO 10% TBP temperature (°F)  
  215.65  
  221.73  
  228.51  
  223.07
- HV-ISO 90% TBP temperature (°F)  
  366.13  
  374.91  
  376.10  
  387.78
- LT-DIST 10% TBP temperature (°F)  
  337.53  
  342.12  
  340.75  
  349.64
- LT-DIST 90% TBP temperature (°F)  
  554.13  
  554.64  
  553.86  
  553.98

*constraint upper bound active

*constraint upper bound violated

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... Table A.11 continued from the previous page

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<th>Summer Prices</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>5</td>
</tr>
</tbody>
</table>
| **Product Standard Volume Flows After Economic Optimization:**
| Vapour Product (bbl/day) | 978.44 | 912.94 | 855.61 | 801.29 |
| C₄-Distillate Product (bbl/day) | 977.83 | 1021.41 | 1065.87 | 1115.14 |
| Light Iso Product (bbl/day) | 2051.35 | 2155.37 | 2267.20 | 2381.49 |
| Heavy Iso Product (bbl/day) | 3826.05 | 3930.12 | 3797.74 | 3971.45 |
| Light Distillate Product (bbl/day) | 3317.84 | 3226.82 | 3433.12 | 3281.81 |
| Splitter Bottoms Product (bbl/day) | 10754.64 | 10665.10 | 10489.92 | 10373.86 |
| **Reboiler Heat Duties After Economic Optimization:**
| Stabilizer (C1) Reboiler (MMBTU/hr) | 22.8092 | 22.3782 | 22.1024 | 21.8891 |
| Splitter (C2) Reboiler (MMBTU/hr) | 18.8549 | 19.1314 | 19.7082 | 21.3738 |
| **Economic Optimization Marginal Stream Values:**
| Light Iso Marginal Stream Value ($/m³) | 187.12 | 187.01 | 187.13 | 187.33 |

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### Economic Optimization:

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<td><strong>Profit ($/hr)</strong></td>
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<td><strong>Optimization iterations</strong></td>
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<td><strong>Total product values ($/hr)</strong></td>
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<td>23713.34</td>
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<td><strong>Total feed cost ($/hr)</strong></td>
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<td><strong>Total utility costs ($/hr)</strong></td>
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### Economic Optimization Set Points:

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<th>Prices</th>
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<tr>
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<td>6356.84</td>
<td>6360.76</td>
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<tr>
<td><strong>C1 tray 3 temperature (°F)</strong></td>
<td>181.75</td>
<td>177.59</td>
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<tr>
<td><strong>DIST-C4 C₅ mole fraction</strong></td>
<td>0.11016</td>
<td>0.08957</td>
</tr>
<tr>
<td><strong>C1 reboiler temperature (°F)</strong></td>
<td>588.60</td>
<td>583.88</td>
</tr>
<tr>
<td><strong>C2 reflux flow (bbl/day)</strong></td>
<td>12448.03</td>
<td>12144.23</td>
</tr>
<tr>
<td><strong>C4 feed flow (bbl/day)</strong></td>
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<td>5697.30</td>
</tr>
<tr>
<td><strong>C5 feed flow (bbl/day)</strong></td>
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<td>4001.39</td>
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<td><strong>C2 reboiler temperature (°F)</strong></td>
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<td>583.88</td>
</tr>
<tr>
<td><strong>HV-ISO 10% TBP temperature (°F)</strong></td>
<td>231.23</td>
<td>234.67</td>
</tr>
<tr>
<td><strong>HV-ISO 90% TBP temperature (°F)</strong></td>
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<td>394.86</td>
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<tr>
<td><strong>LT-DIST 10% TBP temperature (°F)</strong></td>
<td>354.17</td>
<td>357.47</td>
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<tr>
<td><strong>LT-DIST 90% TBP temperature (°F)</strong></td>
<td>354.64</td>
<td>553.74</td>
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### Economic Optimization Inequality Constraints:

<table>
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<tr>
<th></th>
<th>Summer</th>
<th>Prices</th>
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<tbody>
<tr>
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<td>6356.84</td>
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<td>12448.03</td>
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<tr>
<td><strong>C5 feed flow (bbl/day)</strong></td>
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</tr>
<tr>
<td><strong>C1 tray 3 temperature (°F)</strong></td>
<td>181.75</td>
<td>177.59</td>
</tr>
<tr>
<td><strong>C1 reboiler temperature (°F)</strong></td>
<td>588.60</td>
<td>583.88</td>
</tr>
<tr>
<td><strong>C2 tray 2 temperature (°F)</strong></td>
<td>190.85</td>
<td>192.95</td>
</tr>
<tr>
<td><strong>C2 reboiler temperature (°F)</strong></td>
<td>692.96</td>
<td>695.99</td>
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<tr>
<td><strong>DIST-C4 C₅ mole fraction</strong></td>
<td>0.11016</td>
<td>0.08957</td>
</tr>
<tr>
<td><strong>LT-ISO Reid vapour pressure (psi)</strong></td>
<td>9.329</td>
<td>9.763</td>
</tr>
<tr>
<td><strong>LT-ISO bubble point temperature (°F)</strong></td>
<td>141.43</td>
<td>138.87</td>
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<tr>
<td><strong>HV-ISO 10% TBP temperature (°F)</strong></td>
<td>231.23</td>
<td>234.67</td>
</tr>
<tr>
<td><strong>HV-ISO 90% TBP temperature (°F)</strong></td>
<td>390.43</td>
<td>394.86</td>
</tr>
<tr>
<td><strong>LT-DIST 10% TBP temperature (°F)</strong></td>
<td>354.17</td>
<td>357.47</td>
</tr>
<tr>
<td><strong>LT-DIST 90% TBP temperature (°F)</strong></td>
<td>554.64ᵃ</td>
<td>553.74ᵃ</td>
</tr>
</tbody>
</table>

*ᵃconstraint upper bound active

continued on the next page...
... Table A.11 continued from the previous page

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<td><strong>Product Standard Volume Flows After Economic Optimization:</strong></td>
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<tr>
<td>Vapour Product (bbl/day)</td>
<td>779.36</td>
<td>720.09</td>
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<tr>
<td>C₄-Distillate Product (bbl/day)</td>
<td>1190.79</td>
<td>1196.45</td>
<td></td>
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<tr>
<td>Light Iso Product (bbl/day)</td>
<td>2503.26</td>
<td>2632.64</td>
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<tr>
<td>Heavy Iso Product (bbl/day)</td>
<td>3851.53</td>
<td>3919.91</td>
<td></td>
</tr>
<tr>
<td>Light Distillate Product (bbl/day)</td>
<td>3427.78</td>
<td>3325.40</td>
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<tr>
<td>Splitter Bottoms Product (bbl/day)</td>
<td>10161.71</td>
<td>10133.13</td>
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<tr>
<td><strong>Reboiler Heat Duties After Economic Optimization:</strong></td>
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<td></td>
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<tr>
<td>Stabilizer (C1) Reboiler (MMBTU/hr)</td>
<td>22.3948</td>
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<tr>
<td>Splitter (C2) Reboiler (MMBTU/hr)</td>
<td>21.9934</td>
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<td><strong>Economic Optimization Marginal Stream Values:</strong></td>
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<tr>
<td>Light Iso Marginal Stream Value ($/m³)</td>
<td>188.57</td>
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Table A.12: ASPEN PLUS real time optimizer run with external condenser disturbances.

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<td><strong>Economic Optimization:</strong></td>
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<td></td>
</tr>
<tr>
<td>Profit ($/hr)</td>
<td>-9.84</td>
<td>204.71</td>
<td>136.48</td>
<td>103.64</td>
</tr>
<tr>
<td>Optimization iterations</td>
<td>10</td>
<td>7</td>
<td>14</td>
<td>6</td>
</tr>
<tr>
<td>Total product values ($/hr)</td>
<td>23035.02</td>
<td>23124.08</td>
<td>23027.42</td>
<td>22988.36</td>
</tr>
<tr>
<td>Total feed cost ($/hr)</td>
<td>22928.41</td>
<td>22796.18</td>
<td>22762.67</td>
<td>22751.29</td>
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<tr>
<td>Total utility costs ($/hr)</td>
<td>116.45</td>
<td>123.19</td>
<td>128.27</td>
<td>133.43</td>
</tr>
<tr>
<td><strong>Economic Optimization Set Points:</strong></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C1 reflux flow (bbl/day)</td>
<td>6913.71</td>
<td>7574.51</td>
<td>8090.61</td>
<td>8673.31</td>
</tr>
<tr>
<td>C1 tray 3 temperature (°F)</td>
<td>181.26</td>
<td>173.04</td>
<td>174.54</td>
<td>173.11</td>
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<tr>
<td>DIST-C4 C5 mole fraction</td>
<td>0.11882</td>
<td>0.06681</td>
<td>0.07033</td>
<td>0.06068</td>
</tr>
<tr>
<td>C1 reboiler temperature (°F)</td>
<td>595.10</td>
<td>601.80</td>
<td>612.81</td>
<td>617.63</td>
</tr>
<tr>
<td>C2 reflux flow (bbl/day)</td>
<td>13951.69</td>
<td>13967.29</td>
<td>13622.78</td>
<td>13407.55</td>
</tr>
<tr>
<td>C4 feed flow (bbl/day)</td>
<td>5998.29</td>
<td>6447.35</td>
<td>6345.58</td>
<td>6072.69</td>
</tr>
<tr>
<td>C5 feed flow (bbl/day)</td>
<td>3334.48</td>
<td>3483.00</td>
<td>3236.97</td>
<td>3010.71</td>
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<tr>
<td>C2 reboiler temperature (°F)</td>
<td>595.10</td>
<td>601.80</td>
<td>612.81</td>
<td>617.63</td>
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<tr>
<td>HV-ISO 10% TBP temperature (°F)</td>
<td>197.38</td>
<td>198.46</td>
<td>197.74</td>
<td>193.32</td>
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<tr>
<td>HV-ISO 90% TBP temperature (°F)</td>
<td>351.62</td>
<td>368.63</td>
<td>367.62</td>
<td>365.04</td>
</tr>
<tr>
<td>LT-DIST 10% TBP temperature (°F)</td>
<td>338.26</td>
<td>355.20</td>
<td>359.43</td>
<td>357.30</td>
</tr>
<tr>
<td>LT-DIST 90% TBP temperature (°F)</td>
<td>496.25</td>
<td>554.11</td>
<td>554.10</td>
<td>552.19</td>
</tr>
</tbody>
</table>

**Economic Optimization Inequality Constraints:**

| C1 reflux flow (bbl/day) | 6913.71 | 7574.51 | 8090.61 | 8673.31 |
| C2 reflux flow (bbl/day) | 13951.69 | 13967.29 | 13622.78 | 13407.55 |
| C4 feed flow (bbl/day) | 5998.29 | 6447.35 | 6345.58 | 6072.69 |
| C5 feed flow (bbl/day) | 3334.48 | 3483.00 | 3236.97 | 3010.71 |
| C1 tray 3 temperature (°F) | 181.26 | 173.04 | 174.54 | 173.11 |
| C1 reboiler temperature (°F) | 595.10 | 601.80 | 612.81 | 617.63 |
| C2 tray 2 temperature (°F) | 153.02 | 153.83 | 154.55 | 151.63 |
| C2 reboiler temperature (°F) | 651.22 | 663.09 | 645.76 | 634.25 |
| DIST-C4 C5 mole fraction | 0.11882 | 0.06681 | 0.07033 | 0.06068 |
| LT-ISO Reid vapour pressure (psi) | 14.000* | 12.436 | 11.659 | 11.988 |
| LT-ISO bubble point temperature (°F) | 115.05 | 121.22 | 124.63 | 122.72 |
| HV-ISO 10% TBP temperature (°F) | 197.38 | 198.46 | 197.74 | 193.32 |
| HV-ISO 90% TBP temperature (°F) | 351.62 | 368.63 | 367.62 | 365.04 |
| LT-DIST 10% TBP temperature (°F) | 338.26 | 355.20 | 359.43 | 357.30 |
| LT-DIST 90% TBP temperature (°F) | 496.25 | 554.11* | 554.10* | 552.19 |

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<table>
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<tr>
<th>Cycle</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
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</thead>
<tbody>
<tr>
<td><strong>Product Standard Volume Flows After Economic Optimization:</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Vapour Product (bbl/day)</td>
<td>1024.90</td>
<td>1001.83</td>
<td>1010.12</td>
<td>993.86</td>
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<tr>
<td>C₄-Distillate Product (bbl/day)</td>
<td>902.05</td>
<td>900.70</td>
<td>921.20</td>
<td>926.90</td>
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<tr>
<td>Light Iso Product (bbl/day)</td>
<td>1559.61</td>
<td>1565.83</td>
<td>1517.12</td>
<td>1446.06</td>
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<tr>
<td>Heavy Iso Product (bbl/day)</td>
<td>4202.01</td>
<td>4627.11</td>
<td>4608.50</td>
<td>4587.07</td>
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<td>Light Distillate Product (bbl/day)</td>
<td>1952.44</td>
<td>2474.43</td>
<td>2167.61</td>
<td>2031.50</td>
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<tr>
<td>Splitter Bottoms Product (bbl/day)</td>
<td>12218.00</td>
<td>11161.76</td>
<td>11476.82</td>
<td>11704.48</td>
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<tr>
<td><strong>Reboiler Heat Duties After Economic Optimization:</strong></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Stabilizer (C1) Reboiler (MMBTU/hr)</td>
<td>21.2420</td>
<td>23.3510</td>
<td>26.7621</td>
<td>29.2489</td>
</tr>
<tr>
<td>Splitter (C2) Reboiler (MMBTU/hr)</td>
<td>18.0814</td>
<td>18.2495</td>
<td>16.8149</td>
<td>15.8111</td>
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<tr>
<td><strong>Economic Optimization Marginal Stream Values:</strong></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Light Iso Marginal Stream Value ($/m³)</td>
<td>182.78</td>
<td>184.72</td>
<td>185.68</td>
<td>185.27</td>
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<tr>
<td><strong>Data Reconciliation:</strong></td>
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<td>Final objective function value</td>
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<td>17.926</td>
<td>13.634</td>
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<td>11</td>
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Table A.13: ASPEN PLUS real time optimizer run with external condenser disturbances and no measurement noise.

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<tbody>
<tr>
<td><strong>Economic Optimization:</strong></td>
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</tr>
<tr>
<td>Profit ($/hr)</td>
<td>-9.84</td>
<td>141.59</td>
<td>116.81</td>
</tr>
<tr>
<td>Optimization iterations</td>
<td>10</td>
<td>16</td>
<td>7</td>
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<tr>
<td>Total product values ($/hr)</td>
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<td>23160.33</td>
<td>23114.22</td>
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<td>Total feed cost ($/hr)</td>
<td>22928.41</td>
<td>22905.32</td>
<td>22881.38</td>
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<tr>
<td>Total utility costs ($/hr)</td>
<td>116.45</td>
<td>113.42</td>
<td>116.02</td>
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| **Economic Optimization Set Points:** |              |              |              |
| C1 reflux flow (bbl/day) | 6913.71 | 6727.41 | 6834.17 |
| C1 tray 3 temperature (°F) | 181.26 | 184.02 | 185.89 |
| DIST-C4 C5 mole fraction | 0.11882 | 0.13807 | 0.13206 |
| C1 reboiler temperature (°F) | 595.10 | 596.31 | 596.90 |
| C2 reflux flow (bbl/day) | 13951.69 | 13807.65 | 13747.68 |
| C4 feed flow (bbl/day) | 5998.29 | 6337.05 | 6495.17 |
| C5 feed flow (bbl/day) | 3334.48 | 3623.67 | 3457.30 |
| C2 reboiler temperature (°F) | 595.10 | 596.31 | 596.90 |
| HV-ISO 10% TBP temperature (°F) | 197.38 | 193.81 | 200.13 |
| HV-ISO 90% TBP temperature (°F) | 351.62 | 361.98 | 372.89 |
| LT-DIST 10% TBP temperature (°F) | 338.26 | 353.10 | 366.03 |
| LT-DIST 90% TBP temperature (°F) | 496.25 | 553.68 | 356.51 |

| **Economic Optimization Inequality Constraints:** |              |              |              |
| C1 reflux flow (bbl/day) | 6913.71 | 6727.41 | 6834.17 |
| C2 reflux flow (bbl/day) | 13951.69 | 13807.65 | 13747.68 |
| C4 feed flow (bbl/day) | 5998.29 | 6337.05 | 6495.17 |
| C5 feed flow (bbl/day) | 3334.48 | 3623.67 | 3457.30 |
| C1 tray 3 temperature (°F) | 181.26 | 184.02 | 185.89 |
| C1 reboiler temperature (°F) | 595.10 | 596.31 | 596.90 |
| C2 tray 2 temperature (°F) | 153.02 | 155.38 | 157.21 |
| C2 reboiler temperature (°F) | 651.22 | 657.44 | 661.89 |
| DIST-C4 C5 mole fraction | 0.11882 | 0.13807 | 0.15206a |
| LT-ISO Reid vapour pressure (psi) | 14.000a | 13.990a | 14.028a |
| LT-ISO bubble point temperature (°F) | 115.05 | 115.42 | 115.42 |
| HV-ISO 10% TBP temperature (°F) | 197.38 | 193.81 | 200.13 |
| HV-ISO 90% TBP temperature (°F) | 351.62 | 361.98 | 372.89 |
| LT-DIST 10% TBP temperature (°F) | 338.26 | 353.10 | 366.03 |
| LT-DIST 90% TBP temperature (°F) | 496.25 | 553.58a | 556.51a |

*constraint upper bound active

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... Table A.13 continued from the previous page

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<td><strong>Product Standard Volume Flows After Economic Optimization:</strong></td>
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<tr>
<td>Vapour Product (bbl/day)</td>
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<td>984.36</td>
<td>1057.79</td>
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<tr>
<td>C₄-Distillate Product (bbl/day)</td>
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<td>957.58</td>
<td>879.47</td>
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<td>Light Iso Product (bbl/day)</td>
<td>1559.61</td>
<td>1615.82</td>
<td>1677.26</td>
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<tr>
<td>Heavy Iso Product (bbl/day)</td>
<td>4202.01</td>
<td>4420.61</td>
<td>4653.28</td>
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<td>Light Distillate Product (bbl/day)</td>
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<td>2136.40</td>
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<tr>
<td>Splitter Bottoms Product (bbl/day)</td>
<td>12218.00</td>
<td>11453.92</td>
<td>11410.01</td>
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<td><strong>Reboiler Heat Duties After Economic Optimization:</strong></td>
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<tr>
<td>Stabilizer (C1) Reboiler (MMBTU/hr)</td>
<td>21.2420</td>
<td>20.5632</td>
<td>19.8622</td>
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<td>Splitter (C2) Reboiler (MMBTU/hr)</td>
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<td>19.3180</td>
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<td><strong>Economic Optimization Marginal Stream Values:</strong></td>
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<tr>
<td>Light Iso Marginal Stream Value ($/m³)</td>
<td>182.78</td>
<td>182.79</td>
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<td><strong>Economic Optimization:</strong></td>
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<tr>
<td>Profit ($/hr)</td>
<td>162.95</td>
<td>175.54</td>
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<tr>
<td>Optimization iterations</td>
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<tr>
<td>Total product values ($/hr)</td>
<td>23179.09</td>
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</tr>
<tr>
<td>Total feed cost ($/hr)</td>
<td>22897.08</td>
<td>22881.78</td>
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<tr>
<td>Total utility costs ($/hr)</td>
<td>119.07</td>
<td>121.34</td>
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</tbody>
</table>

| **Economic Optimization Set Points:** | | |
| C1 reflux flow (bbl/day) | 6740.53 | 6841.06 |
| C1 tray 3 temperature (°F) | 185.62 | 186.50 |
| DIST-C4 C₅ mole fraction | 0.14996 | 0.15707 |
| C1 reboiler temperature (°F) | 594.04 | 593.93 |
| C2 reflux flow (bbl/day) | 13681.67 | 13543.65 |
| C4 feed flow (bbl/day) | 6809.83 | 7009.66 |
| C5 feed flow (bbl/day) | 3304.65 | 3190.03 |
| C2 reboiler temperature (°F) | 594.04 | 593.93 |
| HV-ISO 10% TBP temperature (°F) | 206.14 | 211.14 |
| HV-ISO 90% TBP temperature (°F) | 383.63 | 394.26 |
| LT-DIST 10% TBP temperature (°F) | 375.07 | 391.09 |
| LT-DIST 90% TBP temperature (°F) | 551.84 | 569.22 |

| **Economic Optimization Inequality Constraints:** | | |
| C1 reflux flow (bbl/day) | 6740.53 | 6841.06 |
| C2 reflux flow (bbl/day) | 13681.67 | 13543.65 |
| C4 feed flow (bbl/day) | 6809.83 | 7009.66 |
| C5 feed flow (bbl/day) | 3304.65 | 3190.03 |
| C1 tray 3 temperature (°F) | 185.62 | 186.50 |
| C1 reboiler temperature (°F) | 594.04 | 593.93 |
| C2 tray 2 temperature (°F) | 158.79 | 161.65 |
| C2 reboiler temperature (°F) | 664.63 | 668.60 |
| DIST-C4 C₅ mole fraction | 0.14996* | 0.15707* |
| LT-ISO Reid vapour pressure (psi) | 14.002* | 14.070* |
| LT-ISO bubble point temperature (°F) | 115.64 | 115.44 |
| HV-ISO 10% TBP temperature (°F) | 206.14 | 211.14 |
| HV-ISO 90% TBP temperature (°F) | 383.63 | 394.26 |
| LT-DIST 10% TBP temperature (°F) | 375.07 | 391.09 |
| LT-DIST 90% TBP temperature (°F) | 551.84 | 569.22* |

*constraint upper bound active

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Table A.13 continued from the previous page

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<th>Cycle</th>
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<tbody>
<tr>
<td><strong>Product Standard Volume Flows After Economic Optimization:</strong></td>
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<td></td>
</tr>
<tr>
<td>Vapour Product (bbl/day)</td>
<td>1009.87</td>
<td>1073.29</td>
</tr>
<tr>
<td>C₄-Distillate Product (bbl/day)</td>
<td>921.15</td>
<td>842.52</td>
</tr>
<tr>
<td>Light Iso Product (bbl/day)</td>
<td>1745.48</td>
<td>1819.39</td>
</tr>
<tr>
<td>Heavy Iso Product (bbl/day)</td>
<td>4857.12</td>
<td>5145.37</td>
</tr>
<tr>
<td>Light Distillate Product (bbl/day)</td>
<td>1832.52</td>
<td>1646.03</td>
</tr>
<tr>
<td>Splitter Bottoms Product (bbl/day)</td>
<td>11463.31</td>
<td>11287.83</td>
</tr>
<tr>
<td><strong>Reboiler Heat Duties After Economic Optimization:</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Stabilizer (C1) Reboiler (MMBTU/hr)</td>
<td>19.5769</td>
<td>18.9294</td>
</tr>
<tr>
<td>Splitter (C2) Reboiler (MMBTU/hr)</td>
<td>20.6308</td>
<td>22.0462</td>
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<td><strong>Economic Optimization Marginal Stream Values:</strong></td>
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<tr>
<td>Light Iso Marginal Stream Value ($/m³)</td>
<td>182.77</td>
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Table A.14: Base Case ASPEN PLUS v9.3 real time optimizer run.

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<tr>
<td>Economic Optimization:</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Profit ($/hr)</td>
<td>67.76</td>
<td>241.23</td>
<td>290.75</td>
</tr>
<tr>
<td>Optimization iterations</td>
<td>10</td>
<td>6</td>
<td>12</td>
</tr>
<tr>
<td>Total product values ($/hr)</td>
<td>23195.72</td>
<td>23329.65</td>
<td>23548.59</td>
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<tr>
<td>Total feed cost ($/hr)</td>
<td>23009.43</td>
<td>22970.32</td>
<td>23130.55</td>
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<tr>
<td>Total utility costs ($/hr)</td>
<td>118.52</td>
<td>118.10</td>
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<td>Economic Optimization Set Points:</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>C1 reflux flow (bbl/day)</td>
<td>7012.50</td>
<td>7617.61</td>
<td>8240.18</td>
</tr>
<tr>
<td>C1 tray 3 temperature (°F)</td>
<td>172.15</td>
<td>161.30</td>
<td>157.52</td>
</tr>
<tr>
<td>DIST-C4 C₅ mole fraction</td>
<td>0.06529</td>
<td>0.01995</td>
<td>0.00589</td>
</tr>
<tr>
<td>C1 reboiler temperature (°F)</td>
<td>587.70</td>
<td>594.12</td>
<td>601.79</td>
</tr>
<tr>
<td>C2 reflux flow (bbl/day)</td>
<td>14209.57</td>
<td>14331.62</td>
<td>14627.33</td>
</tr>
<tr>
<td>C4 feed flow (bbl/day)</td>
<td>6206.91</td>
<td>6617.66</td>
<td>6837.97</td>
</tr>
<tr>
<td>C5 feed flow (bbl/day)</td>
<td>3352.91</td>
<td>3476.24</td>
<td>3388.27</td>
</tr>
<tr>
<td>C2 reboiler temperature (°F)</td>
<td>587.70</td>
<td>594.12</td>
<td>601.79</td>
</tr>
<tr>
<td>HV-ISO 10% TBP temperature (°F)</td>
<td>196.98</td>
<td>192.59</td>
<td>190.67</td>
</tr>
<tr>
<td>HV-ISO 90% TBP temperature (°F)</td>
<td>351.81</td>
<td>363.53</td>
<td>370.16</td>
</tr>
<tr>
<td>LT-DIST 10% TBP temperature (°F)</td>
<td>336.20</td>
<td>350.82</td>
<td>356.32</td>
</tr>
<tr>
<td>LT-DIST 90% TBP temperature (°F)</td>
<td>500.44</td>
<td>553.99</td>
<td>553.97</td>
</tr>
<tr>
<td>Economic Optimization Inequality Constraints:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C1 reflux flow (bbl/day)</td>
<td>7012.50</td>
<td>7617.61</td>
<td>8240.18</td>
</tr>
<tr>
<td>C2 reflux flow (bbl/day)</td>
<td>14209.57</td>
<td>14331.62</td>
<td>14627.33</td>
</tr>
<tr>
<td>C4 feed flow (bbl/day)</td>
<td>6206.91</td>
<td>6617.66</td>
<td>6837.97</td>
</tr>
<tr>
<td>C5 feed flow (bbl/day)</td>
<td>3352.91</td>
<td>3476.24</td>
<td>3388.27</td>
</tr>
<tr>
<td>C1 tray 3 temperature (°F)</td>
<td>172.15</td>
<td>161.30</td>
<td>157.52</td>
</tr>
<tr>
<td>C1 reboiler temperature (°F)</td>
<td>587.70</td>
<td>594.12</td>
<td>601.79</td>
</tr>
<tr>
<td>C2 tray 2 temperature (°F)</td>
<td>151.84</td>
<td>149.13</td>
<td>147.14</td>
</tr>
<tr>
<td>C2 reboiler temperature (°F)</td>
<td>652.65</td>
<td>651.44</td>
<td>653.76</td>
</tr>
<tr>
<td>DIST-C4 C₅ mole fraction</td>
<td>0.06529</td>
<td>0.01995</td>
<td>0.00589&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>LT-ISO Reid vapour pressure (psi)</td>
<td>14.00&lt;sup&gt;b&lt;/sup&gt;</td>
<td>12.977</td>
<td>12.869</td>
</tr>
<tr>
<td>LT-ISO bubble point temperature (°F)</td>
<td>116.54</td>
<td>120.83</td>
<td>121.25</td>
</tr>
<tr>
<td>HV-ISO 10% TBP temperature (°F)</td>
<td>196.98</td>
<td>192.59</td>
<td>190.67</td>
</tr>
<tr>
<td>HV-ISO 90% TBP temperature (°F)</td>
<td>351.81</td>
<td>363.53</td>
<td>370.16</td>
</tr>
<tr>
<td>LT-DIST 10% TBP temperature (°F)</td>
<td>336.20</td>
<td>350.82</td>
<td>356.32</td>
</tr>
<tr>
<td>LT-DIST 90% TBP temperature (°F)</td>
<td>500.44</td>
<td>553.99&lt;sup&gt;b&lt;/sup&gt;</td>
<td>553.97&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
</tbody>
</table>

<sup>a</sup>constraint lower bound active
<sup>b</sup>constraint upper bound active
... Table A.14 continued from the previous page

<table>
<thead>
<tr>
<th>Cycle</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Product Standard Volume Flows After Economic Optimization:</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Vapour Product (bbl/day)</td>
<td>992.10</td>
<td>969.83</td>
<td>954.94</td>
</tr>
<tr>
<td>C₄-Distillate Product (bbl/day)</td>
<td>876.51</td>
<td>894.98</td>
<td>919.96</td>
</tr>
<tr>
<td>Light Iso Product (bbl/day)</td>
<td>1623.72</td>
<td>1521.54</td>
<td>1481.84</td>
</tr>
<tr>
<td>Heavy Iso Product (bbl/day)</td>
<td>4201.09</td>
<td>4599.76</td>
<td>4864.68</td>
</tr>
<tr>
<td>Light Distillate Product (bbl/day)</td>
<td>2124.86</td>
<td>2576.41</td>
<td>2548.58</td>
</tr>
<tr>
<td>Splitter Bottoms Product (bbl/day)</td>
<td>12117.93</td>
<td>11336.73</td>
<td>11281.92</td>
</tr>
<tr>
<td><strong>Reboiler Heat Duties After Economic Optimization:</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Stabilizer (C1) Reboiler (MMBTU/hr)</td>
<td>21.7576</td>
<td>24.4127</td>
<td>27.2240</td>
</tr>
<tr>
<td>Splitter (C2) Reboiler (MMBTU/hr)</td>
<td>18.2673</td>
<td>15.4697</td>
<td>15.7629</td>
</tr>
<tr>
<td><strong>Economic Optimization Marginal Stream Values:</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Light Iso Marginal Stream Value ($/m³)</td>
<td>182.78</td>
<td>184.05</td>
<td>184.18</td>
</tr>
<tr>
<td><strong>Data Reconciliation:</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Final objective function value</td>
<td>47.154</td>
<td>11.281</td>
<td>13.312</td>
</tr>
<tr>
<td>Initial objective function value</td>
<td>257.281</td>
<td>31.389</td>
<td>31.392</td>
</tr>
<tr>
<td>Data reconciliation iterations</td>
<td>16</td>
<td>19</td>
<td>12</td>
</tr>
</tbody>
</table>
NOTE TO USERS

Page(s) missing in number only; text follows. Microfilmed as received.

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UMI
Appendix B

ASPN PLUS Real Time Optimizer Documentation

B.1 Purpose

This program performs a given number of cycles of a real time optimizer on the stabilizer-splitter flowsheet given in Figure B.1 using ASPEN PLUS to perform the data reconciliation and optimization.

B.2 Specification

To setup the real time optimizer for a run, use the command:

setup

or

nohup setup &

This command must be given before running the real time optimizer, and the files listed in Table B.1 must already exist on the paths specified.

To run the real time optimizer for a given number of cycles, \( n \), use the command:
Figure B.1: Stabilizer-splitter process flowsheet (including measurement tag numbers).
run n

or

nohup run n &

The real time optimizer must already have been either setup or run prior to using this command.

B.3 Description

The ASPEN PLUS real time optimizer performs data reconciliation and optimization on the stabilizer-splitter flowsheet given in Figure B.1. Detailed information about this optimizer is covered by Naysmith [1].

Before running the real time optimizer, the program setup must be run first. This program translates and compiles the ASPEN PLUS simulations, and compiles the FORTRAN77 routines used. The files listed in Table B.1 must exist on the paths specified, and the NAG FORTRAN Library Routines must be available. The program setup only needs to be run once.

The program run runs a specified number of cycles (or iterations) of the real time optimizer. The steps used by this program are summarised in Figure B.2.

The data reconciliation uses a weighted least squares objective function to reconcile 28 measured variables (all variables shown in Figure B.1 except T11):

\[
\min_x \left[ \sum_{i=1}^{28} w_i \left( \frac{y_i - x_i}{s_i} \right)^2 \right] \tag{B.1}
\]

subject to \( h(x) = 0 \)

where

\( w = \) weighting factor associated with each measured variable;

\( y = \) the measured variable;

\( x = \) the estimated true (reconciled) variable value;

\( s = \) the standard deviation of the measurements;
Figure B.2: ASPEN PLUS real time optimization program flow chart.
\[ h(x) = \text{the set of equality constraints representing the process model.} \]

The optimization algorithm used is the built in ASPEN PLUS SQP algorithm. This objective function is minimized by varying 15 free variables.

The economic optimization maximizes profit using the following objective function:

\[
\max \left[ \sum (\text{product values}) - (\text{feed cost}) - (\text{reboiler fuel oil cost}) \right]
\]

subject to \( h(x) = 0 \)

\[ g(x) \geq 0 \quad (B.2) \]

where \( h(x) = \text{the set of equality constraints representing the process model:} \)

\[ g(x) = \text{product quality and operating inequality constraints.} \]

The optimization algorithm used is the built in ASPEN PLUS SQP algorithm. The objective function is maximized by varying 13 free variables subject to 25 inequality constraints and 2 equality constraints on condenser heat duties.

Normally distributed random noise is added to the plant data calculated in the plant simulation before being returned to the real time optimizer for the next iteration. The noise has a mean of zero, and a given standard deviation for each of the 28 measured variables.

### B.4 References


### B.5 Files

The files required to run ASPEN PLUS real time optimizer are listed in Table B.1.
<table>
<thead>
<tr>
<th>File</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>run</td>
<td>Runs the real time optimizer (C-shell script, executable)</td>
</tr>
<tr>
<td>setup</td>
<td>Sets up the real time optimizer prior to being run (C-shell script, executable)</td>
</tr>
<tr>
<td>plant/plant6.inp</td>
<td>&quot;Plant&quot; simulation (ASPE-PLUS input file)</td>
</tr>
<tr>
<td>plant/randata.f</td>
<td>Adds normally distributed random noise to the measured plant data (FORTRAN77 input file, requires the NAG FORTRAN Library Routines)</td>
</tr>
<tr>
<td>plant/RV-RNC.DAT</td>
<td>Contains the random noise standard deviations for the measured plant data</td>
</tr>
<tr>
<td>rto/ICN-NSTR.DAT</td>
<td>Contains the optimization inequality constraint upper and lower bounds</td>
</tr>
<tr>
<td>rto/IDF-FREE.DAT</td>
<td>Contains the data reconciliation free variable bound ranges</td>
</tr>
<tr>
<td>rto/IME-AS.DAT</td>
<td>Contains the measured variable data from the plant (with noise added)</td>
</tr>
<tr>
<td>rto/IOBJ-F\N.DAT</td>
<td>Contains the optimization objective function parameters</td>
</tr>
<tr>
<td>rto/IOF-FREE.DAT</td>
<td>Contains the optimization free variable bound ranges</td>
</tr>
<tr>
<td>rto/ISM-ST.DAT</td>
<td>Contains the initial simulation settings and parameters for starting the ASPE-PLUS real time optimization simulation</td>
</tr>
<tr>
<td>rto/IV-RNC.DAT</td>
<td>Contains the measured variable standard deviations for the data reconciliation</td>
</tr>
<tr>
<td>rto/IWG-HT.DAT</td>
<td>Contains the measured variable weights for the data reconciliation</td>
</tr>
<tr>
<td>rto/rto-6.inp</td>
<td>Data reconciliation and optimization simulation (ASPE-PLUS input file)</td>
</tr>
</tbody>
</table>
B.6 Input File Specifications

All input files are formatted in the same way using the following FORTRAN format statement:

```
FORMAT(A13, 2X, E15.8)
```

The first 13 columns of each line contain a descriptive label. The next 2 columns are blank and the last 15 columns contain the corresponding numerical value. Example input files are given in section B.8.

B.6.1 IMEAS.DAT, IVARNC.DAT and IWGHT.DAT

IMEAS.DAT, IVARNC.DAT and IWGHT.DAT contain the measured values, standard deviations and weights for data reconciliation corresponding to the 28 measured plant variables respectively. The 28 variables are given in the same order as presented in Table B.2 for all three files. The units given are for the measured variables and standard deviations. The variable names are the same as those used in Figure B.1.

B.6.2 IDFREE.DAT

IDFREE.DAT contains the free variable ranges for data reconciliation. The upper and lower are free variable bounds are calculated using the following formulae:

\[
\begin{align*}
    x_{UB} &= x^{(0)} + r \\
    x_{LB} &= x^{(0)} - r
\end{align*}
\]  

(B.3)

where \( x_{UB} \) = free variable upper bound;
\( x_{UB} \) = free variable lower bound;
\( x^{(0)} \) = initial free variable value;
\( r \) = free variable range as specified in IDFREE.DAT.

The free variable range specifications are given in the order shown in Table B.3.
<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>F01</td>
<td>STAB stream standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F11</td>
<td>VAP stream standard vapour volume flow</td>
<td>cuft/hr</td>
</tr>
<tr>
<td>F12</td>
<td>C1 reflux standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F13</td>
<td>DIST-C4 stream standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F21</td>
<td>C1 reboiler standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F22</td>
<td>E1 outlet standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F31</td>
<td>LT-ISO stream standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F32</td>
<td>C2 reflux standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F41</td>
<td>C4 feed standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F42</td>
<td>HV-ISO stream standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F51</td>
<td>C5 feed standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F52</td>
<td>LT-DIST stream standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F61</td>
<td>C2 reboiler standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F62</td>
<td>SSFEED stream standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>T01</td>
<td>STAB stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T12</td>
<td>C1 tray 2 temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T13</td>
<td>C1 condenser temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T21</td>
<td>C1 bottoms stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T22</td>
<td>C1 reboiler outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T23</td>
<td>E1 outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T31</td>
<td>C2 tray 2 temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T32</td>
<td>LT-ISO stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T41</td>
<td>C4 feed stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T42</td>
<td>HV-ISO stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T51</td>
<td>C5 feed stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T52</td>
<td>LT-DIST stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T61</td>
<td>C2 bottoms stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T62</td>
<td>C2 reboiler outlet temperature</td>
<td>°F</td>
</tr>
</tbody>
</table>
Table B.3: Data reconciliation free variable ranges used in the ASPEN PLUS real time optimizer input file IDFREE.DAT.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>STAB-MOLEFLOW</td>
<td>STAB stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>STAB-TEMP</td>
<td>STAB stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C1-RR</td>
<td>C1 molar reflux ratio</td>
<td>lbmol/lbmol</td>
</tr>
<tr>
<td>C1-RDV</td>
<td>C1 condenser molar vapour fraction</td>
<td>lbmol/lbmol</td>
</tr>
<tr>
<td>C1-REBL-FLOW</td>
<td>C1 reboiler mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C1-REBL-TEMP</td>
<td>C1 reboiler outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>E1-TEMP</td>
<td>E1 outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C2-MOLE-D</td>
<td>C2 liquid distillate mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2-REBL-FLOW</td>
<td>C2 reboiler mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2-REBL-TEMP</td>
<td>C2 reboiler outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C2-SC-TEMP</td>
<td>C2 condenser sub-cooled temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C4-QN</td>
<td>C4 reboiler heat duty</td>
<td>MMBTU/hr</td>
</tr>
<tr>
<td>C5-QN</td>
<td>C5 reboiler heat duty</td>
<td>MMBTU/hr</td>
</tr>
<tr>
<td>C2-C4-FLOW</td>
<td>C4 feed stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2-C5-FLOW</td>
<td>C5 feed stream mole flow</td>
<td>lbmol/hr</td>
</tr>
</tbody>
</table>
B.6.3 ISMST.DAT

The file ISMST.DAT contains all the simulation settings to initialize the ASPEN PLUS real time optimization simulation. Table B.4 summarises the variable in this file. Variables which are vectors, such as compositions and temperature profiles, use n lines in the input file as specified in Table B.4.

B.6.4 IOBJFN.DAT

IOBJFN.DAT contains the parameters used in calculating the economic objective function. Table B.5 summarises the order in which these parameters must appear in the file IOBJFN.DAT.

B.6.5 ICNSTR.DAT

ICNSTR.DAT contains the upper and lower bounds for all the inequality constraints in the optimization. Table B.6 summarises the order in which these bounds must appear in the file ICNSTR.DAT.

B.6.6 IOFREE.DAT

IOFREE.DAT contains the free variable ranges for optimization. The upper and lower are free variable bounds are calculated using the following formulae for all free variables except temperatures:

\[ x_{UB} = x^{(0)} + qx^{(0)} \]
\[ x_{LB} = x^{(0)} - qx^{(0)} \]  \hspace{1cm} (B.4)

where \( q \) = free variable range as a fraction of the initial variable value.

Temperature free variable bounds are calculated using the formulae given in equation (B.3). The free variable range specifications are given in the order shown in Table B.7. Free variable bounds calculated using equation (B.4) have the character ‘%’ at the end of their variable name.
Table B.4: Simulation settings used in the ASPEN PLUS real time optimizer input file ISMST.DAT.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>STAB MOLEFLOW</td>
<td>STAB stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>STAB TEMP</td>
<td>STAB stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>STAB PRESS</td>
<td>STAB stream pressure</td>
<td>psia</td>
</tr>
<tr>
<td>STAB Z n</td>
<td>STAB stream composition ($n = 1 \ldots 23$)</td>
<td>lbmol/lbmol</td>
</tr>
<tr>
<td>C2REBL FLOW</td>
<td>C2 reboiler outlet mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2REBL TEMP</td>
<td>C2 reboiler outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C2REBL PRESS</td>
<td>C2 reboiler outlet pressure</td>
<td>psia</td>
</tr>
<tr>
<td>C2REBL Z n</td>
<td>C2 reboiler outlet composition</td>
<td>lbmol/lbmol</td>
</tr>
<tr>
<td></td>
<td>($n = 1 \ldots 23$)</td>
<td></td>
</tr>
<tr>
<td>E1 TEMP</td>
<td>E1 outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>E1 PRESS</td>
<td>E1 outlet pressure</td>
<td>psia</td>
</tr>
<tr>
<td>C1 RFLX RATIO</td>
<td>C1 molar reflux ratio</td>
<td>lbmol/lbmol</td>
</tr>
<tr>
<td>C1 VAP/DIST</td>
<td>C1 condenser molar vapour fraction</td>
<td>lbmol/lbmol</td>
</tr>
<tr>
<td>C1 REBL FLOW</td>
<td>C1 reboiler outlet mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C1 REBL TEMP</td>
<td>C1 reboiler outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C1 COL P DROP</td>
<td>C1 column pressure drop</td>
<td>psi</td>
</tr>
<tr>
<td>C1 TOP TRAY P</td>
<td>C1 condenser pressure</td>
<td>psia</td>
</tr>
<tr>
<td>C1 2ND TRAY P</td>
<td>C1 tray 2 pressure</td>
<td>psia</td>
</tr>
<tr>
<td>C2 DIST FLOW</td>
<td>LT-ISO stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2 COND SC T</td>
<td>C2 condenser subcooled temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C2 COL P DROP</td>
<td>C2 column pressure drop</td>
<td>psi</td>
</tr>
<tr>
<td>C2 TOP TRAY P</td>
<td>C2 condenser pressure</td>
<td>psia</td>
</tr>
<tr>
<td>C2 2ND TRAY P</td>
<td>C2 tray 2 pressure</td>
<td>psia</td>
</tr>
<tr>
<td>C2-C4 IC FLOW</td>
<td>C4 feed stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2-C5 IC FLOW</td>
<td>C5 feed stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C4 REBL DUTY</td>
<td>C4 reboiler heat duty</td>
<td>MMBTU/hr</td>
</tr>
</tbody>
</table>

continued on the next page...
Table B.4 continued from the previous page

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>C5 T, TRAY n</td>
<td>C5 reboiler heat duty</td>
<td>MMBTU/hr</td>
</tr>
<tr>
<td>C1 T, TRAY n</td>
<td>C1 temperature profile (n = 1...29)</td>
<td>°F</td>
</tr>
<tr>
<td>C2 T, TRAY n</td>
<td>C2 temperature profile (n = 1...24)</td>
<td>°F</td>
</tr>
<tr>
<td>C4 T, TRAY n</td>
<td>C4 temperature profile (n = 1...3)</td>
<td>°F</td>
</tr>
<tr>
<td>C5 T, TRAY n</td>
<td>C5 temperature profile (n = 1...3)</td>
<td>°F</td>
</tr>
<tr>
<td>C1 L, TRAY n</td>
<td>C1 liquid flow profile (n = 1...29)</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C1 V, TRAY n</td>
<td>C1 vapour flow profile (n = 1...29)</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2 L, TRAY n</td>
<td>C2 liquid flow profile (n = 1...24)</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2 V, TRAY n</td>
<td>C2 vapour flow profile (n = 1...24)</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C4 L, TRAY n</td>
<td>C4 liquid flow profile (n = 1...3)</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C4 V, TRAY n</td>
<td>C4 vapour flow profile (n = 1...3)</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C5 L, TRAY n</td>
<td>C5 liquid flow profile (n = 1...3)</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C5 V, TRAY n</td>
<td>C5 vapour flow profile (n = 1...3)</td>
<td>lbmol/hr</td>
</tr>
</tbody>
</table>

B.6.7 **RVARNC.DAT**

RVARNC.DAT contains standard deviations used to determine the normal distributions for the random noise to be added to the plant measurements. This input file has the same format as IVARNC.DAT, with the 28 variances given in the same order as presented in Table B.2.

B.7 **Results**

Results from the real time optimizer are stored in series of directories under the directory results/ for each iteration, e.g., for the first iteration the results are stored in results/itr1/. The results files stored after each iteration are summarised in Table B.8.
Table B.5: Optimization parameters used in the ASPEN PLUS real time optimizer input file IOBJFN.DAT.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>PRMVP</td>
<td>Reid vapour pressure premium</td>
<td>$/m^3/kPa</td>
</tr>
<tr>
<td>SPCRVP</td>
<td>Reid vapour pressure specification below which a quality premium is added to</td>
<td>kPa</td>
</tr>
<tr>
<td></td>
<td>the LT-ISO stream price</td>
<td></td>
</tr>
<tr>
<td>DVAP</td>
<td>VAP stream price</td>
<td>$/m^3</td>
</tr>
<tr>
<td>DDIST</td>
<td>DIST-C4 stream price</td>
<td>$/m^3</td>
</tr>
<tr>
<td>DLTISO</td>
<td>LT-ISO stream price</td>
<td>$/m^3</td>
</tr>
<tr>
<td>DHISO</td>
<td>HV-ISO stream price</td>
<td>$/m^3</td>
</tr>
<tr>
<td>DLTDST</td>
<td>LT-DIST stream price</td>
<td>$/m^3</td>
</tr>
<tr>
<td>DSSFED</td>
<td>SSFEED stream price</td>
<td>$/m^3</td>
</tr>
<tr>
<td>DSTAB</td>
<td>STAB feed stream price</td>
<td>$/m^3</td>
</tr>
<tr>
<td>DFO</td>
<td>Fuel oil price</td>
<td>$/LFEm³</td>
</tr>
<tr>
<td>F1EFF</td>
<td>C1 reboiler furnace efficiency</td>
<td>—</td>
</tr>
<tr>
<td>F2EFF</td>
<td>C2 reboiler furnace efficiency</td>
<td>—</td>
</tr>
</tbody>
</table>

Table B.6: Constraint bounds used in the ASPEN PLUS real time optimizer input file ICNSTR.DAT.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>A11U</td>
<td>DIST-C4 C5's mole fraction upper bound</td>
<td>lbmol/lbmol</td>
</tr>
<tr>
<td>A11L</td>
<td>DIST-C4 C5's mole fraction lower bound</td>
<td>lbmol/lbmol</td>
</tr>
<tr>
<td>A31UR</td>
<td>LT-ISO Reid vapour pressure upper bound</td>
<td>psi</td>
</tr>
<tr>
<td>A31LT</td>
<td>C2 condenser bubble point temperature lower bound</td>
<td>°F</td>
</tr>
<tr>
<td>A41U1</td>
<td>HV-ISO 10% TBP (true boiling point) temperature upper bound</td>
<td>°F</td>
</tr>
<tr>
<td>A41L1</td>
<td>HV-ISO 10% TBP temperature lower bound</td>
<td>°F</td>
</tr>
</tbody>
</table>

continued on the next page...
Table B.6 continued from the previous page

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>A41U9</td>
<td>HV-ISO 90% TBP temperature upper bound</td>
<td>°F</td>
</tr>
<tr>
<td>A41L9</td>
<td>HV-ISO 90% TBP temperature lower bound</td>
<td>°F</td>
</tr>
<tr>
<td>A51U1</td>
<td>LT-DIST 10% TBP temperature upper bound</td>
<td>°F</td>
</tr>
<tr>
<td>A51L1</td>
<td>LT-DIST 10% TBP temperature lower bound</td>
<td>°F</td>
</tr>
<tr>
<td>A51U9</td>
<td>LT-DIST 90% TBP temperature upper bound</td>
<td>°F</td>
</tr>
<tr>
<td>A51L9</td>
<td>LT-DIST 90% TBP temperature lower bound</td>
<td>°F</td>
</tr>
<tr>
<td>F12U</td>
<td>C1 reflux standard liquid volume flow upper bound</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F12L</td>
<td>C1 reflux standard liquid volume flow lower bound</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F32U</td>
<td>C2 reflux standard liquid volume flow upper bound</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F41U</td>
<td>C4 feed stream standard liquid volume flow upper bound</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F51U</td>
<td>C5 feed stream standard liquid volume flow upper bound</td>
<td>bbl/day</td>
</tr>
<tr>
<td>T11U</td>
<td>C1 tray 3 temperature upper bound</td>
<td>°F</td>
</tr>
<tr>
<td>T11L</td>
<td>C1 tray 3 temperature lower bound</td>
<td>°F</td>
</tr>
<tr>
<td>T22U</td>
<td>C1 reboiler outlet temperature upper bound</td>
<td>°F</td>
</tr>
<tr>
<td>T22L</td>
<td>C1 reboiler outlet temperature lower bound</td>
<td>°F</td>
</tr>
<tr>
<td>T31U</td>
<td>C2 tray 2 temperature upper bound</td>
<td>°F</td>
</tr>
<tr>
<td>T31L</td>
<td>C2 tray 2 temperature lower bound</td>
<td>°F</td>
</tr>
<tr>
<td>T62U</td>
<td>C2 reboiler outlet temperature upper bound</td>
<td>°F</td>
</tr>
<tr>
<td>T62L</td>
<td>C2 reboiler outlet temperature lower bound</td>
<td>°F</td>
</tr>
</tbody>
</table>
Table B.7: Optimization free variable ranges used in the ASPEN PLUS real time optimizer input file I0FREE.DAT.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1-RR%</td>
<td>C1 molar reflux ratio</td>
<td>—</td>
</tr>
<tr>
<td>C1-RDV%</td>
<td>C1 condenser molar vapour fraction</td>
<td>—</td>
</tr>
<tr>
<td>C1-REBL-FLOW%</td>
<td>C1 reboiler mole flow</td>
<td>—</td>
</tr>
<tr>
<td>C1-REBL-TEMP</td>
<td>C1 reboiler outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>E1-TEMP</td>
<td>E1 outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C2-MOLE-D%</td>
<td>C2 liquid distillate mole flow</td>
<td>—</td>
</tr>
<tr>
<td>C2-REBL-FLOW%</td>
<td>C2 reboiler mole flow</td>
<td>—</td>
</tr>
<tr>
<td>C2-REBL-TEMP</td>
<td>C2 reboiler outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C2-SC-TEMP</td>
<td>C2 condenser sub-cooled temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C4-QN%</td>
<td>C4 reboiler heat duty</td>
<td>—</td>
</tr>
<tr>
<td>C5-QN%</td>
<td>C5 reboiler heat duty</td>
<td>—</td>
</tr>
<tr>
<td>C2-C4-FLOW%</td>
<td>C4 feed stream mole flow</td>
<td>—</td>
</tr>
<tr>
<td>C2-C5-FLOW%</td>
<td>C5 feed stream mole flow</td>
<td>—</td>
</tr>
</tbody>
</table>

Table B.8: ASPEN PLUS real time optimizer results files.

<table>
<thead>
<tr>
<th>File</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RDVARS.DAT</td>
<td>Reconciled variables (in the same format as IMEAS.DAT)</td>
</tr>
<tr>
<td>RDOFF.DAT</td>
<td>Reconciled variable offsets (reconciled – measured)</td>
</tr>
<tr>
<td>RDERR.DAT</td>
<td>Data reconciliation error contributions for each variable</td>
</tr>
<tr>
<td>ROVARS.DAT</td>
<td>Predicted values of the measured variables after optimization</td>
</tr>
<tr>
<td>ROCNST.DAT</td>
<td>Inequality constraint results summary</td>
</tr>
<tr>
<td>ROOPFN.DAT</td>
<td>Optimization objective function results summary</td>
</tr>
<tr>
<td>ROPTPT.DAT</td>
<td>Set point results summary</td>
</tr>
<tr>
<td>ROSMST.DAT</td>
<td>ASPEN PLUS simulation settings after optimization</td>
</tr>
<tr>
<td>PLVARS.DAT</td>
<td>Measures variables from the plant simulation</td>
</tr>
<tr>
<td>IMEAS.DAT</td>
<td>Measured variables from the plant with noise added for the next iteration of the real time optimizer</td>
</tr>
</tbody>
</table>
B.8 Example

B.8.1 Input Files

The eight input files required to run an ASPEN PLUS real time optimization run are listed below. They have been printed in two columns to save paper, but appear in a single column in the actual input file.

IMEAS.DAT

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>F01</td>
<td>2.0863014E+05</td>
</tr>
<tr>
<td>F11</td>
<td>7.5209442E+05</td>
</tr>
<tr>
<td>F12</td>
<td>7.0246257E+04</td>
</tr>
<tr>
<td>F13</td>
<td>8.8440222E+03</td>
</tr>
<tr>
<td>F21</td>
<td>3.1955347E+05</td>
</tr>
<tr>
<td>F22</td>
<td>1.9080626E+05</td>
</tr>
<tr>
<td>F31</td>
<td>1.5802698E+04</td>
</tr>
<tr>
<td>F32</td>
<td>1.2862473E+05</td>
</tr>
<tr>
<td>F41</td>
<td>5.0296623E+04</td>
</tr>
<tr>
<td>F42</td>
<td>3.8176940E+04</td>
</tr>
<tr>
<td>F51</td>
<td>3.2645036E+04</td>
</tr>
<tr>
<td>F52</td>
<td>1.8477370E+04</td>
</tr>
<tr>
<td>F61</td>
<td>2.9933726E+05</td>
</tr>
<tr>
<td>F62</td>
<td>1.2250671E+05</td>
</tr>
<tr>
<td>T01</td>
<td>4.1295470E+03</td>
</tr>
<tr>
<td>T12</td>
<td>1.5233838E+03</td>
</tr>
<tr>
<td>T13</td>
<td>9.6372107E+02</td>
</tr>
<tr>
<td>T21</td>
<td>5.1601320E+03</td>
</tr>
<tr>
<td>T22</td>
<td>5.8608488E+03</td>
</tr>
<tr>
<td>T23</td>
<td>4.7969655E+03</td>
</tr>
<tr>
<td>T31</td>
<td>1.2835124E+03</td>
</tr>
<tr>
<td>T32</td>
<td>8.4722528E+02</td>
</tr>
<tr>
<td>T41</td>
<td>2.4031157E+03</td>
</tr>
<tr>
<td>T42</td>
<td>2.6107760E+03</td>
</tr>
<tr>
<td>T51</td>
<td>3.5619866E+03</td>
</tr>
<tr>
<td>T52</td>
<td>4.2389816E+03</td>
</tr>
<tr>
<td>T61</td>
<td>6.2344743E+03</td>
</tr>
<tr>
<td>T62</td>
<td>6.8389991E+03</td>
</tr>
</tbody>
</table>

IVARNC.DAT

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>VF01</td>
<td>1.0431507E+04</td>
</tr>
<tr>
<td>VF11</td>
<td>3.7604721E+04</td>
</tr>
</tbody>
</table>
VF12  .35123129E+03
VF13  .44220110E+02
VF21  .15977674E+04
VF22  .95403132E+03
VF31  .79013490E+02
VF32  .64312363E+03
VF41  .25148312E+03
VF42  .19088470E+03
VF51  .16322518E+03
VF52  .92386852E+02
VF61  .14966863E+04
VF62  .61253356E+03
VT01  .20647735E+02
VT12  .76269189E+01
VT13  .48186054E+01
VT21  .25800660E+02
VT22  .29304244E+02
VT23  .23984827E+02
VT31  .64175619E+01
VT32  .42361264E+01
VT41  .12015579E+02
VT42  .13053860E+02
VT51  .17809933E+02
VT52  .21194908E+02
VT61  .31172371E+02
VT62  .34194995E+02

IWGHT.DAT

WF01  .10000000E+01
WF11  .10000000E+01
WF12  .10000000E+01
WF13  .10000000E+01
WF21  .10000000E+01
WF22  .10000000E+01
WF31  .10000000E+01
WF32  .10000000E+01
WF41  .10000000E+01
WF42  .10000000E+01
WF51  .10000000E+01
WF52  .10000000E+01
WF61  .10000000E+01
WF62  .10000000E+01
WT01  .10000000E+01
WT12  .10000000E+01
WT13 .100000000E+01
WT21 .100000000E+01
WT22 .100000000E+01
WT23 .100000000E+01
WT31 .100000000E+01
WT32 .100000000E+01
WT41 .100000000E+01
WT42 .100000000E+01
WT51 .100000000E+01
WT52 .100000000E+01
WT61 .100000000E+01
WT62 .100000000E+01

IDFREE.DAT

STAB-MOLEFLOW .100000000E+03
STAB-TEMP .300000000E+02
C1-RR .100000000E+01
C1-RDV .300000000E+00
C1-REBL-FLOW .400000000E+03
C1-REBL-TEMP .300000000E+02
E1-TEMP .200000000E+02
C2-MOLE-D .500000000E+02
C2-REBL-FLOW .200000000E+03
C2-REBL-TEMP .400000000E+02
C2-SC-TEMP .100000000E+02
C4-QN .150000000E+01
C5-QN .100000000E+01
C2-C4-FLOW .150000000E+03
C2-C5-FLOW .100000000E+03

ISMST.DAT

STAB-MOLEFLOW .148717717E+04
STAB-TEMP .412954700E+03
STAB-PRESS .200000000E+03
STAB Z 1 .703680230E-03
STAB Z 2 .246830080E-01
STAB Z 3 .473640150E-01
STAB Z 4 .387240120E-01
STAB Z 5 .535310170E-01
STAB Z 6 .312790100E-01
STAB Z 7 .351930110E-01
STAB Z 8 .161490050E-01
<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>STAB Z 9</td>
<td>0.47256015E-01</td>
</tr>
<tr>
<td>STAB Z 10</td>
<td>0.43562014E-01</td>
</tr>
<tr>
<td>STAB Z 11</td>
<td>0.49649016E-01</td>
</tr>
<tr>
<td>STAB Z 12</td>
<td>0.53071017E-01</td>
</tr>
<tr>
<td>STAB Z 13</td>
<td>0.52326017E-01</td>
</tr>
<tr>
<td>STAB Z 14</td>
<td>0.48963016E-01</td>
</tr>
<tr>
<td>STAB Z 15</td>
<td>0.44418014E-01</td>
</tr>
<tr>
<td>STAB Z 16</td>
<td>0.41240013E-01</td>
</tr>
<tr>
<td>STAB Z 17</td>
<td>0.60769019E-01</td>
</tr>
<tr>
<td>STAB Z 18</td>
<td>0.53782017E-01</td>
</tr>
<tr>
<td>STAB Z 19</td>
<td>0.59831019E-01</td>
</tr>
<tr>
<td>STAB Z 20</td>
<td>0.62687020E-01</td>
</tr>
<tr>
<td>STAB Z 21</td>
<td>0.56050018E-01</td>
</tr>
<tr>
<td>STAB Z 22</td>
<td>0.52921017E-01</td>
</tr>
<tr>
<td>STAB Z 23</td>
<td>0.25848008E-01</td>
</tr>
<tr>
<td>C2REBL FLOW</td>
<td>1.3271950E+04</td>
</tr>
<tr>
<td>C2REBL TEMP</td>
<td>0.68389991E+03</td>
</tr>
<tr>
<td>C2REBL PRESS</td>
<td>0.35658100E+02</td>
</tr>
<tr>
<td>C2REBL Z 1</td>
<td>0.00000000E+00</td>
</tr>
<tr>
<td>C2REBL Z 2</td>
<td>0.22332348E-19</td>
</tr>
<tr>
<td>C2REBL Z 3</td>
<td>0.37670678E-14</td>
</tr>
<tr>
<td>C2REBL Z 4</td>
<td>0.34882008E-10</td>
</tr>
<tr>
<td>C2REBL Z 5</td>
<td>0.23324335E-07</td>
</tr>
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| C5 V, TRAY 3 | .13035573E+03 |

**IOBJFN.DAT**

| PRMRVP            | -1.8000000E+00 |
| SPCRVVP           | .97000000E+02 |
| DVAP              | .15000000E+00 |
| DDIST             | .10007000E+03 |
| DLTISO            | .18269000E+03 |
| DHVISQ            | .19389000E+03 |
| DLTDST            | .18052000E+03 |
| DSSFED            | .15834000E+03 |
| DSTAR             | .15834000E+03 |
| DFO               | .82140000E+02 |
| F1EFF             | .70000000E+00 |
| F2EFF             | .70000000E+00 |

**ICNSTR.DAT**

| A11U              | .15000000E+00 |
| A11L              | .50000000E-02 |
| A31UR             | .14000000E+02 |
| A31LT             | .11000000E+03 |
| A41U1             | .26600000E+03 |
| A41L1             | .17600000E+03 |
| A41U9             | .46400000E+03 |
| A41L9             | .28400000E+03 |
| A51U1             | .55400000E+03 |
| A51L1             | .30200000E+03 |
| A51U9             | .55400000E+03 |
| A51L9             | .30200000E+03 |
| F12U              | .90000000E+04 |
| F12L              | .10000000E+04 |
| F32U              | .25000000E+05 |
F41U   .10604000E+05  
F51U   .60000000E+04  
T11U   .22000000E+03  
T11L   .12500000E+03  
T22U   .67500000E+03  
T22L   .53000000E+03  
T31U   .25000000E+03  
T31L   .12000000E+03  
T62U   .70000000E+03  
T62L   .55000000E+03  

IOFREE.DAT

C1-RR%  .50000000E-01  
C1-RDV%  .50000000E-01  
C1-REBL-FLOW%  .50000000E-01  
C1-REBL-TEMP  .50000000E-01  
E1-TEMP  .50000000E+01  
C2-MOLE-D%  .50000000E-01  
C2-REBL-FLOW%  .50000000E-01  
C2-REBL-TEMP  .50000000E+01  
C2-SC-TEMP  .50000000E+01  
C4-QN%  .50000000E-01  
C5-QN%  .50000000E-01  
C2-C4-FLOW%  .50000000E-01  
C2-C5-FLOW%  .50000000E-01  

RVARNC.DAT

VF01   .10431507E+04  
VF11   .37604721E+04  
VF12   .35123129E+03  
VF13   .44220110E+02  
VF21   .15977674E+04  
VF22   .95403132E+03  
VF31   .79013490E+02  
VF32   .64312363E+03  
VF41   .25148312E+03  
VF42   .19088470E+03  
VF51   .16322518E+03  
VF52   .92386852E+02  
VF61   .14966863E+04  
VF62   .61253356E+03  
VT01   .20647735E+02  

VT12  .76269189E+01
VT13  .48186054E+01
VT21  .25800660E+02
VT22  .29304244E+02
VT23  .23984827E+02
VT31  .64175619E+01
VT32  .42361264E+01
VT41  .12015579E+02
VT42  .13053880E+02
VT51  .17809933E+02
VT52  .21194908E+02
VT61  .31172371E+02
VT62  .34194995E+02

B.8.2 Command Line

If it the ASPEN PLUS real time optimizer has not already been setup, then type the command:

setup

When completed, type the command:

nohup nice run 1 &

to run one cycle of the real time optimizer.

B.8.3 Results

The following results will be present in the results/itn1/ directory.

RDVARS.DAT

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>F01</td>
<td>.21859091E+05</td>
</tr>
<tr>
<td>F11</td>
<td>.69854292E+05</td>
</tr>
<tr>
<td>F12</td>
<td>.70514797E+04</td>
</tr>
<tr>
<td>F13</td>
<td>.82877958E+03</td>
</tr>
<tr>
<td>F21</td>
<td>.31262989E+05</td>
</tr>
<tr>
<td>F22</td>
<td>.19958397E+05</td>
</tr>
<tr>
<td>F31</td>
<td>.14784074E+04</td>
</tr>
<tr>
<td>F32</td>
<td>.14148616E+05</td>
</tr>
<tr>
<td></td>
<td>QM</td>
</tr>
<tr>
<td>----</td>
<td>--------</td>
</tr>
<tr>
<td>F41</td>
<td>0.55771892E+04</td>
</tr>
<tr>
<td>F42</td>
<td>0.38080990E+04</td>
</tr>
<tr>
<td>F51</td>
<td>0.33253764E+04</td>
</tr>
<tr>
<td>F52</td>
<td>0.18961467E+04</td>
</tr>
<tr>
<td>F61</td>
<td>0.27970047E+05</td>
</tr>
<tr>
<td>F62</td>
<td>0.12775711E+05</td>
</tr>
<tr>
<td>T01</td>
<td>0.43103635E+03</td>
</tr>
<tr>
<td>T12</td>
<td>0.15716275E+03</td>
</tr>
<tr>
<td>T13</td>
<td>0.94728241E+02</td>
</tr>
<tr>
<td>T21</td>
<td>0.52429749E+03</td>
</tr>
<tr>
<td>T22</td>
<td>0.59027415E+03</td>
</tr>
<tr>
<td>T23</td>
<td>0.46081466E+03</td>
</tr>
<tr>
<td>T31</td>
<td>0.14812960E+03</td>
</tr>
<tr>
<td>T32</td>
<td>0.82876202E+02</td>
</tr>
<tr>
<td>T41</td>
<td>0.26395977E+03</td>
</tr>
<tr>
<td>T42</td>
<td>0.28408165E+03</td>
</tr>
<tr>
<td>T51</td>
<td>0.36881493E+03</td>
</tr>
<tr>
<td>T52</td>
<td>0.42521338E+03</td>
</tr>
<tr>
<td>T61</td>
<td>0.60180580E+03</td>
</tr>
<tr>
<td>T62</td>
<td>0.64621622E+03</td>
</tr>
</tbody>
</table>

RDOFF.DAT

| OFFF01 | 0.99607672E+03 |
| OFFF11 | -0.53551503E+04 |
| OFFF12 | 0.26854007E+02 |
| OFFF13 | -0.55622538E+02 |
| OFFF21 | -0.69235822E+03 |
| OFFF22 | 0.87777126E+03 |
| OFFF31 | -0.10186238E+03 |
| OFFF32 | 0.12861433E+04 |
| OFFF41 | 0.54752691E+03 |
| OFFF42 | -0.95949819E+01 |
| OFFF51 | 0.60872806E+02 |
| OFFF52 | 0.48409696E+02 |
| OFFF61 | -0.19636790E+04 |
| OFFF62 | 0.52504041E+03 |
| OFFT01 | 0.18081649E+02 |
| OFFT12 | 0.48243656E+01 |
| OFFT13 | -0.16438662E+01 |
| OFFT21 | 0.82842879E+01 |
| OFFT22 | 0.41892701E+01 |
| OFFT23 | -0.18881893E+02 |
| OFFT31 | 0.19778362E+02 |
| OFFT32 | -0.18463257E+01 |
OFFT41  .23648201E+02
OFFT42  .23004048E+02
OFFT51  .12616267E+02
OFFT52  .13152236E+01
OFFT61  -.21641631E+02
OFFT62  -.37683687E+02

RDERR.DAT
ERRF01  .91178296E+00
ERRF11  .20279563E+01
ERRF12  .58456362E-02
ERRF13  .15822021E+01
ERRF21  .18777363E+00
ERRF22  .84652043E+00
ERRF31  .16619775E+01
ERRF32  .39993532E+01
ERRF41  .47401629E+01
ERRF42  .25266558E-02
ERRF51  .13908245E+00
ERRF52  .27456449E+00
ERRF61  .17213905E+01
ERRF62  .73472647E+00
ERRT01  .76688675E+00
ERRT12  .40011255E+00
ERRT13  .11638317E+00
ERRT21  .10309764E+00
ERRT22  .20436931E-01
ERRT23  .61975195E+00
ERRT31  .94981828E+01
ERRT32  .18996729E+00
ERRT41  .38735289E+01
ERRT42  .31054840E+01
ERRT51  .50180755E+00
ERRT52  .38506686E-02
ERRT61  .48199253E+00
ERRT62  .12144557E+01

ROVARS.DAT
F01  .21859091E+05
F11  .67107186E+05
F12  .69137124E+04
F13  .90205497E+03
ROOPFN.DAT

OBFUN-PROFIT - .98374539E+01
TOT PROD VALS .23035020E+05
TOT FEED COST .22928410E+05
TOT UTIL COST .11644748E+03
VAP SVOLFLOW .10249031E+04
DISTC4 SVOLFL .90205497E+03
LTISO SVOLFL .15596100E+04
HVIS0 SVOLFL .42020112E+04
LTDIST SVOLFL .19524427E+04
SSFEED SVOLFL .12218003E+05
STAB SVOLFLOW .21859091E+05
C1 REBL DUTY .21242019E+02
C2 REBL DUTY .18081425E+02
LT-ISO MARG .18277511E+03
LT-ISO RVP .13999996E+02
**ROCNST.DAT**

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>F12</td>
<td>69137124E+04</td>
</tr>
<tr>
<td>F32</td>
<td>13951685E+05</td>
</tr>
<tr>
<td>F41</td>
<td>59982861E+04</td>
</tr>
<tr>
<td>F51</td>
<td>33344776E+04</td>
</tr>
<tr>
<td>T11</td>
<td>18125698E+03</td>
</tr>
<tr>
<td>T22</td>
<td>59510129E+03</td>
</tr>
<tr>
<td>T31</td>
<td>15302258E+03</td>
</tr>
<tr>
<td>T62</td>
<td>65121622E+03</td>
</tr>
<tr>
<td>A11 (CSS)</td>
<td>11881676E+00</td>
</tr>
<tr>
<td>A31 (RVP)</td>
<td>13999996E+02</td>
</tr>
<tr>
<td>A31 (TBUB)</td>
<td>11505224E+03</td>
</tr>
<tr>
<td>A41 (TBP10)</td>
<td>19737562E+03</td>
</tr>
<tr>
<td>A41 (TBP90)</td>
<td>35162453E+03</td>
</tr>
<tr>
<td>A51 (TBP10)</td>
<td>33825622E+03</td>
</tr>
<tr>
<td>A51 (TBP90)</td>
<td>49624756E+03</td>
</tr>
</tbody>
</table>

**ROSTPT.DAT**

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1 REFLUX FLOW (F12) [BBL/DAY]</td>
<td>69137124E+04</td>
</tr>
<tr>
<td>C1 TRAY 3 TEMPERATURE (T11) [F]</td>
<td>18125698E+03</td>
</tr>
<tr>
<td>DIST-C4 CS MOLE FRACTION (A11)</td>
<td>11881676E+00</td>
</tr>
<tr>
<td>C1 REBOILER TEMPERATURE (T22) [F]</td>
<td>59510129E+03</td>
</tr>
<tr>
<td>C2 REFLUX FLOW (F32) [BBL/DAY]</td>
<td>13951685E+05</td>
</tr>
<tr>
<td>C4 FEED FLOW (F41) [BBL/DAY]</td>
<td>59982861E+04</td>
</tr>
<tr>
<td>C5 FEED FLOW (F51) [BBL/DAY]</td>
<td>33344776E+04</td>
</tr>
<tr>
<td>C2 REBOILER TEMPERATURE (T62) [F]</td>
<td>65121622E+03</td>
</tr>
<tr>
<td>HV-ISD 10% TBP TEMPERATURE (A41) [F]</td>
<td>19737562E+03</td>
</tr>
<tr>
<td>HV-ISD 90% TBP TEMPERATURE (A41) [F]</td>
<td>35162453E+03</td>
</tr>
<tr>
<td>LT-DIST 10% TBP TEMPERATURE (A51) [F]</td>
<td>33825622E+03</td>
</tr>
<tr>
<td>LT-DIST 90% TBP TEMPERATURE (A51) [F]</td>
<td>49624756E+03</td>
</tr>
</tbody>
</table>
Appendix C

SPEEDUP Real Time Optimizer Documentation

C.1 Purpose

This program performs a given number of cycles of a real time optimizer on the stabilizer-splitter flowsheet given in Figure C.1 using SPEEDUP to perform the data reconciliation and optimization.

C.2 Specification

To setup the real time optimizer for a run, use the command:

```
setup
```

or

```
nohup setup &
```

This command must be given before running the real time optimizer, and the files listed in Table C.1 must already exist on the paths specified.

To run the real time optimizer for a given number of cycles, \( n \), use the command:
Figure C.1: Stabilizer-splitter process flowsheet (including measurement tag numbers).
run n

or

nohup run n &

The real time optimizer must already have been either setup or run prior to using this command.

C.3 Description

The SPEEDUP real time optimizer performs data reconciliation and optimization on the stabilizer-splitter flowsheet given in Figure C.1. Detailed information about this optimizer is covered by Naysmith [1].

Before running the real time optimizer, the program setup must be run first. This program translates and compiles the SPEEDUP and ASPEN PLUS simulations, and compiles the FORTRAN77 routines used. The files listed in Table C.1 must exist on the paths specified, and the NAG FORTRAN Library Routines must be available. The program setup only needs to be run once.

The program run runs a specified number of cycles (or iterations) of the real time optimizer. The steps used by this program are summarised in Figure C.2.

The data reconciliation uses a weighted least squares objective function to reconcile 28 measured variables (all variables shown in Figure C.1 except T11):

\[
\min_{x} \left[ \sum_{i=1}^{38} w_{i} \left( \frac{y_{i} - x_{i}}{s_{i}} \right)^{2} \right] \quad (C.1)
\]

subject to \( h(x) = 0 \)

where \( w \) = weighting factor associated with each measured variable;

\( y \) = the measured variable;

\( x \) = the estimated true (reconciled) variable value;
Figure C.2: SPEEDUP real time optimization program flow chart.
\[ s = \text{the standard deviation of the measurements}; \]
\[ h(x) = \text{the set of equality constraints representing the process model}. \]

The optimization algorithm used is the SRQP (sequential reduced quadratic programming) algorithm using a line search method with a modified Lagrangian function. This objective function is minimized by varying 15 free variables.

The economic optimization maximizes profit using the following objective function:

\[
\max \left[ \sum \text{(product values)} - \text{(feed cost)} - \text{(reboiler fuel oil cost)} \right]
\]
subject to \( h(x) = 0 \)

\[ g(x) \geq 0 \]  \hspace{1cm} (C.2)

where \( h(x) = \text{the set of equality constraints representing the process model}; \)

\[ g(x) = \text{product quality and operating inequality constraints}. \]

The optimization algorithm used is the SRQP algorithm using a line search method with a modifies augmented Lagrangian function. The objective function is maximized by varying 11 free variables subject to 25 inequality constraints.

Normally distributed random noise is added to the plant data calculated in the plant simulation before being returned to the real time optimizer for the next iteration. The noise has a mean of zero, and a given standard deviation for each of the 28 measured variables.

### C.4 References

C.5 Files

The files required to run SPEEDUP real time optimizer are listed in Table C.1.

C.6 Input File Specifications

All input files are formatted in the same way, except ISET.DAT, using the following FORTRAN format statement:

```
FORMAT(A13, 2X, E15.8)
```

The first 13 columns of each line contain a descriptive label. The next 2 columns are blank and the last 15 columns contain the corresponding numerical value. ISET.DAT is formatted using the following FORTRAN format statement:

```
FORMAT(A40, 2X, E15.8)
```

In this case, first the 40 columns of each line contain a descriptive label. the next 2 columns are blank and the last 15 columns contain the corresponding numerical value. Example input files are given in section C.8.

C.6.1 IMEAS.DAT, IVARNC.DAT and IWGHT.DAT

IMEAS.DAT, IVARNC.DAT and IWGHT.DAT contain the measured values, standard deviations and weights for data reconciliation corresponding to the 28 measured plant variables respectively. The 28 variables are given in the same order as presented in Table C.2 for all three files. The units given are for the measured variables and standard deviations. The variable names are the same as those used in Figure C.1.
<table>
<thead>
<tr>
<th>File</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>run</td>
<td>Runs the real time optimizer (C-shell script. executable)</td>
</tr>
<tr>
<td>setup</td>
<td>Sets up the real time optimizer prior to being run (C-shell script. executable)</td>
</tr>
<tr>
<td>plant/plant6.inp</td>
<td>Steady state plant simulation (ASPEX PLUS input file)</td>
</tr>
<tr>
<td>plant/randata.f</td>
<td>Adds normally distributed random noise to the measured plant data (FORTRAN77 input file. requires the NAG FORTRAN Library Routines)</td>
</tr>
<tr>
<td>plant/RVARNC.DAT</td>
<td>Contains the random noise standard deviations for the measured plant data</td>
</tr>
<tr>
<td>props/prop6.inp</td>
<td>Properties for both the data reconciliation and optimization SPEEDUP simulations (PROPERTIES PLUS input file)</td>
</tr>
<tr>
<td>rtdr/</td>
<td>Results from a previous run used to initialize the data reconciliation simulation (SPEEDUP saved results file)</td>
</tr>
<tr>
<td>drpreset.speedup</td>
<td></td>
</tr>
<tr>
<td>rtdr/IDFREE.DAT</td>
<td>Contains the data reconciliation free variable bound ranges</td>
</tr>
<tr>
<td>rtdr/IMEAS.DAT</td>
<td>Contains the measured variable data from the plant (with noise added)</td>
</tr>
<tr>
<td>rtdr/ISET.DAT</td>
<td>Contains the initial simulation settings and parameters for starting the SPEEDUP real time optimization simulations</td>
</tr>
<tr>
<td>rtdr/IVARNC.DAT</td>
<td>Contains the measured variable standard deviations for the data reconciliation</td>
</tr>
<tr>
<td>rtdr/IWGHT.DAT</td>
<td>Contains the measured variable weights for the data reconciliation</td>
</tr>
</tbody>
</table>

continued on the next page...
... Table C.1 continued from the previous page

<table>
<thead>
<tr>
<th>File</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>rtodr/</td>
<td>User written models used in the process simulation</td>
</tr>
<tr>
<td>model6x.speedup</td>
<td>flowsheet (SPEEDUP input file)</td>
</tr>
<tr>
<td>rtodr/</td>
<td>User written reports (SPEEDUP input file)</td>
</tr>
<tr>
<td>report6y.speedup</td>
<td>EDI (external data interface) code for receiving and transmitting variables (FORTRAN input file)</td>
</tr>
<tr>
<td>rtodr/rtodr6.f</td>
<td>Data reconciliation simulation (SPEEDUP input file)</td>
</tr>
<tr>
<td>rtodr/rtodr6.run.cmd</td>
<td>SPEEDUP commands used during batch run of the data reconciliation simulation</td>
</tr>
<tr>
<td>rtodr/rtodr6setup.cmd</td>
<td>SPEEDUP commands used during setup of the data reconciliation simulation</td>
</tr>
<tr>
<td>rtodr/speedup.include</td>
<td>File names of FORTRAN object code to be included in the SPEEDUP simulation when compiling</td>
</tr>
<tr>
<td>rtopt/ICNSTR.DAT</td>
<td>Contains the optimization inequality constraint upper and lower bounds</td>
</tr>
<tr>
<td>rtopt/IOBJFN.DAT</td>
<td>Contains the optimization objective function parameters</td>
</tr>
<tr>
<td>rtopt/IOFREE.DAT</td>
<td>Contains the optimization free variable bound ranges</td>
</tr>
<tr>
<td>rtopt/</td>
<td>User written models used in the process simulation</td>
</tr>
<tr>
<td>model6x.speedup</td>
<td>flowsheet (SPEEDUP input file)</td>
</tr>
<tr>
<td>rtopt/</td>
<td>User written reports (SPEEDUP input file)</td>
</tr>
<tr>
<td>report6y.speedup</td>
<td>EDI code for receiving and transmitting variables (FORTRAN input file)</td>
</tr>
</tbody>
</table>

continued on the next page ...
Table C.1 continued from the previous page

<table>
<thead>
<tr>
<th>File</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>rtopt/</td>
<td>Optimization simulation (SPEEDUP input file)</td>
</tr>
<tr>
<td>rtopt6.speedup</td>
<td></td>
</tr>
<tr>
<td>rtopt/</td>
<td>SPEEDUP commands used during batch run of the optimization simulation</td>
</tr>
<tr>
<td>rtopt6run.cmd</td>
<td>SPEEDUP commands used during setup of the optimization simulation</td>
</tr>
<tr>
<td>rtopt/</td>
<td></td>
</tr>
<tr>
<td>rtopt6setup.cmd</td>
<td>File names of FORTRAN object code to be included in the SPEEDUP simulation when compiling</td>
</tr>
</tbody>
</table>

C.6.2 IDFREE.DAT

IDFREE.DAT contains the free variable ranges for data reconciliation. The upper and lower are free variable bounds are calculated using the following formulae:

\[
\begin{align*}
  x_{UB} &= x^{(0)} + r \\
  x_{LB} &= x^{(0)} - r
\end{align*}
\]  

where \( x_{UB} \) = free variable upper bound;
\( x_{LB} \) = free variable lower bound;
\( x^{(0)} \) = initial free variable value;
\( r \) = free variable range as specified in IDFREE.DAT.

The free variable range specifications are given in the order shown in Table C.3.

C.6.3 ISET.DAT

The file ISET.DAT contains all the simulation settings to initialize the SPEEDUP real time optimization simulation. Table C.4 summarises the variable in this file. Variables which are vectors, such as compositions, use \( n \) lines in the
Table C.2: Variable order used in the SPEEDUP real time optimizer input files IMEAS.DAT, IVARNC.DAT and IWGHT.DAT.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>F01</td>
<td>STAB stream standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F11</td>
<td>VAP stream standard vapour volume flow</td>
<td>cuft/hr</td>
</tr>
<tr>
<td>F12</td>
<td>C1 reflux standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F13</td>
<td>DIST-C4 stream standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F21</td>
<td>C1 reboiler standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F22</td>
<td>E1 outlet standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F31</td>
<td>LT-ISO stream standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F32</td>
<td>C2 reflux standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F41</td>
<td>C4 feed standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F42</td>
<td>HV-ISO stream standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F51</td>
<td>C5 feed standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F52</td>
<td>LT-DIST stream standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F61</td>
<td>C2 reboiler standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F62</td>
<td>SSFEED stream standard liquid volume flow</td>
<td>bbl/day</td>
</tr>
<tr>
<td>T01</td>
<td>STAB stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T12</td>
<td>C1 tray 2 temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T13</td>
<td>C1 condenser temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T21</td>
<td>C1 bottoms stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T22</td>
<td>C1 reboiler outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T23</td>
<td>E1 outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T31</td>
<td>C2 tray 2 temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T32</td>
<td>LT-ISO stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T41</td>
<td>C4 feed stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T42</td>
<td>HV-ISO stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T51</td>
<td>C5 feed stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T52</td>
<td>LT-DIST stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T61</td>
<td>C2 bottoms stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>T62</td>
<td>C2 reboiler outlet temperature</td>
<td>°F</td>
</tr>
</tbody>
</table>
Table C.3: Data reconciliation free variable ranges used in the SPEEDUP real time optimizer input file IDFREE.DAT.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1COND.Q</td>
<td>C1 condenser heat duty</td>
<td>MMBTU/hr</td>
</tr>
<tr>
<td>C1SPL1.L_OUT</td>
<td>DIST-C4 stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C1FT14.F_IN</td>
<td>STAB stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C1FT14.T_IN</td>
<td>STAB stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C1BT29.L_OUT1</td>
<td>E1 inlet mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C1BT29.L_OUT2</td>
<td>C1 reboiler mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2COND.Q</td>
<td>C2 condenser heat duty</td>
<td>MMBTU/hr</td>
</tr>
<tr>
<td>C2COND.T_DROP</td>
<td>C2 condenser subcooled temperature drop (bubble point less subcooled temperature)</td>
<td>°F</td>
</tr>
<tr>
<td>C2FT21.T_IN</td>
<td>E1 outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C2BT24.L_OUT1</td>
<td>SSFEED stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2BT24.L_OUT2</td>
<td>C2 reboiler mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2SPL1.L_OUT1</td>
<td>C4 feed stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2SPL2.L_OUT1</td>
<td>C5 feed stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C4REBL.L_OUT</td>
<td>HV-ISO stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C5REBL.L_OUT</td>
<td>LT-DIST stream mole flow</td>
<td>lbmol/hr</td>
</tr>
</tbody>
</table>
input file as specified in Table C.4. Note that this file is formatted differently to the other input files using the FORTRAN format statement:

\[
\text{FORMAT(A40, 2X, E15.8)}
\]

### C.6.4 IOBJFN.DAT

IOBJFN.DAT contains the parameters used in calculating the economic objective function. Table C.5 summarises the order in which these parameters must appear in the file IOBJFN.DAT.

### C.6.5 ICNSTR.DAT

ICNSTR.DAT contains the upper and lower bounds for all the inequality constraints in the optimization. Table C.6 summarises the order in which these bounds must appear in the file ICNSTR.DAT.

### C.6.6 IOFREE.DAT

IOFREE.DAT contains the free variable ranges for optimization. The upper and lower are free variable bounds are calculated using the following formulae for all free variables except temperatures:

\[
\begin{align*}
  x_{UB} &= x^{(0)} + qx^{(0)} \\
  x_{LB} &= x^{(0)} - qx^{(0)}
\end{align*}
\]  

(C.4)

where \( q \) = free variable range as a fraction of the initial variable value.

Temperature free variable bounds are calculated using the formulae given in equation (C.3). The free variable range specifications are given in the order shown in Table C.7. Free variable bounds calculated using equation (C.4) have the character "%" at the end of their variable name.
Table C.4: Simulation settings used in the SPEEDUP real time optimizer input file ISET.DAT.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>MFEED.Z.OUT(n)</td>
<td>STAB stream composition</td>
<td>lbmol/lbmol</td>
</tr>
<tr>
<td></td>
<td>(n = 1 ... 22) (Note: the 23rd component composition, B395T510, is not included)</td>
<td></td>
</tr>
<tr>
<td>MFEED.P.OUT</td>
<td>STAB stream pressure</td>
<td>psia</td>
</tr>
<tr>
<td>C1COND.P</td>
<td>C1 condenser pressure</td>
<td>psia</td>
</tr>
<tr>
<td>C1COND.Q</td>
<td>C1 condenser heat duty</td>
<td>MMBTU/hr</td>
</tr>
<tr>
<td>C1SPL1.L.OUT1</td>
<td>DIST-C4 stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>&quot;C1S.TRAY_SS(2)&quot;.P</td>
<td>C1 tray 2 pressure</td>
<td>psia</td>
</tr>
<tr>
<td>C1FT14.F.IN</td>
<td>STAB stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C1FT14.T.IN</td>
<td>STAB stream temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C1BT29.L.OUT1</td>
<td>E1 inlet mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C1BT29.L.OUT2</td>
<td>C1 reboiler mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>E1.P.OUT</td>
<td>E1 outlet pressure</td>
<td>psia</td>
</tr>
<tr>
<td>C2COND.P</td>
<td>C2 condenser pressure</td>
<td>psia</td>
</tr>
<tr>
<td>C2COND.Q</td>
<td>C2 condenser heat duty</td>
<td>MMBTU/hr</td>
</tr>
<tr>
<td>C2COND.T.DROP</td>
<td>C2 condenser subcooled temperature drop</td>
<td>°F</td>
</tr>
<tr>
<td>&quot;C2S1.TRAY_SS(2)&quot;.P</td>
<td>C2 tray 2 pressure</td>
<td>psia</td>
</tr>
<tr>
<td>C2FT21.T.IN</td>
<td>E1 outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C2BT24.L.OUT1</td>
<td>SSFEED stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2BT24.L.OUT2</td>
<td>C2 reboiler mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2SPL1.L.OUT1</td>
<td>C4 feed stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C2SPL2.L.OUT1</td>
<td>C5 feed stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C4REBL.L.OUT</td>
<td>HV-ISO stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>C5REBL.L.OUT</td>
<td>LT-DIST stream mole flow</td>
<td>lbmol/hr</td>
</tr>
<tr>
<td>F31.TL.OUT</td>
<td>LT-ISO stream temperature</td>
<td>°F</td>
</tr>
</tbody>
</table>
Table C.5: Optimization parameters used in the SPEEDUP real time optimizer input file I0BJFN.DAT.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>PRMRVP</td>
<td>Reid vapour pressure premium</td>
<td>$/m^3/kPa</td>
</tr>
<tr>
<td>SPCRVP</td>
<td>Reid vapour pressure specification below which a quality premium is added to the LT-ISO stream price</td>
<td>kPa</td>
</tr>
<tr>
<td>DVAP</td>
<td>VAP stream price</td>
<td>$/m^3</td>
</tr>
<tr>
<td>DDIST</td>
<td>DIST-C4 stream price</td>
<td>$/m^3</td>
</tr>
<tr>
<td>DLTISO</td>
<td>LT-ISO stream price</td>
<td>$/m^3</td>
</tr>
<tr>
<td>DHVISQ</td>
<td>HV-ISO stream price</td>
<td>$/m^3</td>
</tr>
<tr>
<td>DLTDST</td>
<td>LT-DIST stream price</td>
<td>$/m^3</td>
</tr>
<tr>
<td>DSSFED</td>
<td>SSFEED stream price</td>
<td>$/m^3</td>
</tr>
<tr>
<td>DSTAB</td>
<td>STAB feed stream price</td>
<td>$/m^3</td>
</tr>
<tr>
<td>DFO</td>
<td>Fuel oil price</td>
<td>$/LFEm^3</td>
</tr>
<tr>
<td>F1EFF</td>
<td>C1 reboiler furnace efficiency</td>
<td>—</td>
</tr>
<tr>
<td>F2EFF</td>
<td>C2 reboiler furnace efficiency</td>
<td>—</td>
</tr>
<tr>
<td>WOBJ</td>
<td>Objective function weight</td>
<td>—</td>
</tr>
</tbody>
</table>

Table C.6: Constraint bounds used in the SPEEDUP real time optimizer input file ICNSTR.DAT.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>A11U</td>
<td>DIST-C4 C5’s mole fraction upper bound</td>
<td>lbmol/lbmol</td>
</tr>
<tr>
<td>A11L</td>
<td>DIST-C4 C5’s mole fraction lower bound</td>
<td>lbmol/lbmol</td>
</tr>
<tr>
<td>A31UR</td>
<td>LT-ISO Reid vapour pressure upper bound</td>
<td>psi</td>
</tr>
<tr>
<td>A31LT</td>
<td>C2 condenser bubble point temperature lower bound</td>
<td>°F</td>
</tr>
<tr>
<td>A41U1</td>
<td>HV-ISO 10% TBP (true boiling point) temperature upper bound</td>
<td>°F</td>
</tr>
<tr>
<td>A41L1</td>
<td>HV-ISO 10% TBP temperature lower bound</td>
<td>°F</td>
</tr>
</tbody>
</table>

continued on the next page
<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>A41U9</td>
<td>HV-ISO 90% TBP temperature upper bound</td>
<td>°F</td>
</tr>
<tr>
<td>A41L9</td>
<td>HV-ISO 90% TBP temperature lower bound</td>
<td>°F</td>
</tr>
<tr>
<td>A51U1</td>
<td>LT-DIST 10% TBP temperature upper bound</td>
<td>°F</td>
</tr>
<tr>
<td>A51L1</td>
<td>LT-DIST 10% TBP temperature lower bound</td>
<td>°F</td>
</tr>
<tr>
<td>A51U9</td>
<td>LT-DIST 90% TBP temperature upper bound</td>
<td>°F</td>
</tr>
<tr>
<td>A51L9</td>
<td>LT-DIST 90% TBP temperature lower bound</td>
<td>°F</td>
</tr>
<tr>
<td>F12U</td>
<td>C1 reflux standard liquid volume flow upper bound</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F12L</td>
<td>C1 reflux standard liquid volume flow lower bound</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F32U</td>
<td>C2 reflux standard liquid volume flow upper bound</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F41U</td>
<td>C4 feed stream standard liquid volume flow upper bound</td>
<td>bbl/day</td>
</tr>
<tr>
<td>F51U</td>
<td>C5 feed stream standard liquid volume flow upper bound</td>
<td>bbl/day</td>
</tr>
<tr>
<td>T11U</td>
<td>C1 tray 3 temperature upper bound</td>
<td>°F</td>
</tr>
<tr>
<td>T11L</td>
<td>C1 tray 3 temperature lower bound</td>
<td>°F</td>
</tr>
<tr>
<td>T22U</td>
<td>C1 reboiler outlet temperature upper bound</td>
<td>°F</td>
</tr>
<tr>
<td>T22L</td>
<td>C1 reboiler outlet temperature lower bound</td>
<td>°F</td>
</tr>
<tr>
<td>T31U</td>
<td>C2 tray 2 temperature upper bound</td>
<td>°F</td>
</tr>
<tr>
<td>T31L</td>
<td>C2 tray 2 temperature lower bound</td>
<td>°F</td>
</tr>
<tr>
<td>T62U</td>
<td>C2 reboiler outlet temperature upper bound</td>
<td>°F</td>
</tr>
<tr>
<td>T62L</td>
<td>C2 reboiler outlet temperature lower bound</td>
<td>°F</td>
</tr>
</tbody>
</table>
Table C.7: Optimization free variable ranges used in the SPEEDUP real time optimizer input file IOFREE.DAT.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1SPL1.L_OUT%</td>
<td>DIST-C4 stream mole flow</td>
<td>—</td>
</tr>
<tr>
<td>C1BT29.L_OUT1%</td>
<td>E1 inlet mole flow</td>
<td>—</td>
</tr>
<tr>
<td>C1BT29.L_OUT2%</td>
<td>C1 reboiler mole flow</td>
<td>—</td>
</tr>
<tr>
<td>C2COND.T_DROP</td>
<td>C2 condenser subcooled temperature drop</td>
<td>°F</td>
</tr>
<tr>
<td>C2FT21.T.IN</td>
<td>E1 outlet temperature</td>
<td>°F</td>
</tr>
<tr>
<td>C2BT24.L_OUT1%</td>
<td>SSFEED stream mole flow</td>
<td>—</td>
</tr>
<tr>
<td>C2BT24.L_OUT2%</td>
<td>C2 reboiler mole flow</td>
<td>—</td>
</tr>
<tr>
<td>C2SPL1.L_OUT1%</td>
<td>C4 feed stream mole flow</td>
<td>—</td>
</tr>
<tr>
<td>C2SPL2.L_OUT1%</td>
<td>C5 feed stream mole flow</td>
<td>—</td>
</tr>
<tr>
<td>C4REBL.L_OUT%</td>
<td>HV-ISO stream mole flow</td>
<td>—</td>
</tr>
<tr>
<td>C5REBL.L_OUT%</td>
<td>LT-DIST stream mole flow</td>
<td>—</td>
</tr>
</tbody>
</table>

C.6.7 RVARNC.DAT

RVARNC.DAT contains standard deviations used to determine the normal distributions for the random noise to be added to the plant measurements. This input file has the same format as IVARNC.DAT, with the 28 variances given in the same order as presented in Table C.2.

C.7 Results

Results from the real time optimizer are stored series of directories under the directory results/ for each iteration, e.g., for the first iteration the results are stored in results/itn1/. The results files stored after each iteration are summarised in Table C.8.
Table C.8: SPEEDUP real time optimizer results files.

<table>
<thead>
<tr>
<th>File</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>rtodr6.lis</td>
<td>Reconciled variables, offsets (reconciled - measured) and data reconciliation error contributions.</td>
</tr>
<tr>
<td>RDSET.DAT</td>
<td>SPEEDUP simulation settings after data reconciliation</td>
</tr>
<tr>
<td>rtopt6.lis</td>
<td>Optimization objective function, inequality constraint and set point summary</td>
</tr>
<tr>
<td>ROSET.DAT</td>
<td>SPEEDUP simulation settings after optimization</td>
</tr>
<tr>
<td>ROSMST.DAT</td>
<td>ASPEN PLUS simulation settings after optimization</td>
</tr>
<tr>
<td>PLVARS.DAT</td>
<td>Measures variables from the plant simulation</td>
</tr>
<tr>
<td>IMEAS.DAT</td>
<td>Measured variables from the plant with noise added for the next iteration of the real time optimizer</td>
</tr>
</tbody>
</table>

C.8 Example

C.8.1 Input Files

The eight input files required to run a SPEEDUP real time optimization run are listed below. They have been printed in two columns to save paper, but appear in a single column in the actual input file.

IMEAS.DAT

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>F01</td>
<td>.20863014E+05</td>
</tr>
<tr>
<td>F11</td>
<td>.75209442E+05</td>
</tr>
<tr>
<td>F12</td>
<td>.70246257E+04</td>
</tr>
<tr>
<td>F13</td>
<td>.88440222E+03</td>
</tr>
<tr>
<td>F21</td>
<td>.31955347E+05</td>
</tr>
<tr>
<td>F22</td>
<td>.19080626E+05</td>
</tr>
<tr>
<td>F31</td>
<td>.15802698E+04</td>
</tr>
<tr>
<td>F32</td>
<td>.12862473E+05</td>
</tr>
<tr>
<td>F41</td>
<td>.50296623E+04</td>
</tr>
<tr>
<td>F42</td>
<td>.38176940E+04</td>
</tr>
<tr>
<td>F51</td>
<td>.32645036E+04</td>
</tr>
<tr>
<td>F52</td>
<td>.18477370E+04</td>
</tr>
<tr>
<td>F61</td>
<td>.29933726E+05</td>
</tr>
<tr>
<td>Symbol</td>
<td>Value</td>
</tr>
<tr>
<td>--------</td>
<td>-----------</td>
</tr>
<tr>
<td>F62</td>
<td>1.2250671E+05</td>
</tr>
<tr>
<td>T01</td>
<td>4.1295470E+03</td>
</tr>
<tr>
<td>T12</td>
<td>1.5233838E+03</td>
</tr>
<tr>
<td>T13</td>
<td>9.6372107E+02</td>
</tr>
<tr>
<td>T21</td>
<td>5.1601320E+03</td>
</tr>
<tr>
<td>T22</td>
<td>5.8608488E+03</td>
</tr>
<tr>
<td>T23</td>
<td>4.7969655E+03</td>
</tr>
<tr>
<td>T31</td>
<td>1.2835124E+03</td>
</tr>
<tr>
<td>T32</td>
<td>8.4722528E+02</td>
</tr>
<tr>
<td>T41</td>
<td>2.4031157E+03</td>
</tr>
<tr>
<td>T42</td>
<td>2.6107760E+03</td>
</tr>
<tr>
<td>T51</td>
<td>3.5619866E+03</td>
</tr>
<tr>
<td>T52</td>
<td>4.2389816E+03</td>
</tr>
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IDFREE.DAT

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| C1FT14.T.IN  | 2.0000000E+02 |
| C1BT29.L.OUT1 | 1.0000000E+03 |
| C1BT29.L.OUT2 | 1.0000000E+03 |
| C2COND.Q  | 1.5000000E+02 |
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| C2FT21.T.IN  | 3.0000000E+02 |
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T31L  .12000000E+03
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IOFREE.DAT

C1SPL1.L_OUT%  .50000000E-01
C1BT29.L_OUT1%  .50000000E-01
C1BT29.L_OUT2%  .50000000E-01
C2COND.T_DROP  .50000000E+01
C2FT21.T_IN    .50000000E+01
C2BT24.L_OUT1%  .50000000E-01
C2BT24.L_OUT2%  .50000000E-01
C2SPL1.L_OUT1%  .50000000E-01
C2SPL2.L_OUT1%  .50000000E-01
C4REBL.L_OUT%  .50000000E-01
CSREBL.L_OUT%  .50000000E-01

RVARNC.DAT

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VF11   .37604721E+04
VF12   .35123129E+03
VF13   .44220110E+02
VF21   .15977674E+04
VF22   .95403132E+03
VF31   .79013490E+02
VF32   .64312363E+03
VF41   .25148312E+03
VF42   .19088470E+03
VF51   .16322518E+03
VF52   .92386852E+02
VF61   .14966863E+04
VF62   .61253356E+03
VT01   .20647735E+02
VT12   .76269189E+01
VT13   .48186054E+01
VT21   .25800660E+02
VT22   .29304244E+02
C.8.2 Command Line

If it the SPEEDUP real time optimizer has not already been setup, then type the command:

setup

When completed, type the command:

nohup nice run 1 &

to run one cycle of the real time optimizer.

C.8.3 Results

The following results will be present in the results/itn1/ directory.

rtodr6.lis

DATA RECONCILIATION SUMMARY REPORT CREATED BY SPEEDUP ON 09:06:97, 20:33:23
Page 1 of 1

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* VARIABLE, OFFSET & ERROR SUMMARY *
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T22 [F]  500.0  566.744151  675.0  
T31 [F]  120.0  167.804627  250.0  
T62 [F]  550.0  668.354528  700.0  
A11 [PERCENT C5's]  0.5  0.676120  15.0  
A31-RVP [PSI]  14.000000  14.0  
A31-TBUBBLE [F]  110.0  115.540881  
A41-TBP Q .10 VOL [F]  176.0  210.961598  266.0  
A41-TBP Q .90 VOL [F]  284.0  362.141645  464.0  
A51-TBP Q .10 VOL [F]  302.0  346.631296  554.0  
A51-TBP Q .90 VOL [F]  302.0  498.932721  554.0  

******************************************************************************
  * OBJECTIVE FUNCTION SUMMARY * 
******************************************************************************

FINAL OBJECTIVE FUNCTION VALUE (PROFIT) [$/HR] = 277.363060

TOTAL PRODUCT VALUES [$/HR] = 21848.829125
TOTAL FEED COSTS [$/HR] = 21456.451340
TOTAL UTILITY COSTS [$/HR] = 115.014725

STREAM  STD-VOL FLOWS  COLUMN  HEAT DUTY 
         [BBL/DAY]          [MMBTU/HR]  
STAB    4785.444846  C1   18.309412  
VAP     192.331490   C2   20.530202  
DIST-C4 185.050479   C2   20.530202  
LT-IS0  493.359652   
HV-IS0  884.070411   
LT-DIST 437.753338   
SSFEED  2604.696657   

-----------------------------------------------------------------------------
OPTIMIZATION SUMMARY REPORT CREATED BY SPEEDUP ON 10:06:97, 00:56:09
Page 2 of 3

******************************************************************************
  * VARIABLE SUMMARY * 
******************************************************************************
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F11 [CUFT/HR]  53952.071977
F12 [BBL/DAY]  6634.956996
F13 [BBL/DAY]  791.064361
F21 [BBL/DAY]  31614.429981
F22 [BBL/DAY]  18894.355852
F31 [BBL/DAY]  2109.042031
F32 [BBL/DAY]  12389.577530
F41 [BBL/DAY]  5418.612740
F42 [BBL/DAY]  3779.274709
F51 [BBL/DAY]  3503.996662
F52 [BBL/DAY]  1871.332985
F61 [BBL/DAY]  30341.849577
F62 [BBL/DAY]  11134.706108
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T61 [F]        628.022466
T62 [F]        668.354528

OPTIMIZATION SUMMARY REPORT CREATED BY SPEEDUP ON 10:06:97, 00:56:20
Page 3 of 3

* SET POINT SUMMARY *

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C1 REFLUX FLOW (F12) [BBL/DAY] = 6634.956996
C1 TRAY 3 TEMPERATURE (T11) [F] = 154.699978
C1 REBOILER TEMPERATURE (T22) [F] = 566.744151
C2 REFLUX FLOW (F32) [BBL/DAY] = 12389.577530
C4 FEED FLOW (F41) [BBL/DAY] = 5418.612740

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<tr>
<td>HV-ISO .90 TBP TEMPERATURE (A41) [F]</td>
<td>362.141645</td>
</tr>
<tr>
<td>LT-DIST .10 TBP TEMPERATURE (A51) [F]</td>
<td>346.631296</td>
</tr>
<tr>
<td>LT-DIST .90 TBP TEMPERATURE (A51) [F]</td>
<td>498.932721</td>
</tr>
</tbody>
</table>
NOTE TO USERS

Page(s) missing in number only; text follows. Microfilmed as received.
Appendix D

ASPEN PLUS Real Time Optimizer Code

D.1 setup

The following executable C-shell script, setup, is used to setup the ASPEN PLUS real time optimizer.

#!/bin/csh
#
# ASPEN PLUS RTO SETUP SCRIPT
#
# Sets up the Aspen Plus RTO simulation and plant simulations in
# preparation for real time optimization runs.
#
echo "=== SETTING UP ASPEN PLUS REAL TIME OPTIMIZER SIMULATIONS ==="
cd plant
# Check if input files all exist
if ( !(-e plant6.inp) ) then
    echo "=== SETUP: ERROR: plant/plant6.inp does not exist ==="
    exit
endif
if ( !(-e randdata.f) ) then
    echo "=== SETUP: ERROR: plant/randdata.f does not exist ==="
    exit
endif
echo "=== SETUP: Setting up ASPEN PLUS plant simulation ==="
aspen plant6 /itonly
echo "=== SETUP: Setting up variable noise FORTRAN ==="
f77 randdata.f -l nag -o randdata.exe
cd ..
cd rto
if (!(-e rto6.inp)) then
  echo "=== SETUP: ERROR: rto/rto6.inp does not exist ==="
  exit
endif
echo "=== SETUP: Setting up ASPEN PLUS RTO simulation ==="
aspen rto6 /itonly
echo "=== SETUP: COMPLETED ==="

D.2  run

The following executable C-shell script, run, is used to run a given number of cycles of the ASPEN PLUS real time optimizer.

#!/bin/csh
#
# ASPEN PLUS RTO RUN SCRIPT
#
# Runs the Aspen Plus RTO simulation and plant simulations.
#
# SYNTAX: run n
#        where n = number of cycles of the real time optimzer to be run
#                (default = 1 if n not given)
#
# echo "=== ASPEN PLUS REAL TIME OPTIMIZER SIMULATION ==="
# Check number of cycles to be performed
if ( "$1" >= 1 ) then
  set MAXITN = $1
else
  set MAXITN = 1
endif
set ITN = 1
# Make results directory, deleting old one first
if ( -e results ) then
  rm -r -f results
endif
mkdir results
cd results
mkdir start
cd ..
while ( $MAXITN >= $ITN )
  echo "=== REAL TIME OPTIMIZER CYCLE $ITN BEGINNING ==="
  cd results
  set RESITN = "itn$ITN"
  mkdir $RESITN
  cd ..
#
# ASPEN RTO6 RUN
#
# cd rto
# Check if input files all exist
if ( !(-e IMEAS.DAT) ) then
  echo "=== RUN: ERROR: rto/IMEAS.DAT does not exist ==="
  exit
endif
if ( !(-e IVARNC.DAT) ) then
  echo "=== RUN: ERROR: rto/IVARNC.DAT does not exist ==="
  exit
endif
if ( !(-e IWGHT.DAT) ) then
  echo "=== RUN: ERROR: rto/IWGHT.DAT does not exist ==="
  exit
endif
if ( !(-e IDFREE.DAT) ) then
  echo "=== RUN: ERROR: rto/IDFREE.DAT does not exist ==="
  exit
endif
if ( !(-e ISMST.DAT) ) then
  echo "=== RUN: ERROR: rto/ISMST.DAT does not exist ==="
  exit
endif
if ( !(-e IOBJFN.DAT) ) then
  echo "=== RUN: ERROR: rto/IOBJFN.DAT does not exist ==="
  exit
endif
if ( !(-e ICNSTR.DAT) ) then
  echo "=== RUN: ERROR: rto/ICNSTR.DAT does not exist ==="
  exit
endif
if ( !(-e IOFREE.DAT) ) then
  echo "=== RUN: ERROR: rto/IOFREE.DAT does not exist ==="
  exit
endif
# Remove any output files if they exist
if ( -e RDVARS.DAT ) then
    rm RDVARS.DAT
endif
if ( -e RDOFF.DAT ) then
    rm RDOFF.DAT
endif
if ( -e RDERR.DAT ) then
    rm RDERR.DAT
endif
if ( -e ROVARS.DAT ) then
    rm ROVARS.DAT
endif
if ( -e ROCNST.DAT ) then
    rm ROCNST.DAT
endif
if ( -e ROOPFN.DAT ) then
    rm ROOPFN.DAT
endif
if ( -e ROSMST.DAT ) then
    rm ROSMST.DAT
endif
if ( -e ROSTPT.DAT ) then
    rm ROSTPT.DAT
endif
# Run Aspen Plus rto6 job
    echo "=== RUN: Starting ASPEN PLUS RTO simulation ==="
    aspen rto6 /sponly
# Check if simulation ran to completion
    if ( !( -e ROSMST.DAT ) ) then
        echo "=== RUN: ERROR: an error occurred running aspen rto6 ==="
        exit
    endif
# Copy run results to results directory
    cp R*.DAT ../results/$RESITN
    if ( "$RESITN" == "itn1" ) then
        cp IMEAS.DAT ../results/start
        cp ISMST.DAT ../results/start
    endif
# Rename files for next cycle
    cp ROSMST.DAT ISMST.DAT
# # ASPEN PLANT6 RUN
# # Set up for plant6 run
    cp ROSMST.DAT ../plant
cd ..
cd plant
# Check if input files all exist
if ( !(-e ROSTM.DAT) ) then
  echo "== RUN: ERROR: plant/ROSTM.DAT does not exist =="
  exit
endif
# Remove any output files if they exist
if ( -e PLVARS.DAT ) then
  rm PLVARS.DAT
endif
# Run Aspen Plus plant6 job
  echo "== RUN: Starting ASPEN PLUS PLANT simulation =="
  aspen plant6 /sponly
# Check if simulation ran to completion
if ( !(-e PLVARS.DAT) ) then
  echo "== RUN: ERROR: an error occurred running aspen plant6 =="
  exit
endif
# Copy run results to results directory
cp PLVARS.DAT ../results/$RESITN
#
# FORTRAN RANDDATA RUN
#
# Check if input files all exist
if ( !(-e PLVARS.DAT) ) then
  echo "== RUN: ERROR: plant/PLVARS.DAT does not exist =="
  exit
endif
if ( !(-e RVARNC.DAT) ) then
  echo "== RUN: ERROR: plant/RVARNC.DAT does not exist =="
  exit
endif
# Remove any output files if they exist
if ( -e IMEAS.DAT ) then
  rm IMEAS.DAT
endif
# Run FORTRAN randdata.exe job
  echo "== RUN: Starting randdata.exe =="
  randdata.exe
# Check if simulation ran to completion
if ( !(-e IMEAS.DAT) ) then
  echo "== RUN: ERROR: an error occurred running randdata.exe =="
  exit
endif
# Copy run results to results directory
   cp IMEAS.DAT ../results/$RESITN
# Send files to Data Rec run, next cycle
   cp IMEAS.DAT ../rto
   cd ..
   set ITN = 'expr $ITN + 1'
end
   cp rto/rto6.rep results
   cp plant/plant6.rep results
   echo "== MAXITN REAL TIME OPTIMIZER CYCLES COMPLETED =="

D.3 rto6.inp

The following ASPEN PLUS input code, rto6.inp, forms both the data reconciliation and optimization simulations.

; ; Input Summary created by ASPEN PLUS Rel. 9.2-1 at 13:31:24 Wed May 14, 1997
; Directory D:\ Fileame D:\rto6.inp
;
TITLE 'STABILIZER-SPLITTER REAL TIME OPTIMIZATION'

IN-UNITS ENG VOLUME-FLOW='BBL/DAY' ENTHALPY-FLO='MMBTU/HR' &
                 VOLUME=BBL HEAD=FT HEAT=MMBTU

DEF-STREAMS CONVEN ALL

DIAGNOSTICS
   HISTORY SYS-LEVEL=3 SIM-LEVEL=2 PROP-LEVEL=1 STREAM-LEVEL=1 &
           CONV-LEVEL=4 COST-LEVEL=0 ECON-LEVEL=0
   TERMINAL SIM-LEVEL=2 CONV-LEVEL=4 COST-LEVEL=0 PROP-LEVEL=1 &
           ECON-LEVEL=0 STREAM-LEVEL=1 SYS-LEVEL=3

SIM-OPTIONS
   IN-UNITS ENG
   SIM-OPTIONS FREE-WATER=NO

RUN-CONTROL MAX-TIME=1.0000E+08 MAX-ERRORS=9999 MAX-FORT-ERR=50

DESCRIPTION "
   STABILIZER (C1): MODELLED BY RADFRAC WITH 29 STAGES WITH A PUMPAROUND
   REBOILER."
SPLITTER (C2, C4, C5): MODELLED BY PETROFRAC WITH A 24 STAGE MAIN COLUMN WITH AN EXTERNAL REBOILER, AND TWO 3 STAGE REBOILED SIDESTRIPPERS (C4 AND C5). EXTERNAL REBOILER CONSISTES OF AN FSPLIT AND A HEATER.

PROPERTIES: 15 PSEUDO-COMPONENTS, 8 CONVENTIONAL COMPONENTS, PENG-ROBINSON E.O.S. (N.B. WATER IS NOT USED - NO FREE WATER CALCS).

BASIS: MOLE BASIS USED (LB/MOL/HR).

DATA RECONCILIATION: USING WEIGHTED LEAST SQUARES OBJECTIVE FUNCTION SOLVED USING SQP OPTIMIZATION ALGORITHM.

OPTIMIZATION: MAXIMIZING A PROFIT OBJECTIVE FUNCTION SOLVED USING SQP OPTIMIZATION ALGORITHM."

DATABANKS ASPENPCD / PURE856 / PURECOMP / AQUEOUS / & SOLIDS / INORGANIC

PROP-SOURCES ASPENPCD / PURE856 / PURECOMP / AQUEOUS / & SOLIDS / INORGANIC

COMPONENTS
H2, H2, H2 / METHANE CH4 METHANE /
ETHANE C2H6 ETHANE /
PROPANE C3H8 PROPANE /
IBUTANE C4H10-2 IBUTANE /
BUTANE C4H10-1 BUTANE /
IPENTANE C5H12-2 IPENTANE /
PENTANE C5H12-1 PENTANE /
B45T65 * B45T65 /
B65T85 * B65T85 /
B85T105 * B85T105 /
B105T125 * B105T125 /
B125T145 * B125T145 /
B145T165 * B145T165 /
B165T185 * B165T185 /
B185T205 * B185T205 /
B205T235 * B205T235 /
B235T265 * B235T265 /
B265T295 * B265T295 /
B295T325 * B295T325 /
B325T355 * B325T355 /
B355T395 * B355T395 /
B395T510 * B395T510

PC-USER
PC-DEF API-METH B45T65 NBP=128.49380 GRAV=.64840 &
MW=85.98380
PC-DEF API-METH B65T85 NBP=167.34120 GRAV=.69060 &
   MW=89.15430
PC-DEF API-METH B85T105 NBP=203.78650 GRAV=.71370 &
   MW=99.91430
PC-DEF API-METH B105T125 NBP=239.16230 GRAV=.7320 &
   MW=110.25780
PC-DEF API-METH B125T145 NBP=275.02460 GRAV=.74760 &
   MW=120.44870
PC-DEF API-METH B145T165 NBP=310.94660 GRAV=.76280 &
   MW=132.08530
PC-DEF API-METH B165T185 NBP=347.01010 GRAV=.77630 &
   MW=144.87180
PC-DEF API-METH B185T205 NBP=383.08250 GRAV=.78560 &
   MW=160.93490
PC-DEF API-METH B205T235 NBP=428.20310 GRAV=.79940 &
   MW=180.13470
PC-DEF API-METH B235T265 NBP=482.06570 GRAV=.81410 &
   MW=204.11590
PC-DEF API-METH B265T295 NBP=537.76350 GRAV=.8240 &
   MW=236.50410
PC-DEF API-METH B295T325 NBP=590.42290 GRAV=.82590 &
   MW=270.94860
PC-DEF API-METH B325T355 NBP=643.56240 GRAV=.83250 &
   MW=307.94140
PC-DEF API-METH B355T395 NBP=704.2320 GRAV=.83780 &
   MW=354.40350
PC-DEF API-METH B395T510 NBP=786.51950 GRAV=.85560 &
   MW=418.92730

FLOWSHEET
  BLOCK C1 IN=STAB OUT=VAP DIST-C4 SPLITFEED C1RFLX C1REBL
  BLOCK C2C4CS IN=SPLIT C2REBL OUT=LT-ISO C2BOT HV-ISO &
    LT-DIST C2RFLX IC1 IC2
  BLOCK E1 IN=SPLITFEED OUT=SPLIT
  BLOCK F2 IN=C2RBFD OUT=C2REBL
  BLOCK C2SPL1 IN=C2BOT OUT=C2RBFD SSFEED

PROPERTIES PENG-ROB SOLU-WATER=2

PROP-SET RVP REIDVP SUBSTREAM=MIXED

PROP-SET STDVOL VLSTDMX UNITS='BBL/DAY' SUBSTREAM=MIXED PHASE=T

PROP-SET TBP-10 TBPT SUBSTREAM=MIXED LVPCT=10.0
PROP-SET TBP-90 TBPT SUBSTREAM=MIXED LVPCT=90.0

PROP-SET TBUB TBUB SUBSTREAM=MIXED

PROP-SET V-STDVOL VMX UNITS='CUFT/HR' SUBSTREAM=MIXED PHASE=V &
TEMP=60.0 PRES=14.6960

PROP-SET VOL VMX UNITS='CUFT/HR' SUBSTREAM=MIXED PHASE=T

STREAM C2REBL
SUBSTREAM MIXED TEMP=683.899910 PRES=35.65810 &
MOLE-FLOW=1327.2170
MOLE-FRAC H2 0.0 / METHANE 1.3091E-18 / ETHANE &
3.9177E-15 / PROPANE 3.4897E-11 / IBUTANE 2.3334E-08 / &
BUTANE 5.2249E-08 / IPENTANE 1.0680E-06 / PENTANE &
6.7323E-07 / B4ST65 5.3548E-06 / B6ST85 0.00013843 / &
B8ST105 .000042311 / B10ST125 .000123760 / B12ST145 &
.000363910 / B14ST165 .00117030 / B16ST185 .00455110 / &
B18ST205 .0187060 / B20ST235 .1040 / B23ST265 .14430 &
/ B26ST295 .16840 / B29ST325 .17710 / B32ST355 &
.15840 / B35ST395 .14950 / B39ST510 .073060

STREAM STAB
SUBSTREAM MIXED TEMP=412.954698 PRES=200.0 &
MOLE-FLOW=1487.17710
MOLE-FRAC H2 .000703680 / METHANE .0246830 / ETHANE &
.0473640 / PROPANE .0387240 / IBUTANE .0535310 / &
BUTANE .0312790 / IPENTANE .0351930 / PENTANE &
.0161490 / B4ST65 .0472560 / B6ST85 .0435620 / &
B8ST105 .0496490 / B10ST125 .0530710 / B12ST145 &
.0523260 / B14ST165 .0489630 / B16ST185 .0444180 / &
B18ST205 .041240 / B20ST235 .0607690 / B23ST265 &
.0537820 / B26ST295 .0598310 / B29ST325 .0626870 / &
B32ST355 .056050 / B35ST395 .0529210 / B39ST510 &
.0258480

BLOCK C2SPL1 FSPLIT
DESCRIPTION "C2 BOTTOMS FLOW SPLITTER"
MOLE-FLOW C2RBFD 1327.2170

BLOCK E1 HEATER
IN-UNITS ENG VOLUME-FLOW='BBL/DAY' ENTHALPY-FLO='MMBTU/HR'
DESCRIPTION "E1 HEAT EXCHANGER"
PARAM TEMP=479.65650 PRES=34.0
BLOCK F2 HEATER
DESCRIPTION "C2 REBOILER FURNACE"
PARAM TEMP=683.899910 PRES=0.0

BLOCK C1 RADFRAC
SUBOBJECTS PUMPAROUND = C1REBL
DESCRIPTION "STABILISER"
PARAM NSTAGE=29 NPA=1
PUMPAROUND C1REBL 29 29 NPHASE=2 MOLE-FLOW=2005.69940 &
TEMP=586.084880
FEEDS STAB 14 ON-STAGE
PRODUCTS VAP 1 V / DIST-C4 1 L / SPLITFEED 29 L
PSEUDO-STREA C1RFLX 1 / C1REBL PA=C1REBL
P-SPEC 1 163.0 / 2 167.0
CDL-SPECS QN=0.0 DP-CDL=6.0 MOLE-RDV=.60262460 &
MOLE-RR=3.15630830
T-EST 1 89.5350 / 2 149.04 / 3 169.260 / 4 182.040 / &
5 192.140 / 6 200.260 / 7 206.640 / 8 211.760 / &
9 216.380 / 10 221.630 / 11 229.350 / 12 243.370 / &
13 275.160 / 14 386.670 / 15 389.440 / 16 391.110 &
17 392.160 / 18 392.890 / 19 393.490 / 20 &
394.060 / 21 394.670 / 22 395.410 / 23 396.360 / &
24 397.680 / 25 399.710 / 26 403.380 / 27 411.850 &
/ 28 436.50 / 29 519.830
L-EST 1 1022.0250 / 2 991.26280 / 3 989.080 / 4 &
974.47260 / 5 962.86240 / 6 955.53050 / 7 949.85040 &
/ 8 942.2590 / 9 928.30430 / 10 900.91910 / 11 &
845.60520 / 12 723.95590 / 13 413.96660 / 14 &
1449.9490 / 15 1500.8610 / 16 1531.4830 / 17 &
1550.3670 / 18 1563.3520 / 19 1573.6410 / 20 &
1583.0950 / 21 1593.0030 / 22 1604.5030 / 23 &
1618.8610 / 24 1637.8240 / 25 1664.3390 / 26 &
1703.9790 / 27 1764.4650 / 28 1818.9030 / 29 &
3205.2810
V-EST 1 173.31230 / 2 1195.3370 / 3 1278.8590 / 4 &
1276.7670 / 5 1262.0680 / 6 1250.4580 / 7 1243.1260 &
/ 8 1237.4460 / 9 1229.8550 / 10 1215.90 / 11 &
1188.5150 / 12 1133.2010 / 13 1011.5520 / 14 &
701.56250 / 15 250.3680 / 16 301.27930 / 17 &
331.90150 / 18 350.78570 / 19 363.77040 / 20 &
374.06010 / 21 383.51360 / 22 393.42180 / 23 &
404.92140 / 24 419.27950 / 25 438.24310 / 26 &
464.75790 / 27 504.39750 / 28 564.88340 / 29 &
619.32170
TRAY-REPORT TRAY-OPTION=ALL-TRAYS WIDE=YES
REPORT NOCOMP NOHYDRAULIC NOENTH NOSPLITS

BLOCK C2C4C5 PETROFRAC
SUBOBJECTS STRIPPER = C4 C5
DESCRIPTION "SPLITTER"
PARAM NP=0 NST=2 NST=26 NST=24 HYDRAULIC=NO
FEEDS SPLIT 21 ON-STAGE / C2REBL 24 ON-STAGE
PRODUCTS LT-ISO 1 L / C2BOT 24 L
COL-SPECS CONDENSER=SUBLICCOOL REBOILER=NONE-BOTFEED &
T1=84.725280 MOLE-D=186.54790 DP-COL=12.70
P-SPEC 1 18.95810 / 2 22.95810
T-EST 1 84.7230 / 2 150.930 / 3 169.420 / 4 181.130 / &
  5 188.750 / 6 194.010 / 7 197.990 / 8 201.440 / &
  9 204.930 / 10 208.970 / 11 214.20 / 12 221.490 / &
  13 232.330 / 14 249.640 / 15 278.020 / 16 320.730 &
  / 17 358.980 / 18 388.210 / 19 415.850 / 20 &
  441.860 / 21 483.390 / 22 531.190 / 23 570.180 / &
  24 626.450
V-EST 1 0.0 / 2 2776.1290 / 3 3094.8350 / 4 3095.9990 &
  / 5 3101.710 / 6 3106.5220 / 7 3108.8040 / 8 &
  3107.4250 / 9 3100.7670 / 10 3086.2130 / 11 &
  3059.6610 / 12 3014.5630 / 13 2939.0650 / 14 &
  2809.8090 / 15 2473.5240 / 16 2206.0180 / 17 &
  2037.2320 / 18 1833.3290 / 19 1747.6360 / 20 &
  1647.220 / 21 1439.3880 / 22 772.39920 / 23 &
  965.84870 / 24 953.74740
L-EST 1 2776.1290 / 2 2908.260 / 3 2909.4240 / 4 &
  2915.1350 / 5 2919.9470 / 6 2922.2390 / 7 2920.850 &
  / 8 2914.1920 / 9 2899.6380 / 10 2873.0860 / 11 &
  2827.9890 / 12 2752.490 / 13 2623.2340 / 14 &
  2410.6880 / 15 2143.1810 / 16 1496.7840 / 17 &
  1408.0990 / 18 1322.4060 / 19 973.77810 / 20 &
  765.94590 / 21 1298.5380 / 22 1491.9880 / 23 &
  1479.8870 / 24 1853.3340
PSEUDO-STREA C2RFLX STAGE=1
STRIPPER C4 NSTAGE=3 LDR=15 VR=14 PRODUCT=HV-ISO &
MOLE-DR=47.61110 Q-REC=1.9090
STRIPPER C5 NSTAGE=3 LDR=18 VR=17 PRODUCT=LT-DIST &
MOLE-DR=248.21130 Q-REC=2.39920
STR-T-EST C4 1 278.790 / C4 2 282.20 / C4 3 292.030 / &
  C5 1 402.780 / C5 2 414.880 / C5 3 429.50
STR-V-EST C4 1 123.70 / C4 2 122.70 / C4 3 123.40 / &
  C5 1 115.20 / C5 2 125.60 / C5 3 130.40
STR-L-EST C4 1 476.60 / C4 2 477.20 / C4 3 353.90 / &
C5 1 258.60 / C5 2 263.40 / C5 3 133.0
STR-PSEUDO-S C4 IC1 SOURCE=FEED DRAW=15 / C5 IC2 &
SOURCE=FEED DRAW=18
TRAY-REPORT TRAY-OPTION=ALL-TRAYS WIDE=YES
REPORT RESULTS NOCOMPS NOHYDRAULIC NOENTH

FORTRAN DRDATA
F COMMON / USRSF1 / SF01, SF11, SF12, SF13, SF21, SF22
F COMMON / USRSF2 / SF31, SF32, SF41, SF42, SF51, SF52, SF61, SF62
F COMMON / USRSR1 / ST01, ST12, ST13, ST21, ST22, ST23
F COMMON / USRSR2 / ST31, ST32, ST41, ST42, ST51, ST52, ST61, ST62
F COMMON / USREF1 / EF01, EF11, EF12, EF13, EF21, EF22
F COMMON / USREF2 / EF31, EF32, EF41, EF42, EF51, EF52, EF61, EF62
F COMMON / USRET1 / ET01, ET12, ET13, ET21, ET22, ET23
F COMMON / USRET2 / ET31, ET32, ET41, ET42, ET51, ET52, ET61, ET62
F LOGICAL THERE
DEFINE F01 STREAM-VAR STREAM=STAB SUBSTREAM=MIXED &
VARIABLE=STDVOL-FLOW
DEFINE F11 STREAM-PROP STREAM=VAP PROPERTY=V-STDVOL
DEFINE F12 STREAM-VAR STREAM=C1RFLX SUBSTREAM=MIXED &
VARIABLE=STDVOL-FLOW
DEFINE F13 STREAM-VAR STREAM=DIST-C4 SUBSTREAM=MIXED &
VARIABLE=STDVOL-FLOW
DEFINE F21 STREAM-VAR STREAM=C1REBL SUBSTREAM=MIXED &
VARIABLE=STDVOL-FLOW
DEFINE F22 STREAM-VAR STREAM=SPLTFEED SUBSTREAM=MIXED &
VARIABLE=STDVOL-FLOW
DEFINE F31 STREAM-VAR STREAM=LT-ISO SUBSTREAM=MIXED &
VARIABLE=STDVOL-FLOW
DEFINE F32 STREAM-VAR STREAM=C2RFLX SUBSTREAM=MIXED &
VARIABLE=STDVOL-FLOW
DEFINE F41 STREAM-VAR STREAM=IC1 SUBSTREAM=MIXED &
VARIABLE=STDVOL-FLOW
DEFINE F42 STREAM-VAR STREAM=HV-ISO SUBSTREAM=MIXED &
VARIABLE=STDVOL-FLOW
DEFINE F51 STREAM-VAR STREAM=IC2 SUBSTREAM=MIXED &
VARIABLE=STDVOL-FLOW
DEFINE F52 STREAM-VAR STREAM=LT-DIST SUBSTREAM=MIXED &
VARIABLE=STDVOL-FLOW
DEFINE F61 STREAM-VAR STREAM=C2REBL SUBSTREAM=MIXED &
VARIABLE=STDVOL-FLOW
DEFINE F62 STREAM-VAR STREAM=SSFEED SUBSTREAM=MIXED &
VARIABLE=STDVOL-FLOW
DEFINE T01 STREAM-VAR STREAM=STAB SUBSTREAM=MIXED &
VARIABLE=TEMP
DEFINE T12 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
SENTENCE=PROFILE ID1=2
DEFINE T13 STREAM-VAR STREAM=DIST-C4 SUBSTREAM=MIXED &
VARIABLE=TEMP
DEFINE T21 STREAM-VAR STREAM=SPLITFEED SUBSTREAM=MIXED &
VARIABLE=TEMP
DEFINE T22 STREAM-VAR STREAM=C1REBL SUBSTREAM=MIXED &
VARIABLE=TEMP
DEFINE T23 STREAM-VAR STREAM=SPLIT SUBSTREAM=MIXED &
VARIABLE=TEMP
DEFINE T31 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=PROFILE ID1=2
DEFINE T32 STREAM-VAR STREAM=LT-ISO SUBSTREAM=MIXED &
VARIABLE=TEMP
DEFINE T41 STREAM-VAR STREAM=IC1 SUBSTREAM=MIXED &
VARIABLE=TEMP
DEFINE T42 STREAM-VAR STREAM=HV-ISO SUBSTREAM=MIXED &
VARIABLE=TEMP
DEFINE T51 STREAM-VAR STREAM=IC2 SUBSTREAM=MIXED &
VARIABLE=TEMP
DEFINE T52 STREAM-VAR STREAM=LT-DIST SUBSTREAM=MIXED &
VARIABLE=TEMP
DEFINE T61 STREAM-VAR STREAM=SSFEED SUBSTREAM=MIXED &
VARIABLE=TEMP
DEFINE T62 STREAM-VAR STREAM=C2REBL SUBSTREAM=MIXED &
VARIABLE=TEMP
F WRITE(NTERM,*) '+++ DATA REC RESULTS FORTRAN STARTED +++'
C WRITE TO FILE MEASURED VARIABLES VALUES AFTER DATA REC
F IF (THERE) THEN
F WRITE(NTERM,*) '+++ ERROR: RDVARS.DAT ALREADY EXISTS +++'
F WRITE(NRPT,*) '+++ ERROR: RDVARS.DAT ALREADY EXISTED +++'
F WRITE(NHSTRY,*) '+++ ERROR: RDVARS.DAT ALREADY EXISTS +++'
F GO TO 50
F ENDIF
F OPEN (UNIT=63, STATUS='NEW', FILE='RDVARS.DAT')
F WRITE(63,100) 'F01', F01
F WRITE(63,100) 'F11', F11
F WRITE(63,100) 'F12', F12
F WRITE(63,100) 'F13', F13
F WRITE(63,100) 'F21', F21
F WRITE(63,100) 'F22', F22
F WRITE(63,100) 'F31', F31
F WRITE(63,100) 'F32', F32
F WRITE(63,100) 'F41', F41
WRITE(63,100) 'F42', F42
WRITE(63,100) 'F51', F51
WRITE(63,100) 'F52', F52
WRITE(63,100) 'F61', F61
WRITE(63,100) 'F62', F62
WRITE(63,100) 'T01', T01
WRITE(63,100) 'T12', T12
WRITE(63,100) 'T13', T13
WRITE(63,100) 'T21', T21
WRITE(63,100) 'T22', T22
WRITE(63,100) 'T23', T23
WRITE(63,100) 'T31', T31
WRITE(63,100) 'T32', T32
WRITE(63,100) 'T41', T41
WRITE(63,100) 'T42', T42
WRITE(63,100) 'T51', T51
WRITE(63,100) 'T52', T52
WRITE(63,100) 'T61', T61
WRITE(63,100) 'T62', T62
CLOSE (UNIT=63)
WRITE(UNIT,=) 'RDVARS.DAT WRITTEN SUCCESSFULLY'
WRITE (NDIM,=) 'WRITE TO FILE MEASURED TO RECONCILED VAR OFFSETS AFTER DATA REC'
WRITE (50,=) (FILE=['RDOFF.DAT', EXIST= THERE)
IF ( THERE) THEN
WRITE (NDIM,=) '*** ERROR: RDOFF.DAT ALREADY EXISTS ***'
WRITE (NRPT,=) '*** ERROR: RDOFF.DAT ALREADY EXISTED ***'
WRITE (NHSTRY,=) '*** ERROR: RDOFF.DAT ALREADY EXISTS ***'
GO TO 52
ENDIF
OPEN (UNIT=63, STATUS='NEW', FILE='RDOFF.DAT')
OFF01 = F01-SF01
OFF11 = F11-SF11
OFF12 = F12-SF12
OFF13 = F13-SF13
OFF21 = F21-SF21
OFF22 = F22-SF22
OFF23 = F23-SF23
OFF41 = F41-SF41
OFF42 = F42-SF42
OFF51 = F51-SF51
OFF52 = F52-SF52
OFF61 = F61-SF61
OFF62 = F62-SF62
OFF71 = T01-ST01
OFFT12 = T12-ST12
OFFT13 = T13-ST13
OFFT21 = T21-ST21
OFFT22 = T22-ST22
OFFT23 = T23-ST23
OFFT31 = T31-ST31
OFFT32 = T32-ST32
OFFT41 = T41-ST41
OFFT42 = T42-ST42
OFFT51 = T51-ST51
OFFT52 = T52-ST52
OFFT61 = T61-ST61
OFFT62 = T62-ST62
WRITE(63,100) 'OFFF01', OFFF01
WRITE(63,100) 'OFFF11', OFFF11
WRITE(63,100) 'OFFF12', OFFF12
WRITE(63,100) 'OFFF13', OFFF13
WRITE(63,100) 'OFFF21', OFFF21
WRITE(63,100) 'OFFF22', OFFF22
WRITE(63,100) 'OFFF31', OFFF31
WRITE(63,100) 'OFFF32', OFFF32
WRITE(63,100) 'OFFF41', OFFF41
WRITE(63,100) 'OFFF42', OFFF42
WRITE(63,100) 'OFFF51', OFFF51
WRITE(63,100) 'OFFF52', OFFF52
WRITE(63,100) 'OFFF61', OFFF61
WRITE(63,100) 'OFFF62', OFFF62
WRITE(63,100) 'OFFT01', OFFT01
WRITE(63,100) 'OFFT12', OFFT12
WRITE(63,100) 'OFFT13', OFFT13
WRITE(63,100) 'OFFT21', OFFT21
WRITE(63,100) 'OFFT22', OFFT22
WRITE(63,100) 'OFFT23', OFFT23
WRITE(63,100) 'OFFT31', OFFT31
WRITE(63,100) 'OFFT32', OFFT32
WRITE(63,100) 'OFFT41', OFFT41
WRITE(63,100) 'OFFT42', OFFT42
WRITE(63,100) 'OFFT51', OFFT51
WRITE(63,100) 'OFFT52', OFFT52
WRITE(63,100) 'OFFT61', OFFT61
WRITE(63,100) 'OFFT62', OFFT62
CLOSE (UNIT=63)
WRITE(1,*) 'RDOFF.DAT WRITTEN SUCCESSFULLY'
WRITE (1,*) 'WRITE TO FILE DATA RECONCILIATION ERROR TERMS
F 52 INQUIRE (FILE='RDELR.DAT', EXIST=HERE)
IF (THERE) THEN
  WRITE(NTERM,*) '*** ERROR: RDERR.DAT ALREADY EXISTS ***'
  WRITE(NRPT,*) '*** ERROR: RDERR.DAT ALREADY EXISTED ***'
  WRITE(NHSTRY,*) '*** ERROR: RDERR.DAT ALREADY EXISTS ***'
  GO TO 54
ENDIF
OPEN (UNIT=63, STATUS='NEW', FILE='RDERR.DAT')
WRITE(63,100) 'ERRF01', EF01
WRITE(63,100) 'ERRF11', EF11
WRITE(63,100) 'ERRF12', EF12
WRITE(63,100) 'ERRF13', EF13
WRITE(63,100) 'ERRF21', EF21
WRITE(63,100) 'ERRF22', EF22
WRITE(63,100) 'ERRF31', EF31
WRITE(63,100) 'ERRF32', EF32
WRITE(63,100) 'ERRF41', EF41
WRITE(63,100) 'ERRF42', EF42
WRITE(63,100) 'ERRF51', EF51
WRITE(63,100) 'ERRF52', EF52
WRITE(63,100) 'ERRF61', EF61
WRITE(63,100) 'ERRF62', EF62
WRITE(63,100) 'ERRT01', ET01
WRITE(63,100) 'ERRT12', ET12
WRITE(63,100) 'ERRT13', ET13
WRITE(63,100) 'ERRT21', ET21
WRITE(63,100) 'ERRT22', ET22
WRITE(63,100) 'ERRT23', ET23
WRITE(63,100) 'ERRT31', ET31
WRITE(63,100) 'ERRT32', ET32
WRITE(63,100) 'ERRT41', ET41
WRITE(63,100) 'ERRT42', ET42
WRITE(63,100) 'ERRT51', ET51
WRITE(63,100) 'ERRT52', ET52
WRITE(63,100) 'ERRT61', ET61
WRITE(63,100) 'ERRT62', ET62
CLOSE (UNIT=63)
WRITE(NTERM,*) 'RDERR.DAT WRITTEN SUCCESSFULLY'
54 WRITE(NTERM,*) '+++ DATA REC RESULTS FORTRAN COMPLETED +++'
C FORMAT STATEMENTS
100 FORMAT(A13, 2X, E15.8)
EXECUTE LAST

FORTRAN DRSPCSET
COMMON / USRSF1 / SF01, SF11, SF12, SF13, SF21, SF22
COMMON / USRSF2 / SF31, SF32, SF41, SF42, SF51, SF52, SF61, SF62
DEFINE STABF STREAM=VAR STREAM=STAB SUBSTREAM=MIXED &
        VARIABLE=MOLE-FLOW
DEFINE STABT STREAM=VAR STREAM=STAB SUBSTREAM=MIXED &
        VARIABLE=TEMP
DEFINE STABP STREAM=VAR STREAM=STAB SUBSTREAM=MIXED &
        VARIABLE=PRES
DEFINE STBZ1 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
        COMPONENT=H2
DEFINE STBZ2 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
        COMPONENT=METHANE
DEFINE STBZ3 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
        COMPONENT=ETHANE
DEFINE STBZ4 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
        COMPONENT=PROPANE
DEFINE STBZ5 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
        COMPONENT=IBUTANE
DEFINE STBZ6 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
        COMPONENT=BUTANE
DEFINE STBZ7 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
        COMPONENT=IPENTANE
DEFINE STBZ8 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
        COMPONENT=PENTANE
DEFINE STBZ9 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
        COMPONENT=B45T65
DEFINE STBZ10 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
        COMPONENT=B65T85
DEFINE STBZ11 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
        COMPONENT=B85T105
DEFINE STBZ12 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
        COMPONENT=B105T125
DEFINE STBZ13 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
COMPONENT=B125T145
DEFINE STBZ14 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
COMPONENT=B145T165
DEFINE STBZ15 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
COMPONENT=B165T185
DEFINE STBZ16 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
COMPONENT=B185T205
DEFINE STBZ17 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
COMPONENT=B205T235
DEFINE STBZ18 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
COMPONENT=B235T265
DEFINE STBZ19 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
COMPONENT=B265T295
DEFINE STBZ20 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
COMPONENT=B295T325
DEFINE STBZ21 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
COMPONENT=B325T355
DEFINE STBZ22 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
COMPONENT=B355T395
DEFINE STBZ23 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
COMPONENT=B395T510
DEFINE C2RB1 BLK-VAR BLOCK=C2SPL1 SENTENCE=MOLE-FLOW &
VARIABLE=FLOW ID1=C2RBFD
DEFINE C2RB2 STREAM-VAR STREAM=C2REBL SUBSTREAM=MIXED &
VARIABLE=MOLE-FLOW
DEFINE C2RB1 BLOCK-VAR BLOCK=F2 VARIABLE=TEMP &
SENTENCE=PARAM
DEFINE C2RB2 STREAM-VAR STREAM=C2REBL SUBSTREAM=MIXED &
VARIABLE=TEMP
DEFINE C2RP1 BLOCK-VAR BLOCK=F2 VARIABLE=PRES &
SENTENCE=PARAM
DEFINE C2RP2 STREAM-VAR STREAM=C2REBL SUBSTREAM=MIXED &
VARIABLE=PRES
DEFINE C2RZ1 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
COMPONENT=H2
DEFINE C2RZ2 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
COMPONENT=METHANE
DEFINE C2RZ3 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
COMPONENT=ETHANE
DEFINE C2RZ4 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
COMPONENT=PROPANE
DEFINE C2RZ5 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
COMPONENT=IBUTANE
DEFINE C2RZ6 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
COMPONENT= BUTANE
DEFINE C2RZ7 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
    COMPONENT=IPENTANE
DEFINE C2RZ8 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
    COMPONENT=PENTANE
DEFINE C2RZ9 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
    COMPONENT=B45T65
DEFINE C2RZ10 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
    COMPONENT=B65T85
DEFINE C2RZ11 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
    COMPONENT=B85T105
DEFINE C2RZ12 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
    COMPONENT=B105T125
DEFINE C2RZ13 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
    COMPONENT=B125T145
DEFINE C2RZ14 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
    COMPONENT=B145T165
DEFINE C2RZ15 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
    COMPONENT=B165T185
DEFINE C2RZ16 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
    COMPONENT=B185T205
DEFINE C2RZ17 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
    COMPONENT=B205T235
DEFINE C2RZ18 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
    COMPONENT=B235T265
DEFINE C2RZ19 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
    COMPONENT=B265T295
DEFINE C2RZ20 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
    COMPONENT=B295T325
DEFINE C2RZ21 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
    COMPONENT=B325T355
DEFINE C2RZ22 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
    COMPONENT=B355T395
DEFINE C2RZ23 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED &
    COMPONENT=B395T510
DEFINE E1T BLOCK-VAR BLOCK=E1 VARIABLE=TEMP SENTENCE=PARAM
DEFINE E1P BLOCK-VAR BLOCK=E1 VARIABLE=PRES SENTENCE=PARAM
DEFINE C1RR BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-RR &
    SENTENCE=COL-SPECS
DEFINE C1RDV BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-RDV &
    SENTENCE=COL-SPECS
DEFINE C1RBL BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=PUMPAROUND ID1=C1REBL
DEFINE C1RBT BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=PUMPAROUND ID1=C1REBL
DEFINE C1P1 BLOCK-VAR BLOCK=C1 VARIABLE=PRES &
SENTENCE=P-SPEC ID1=1
DEFINE C1P2 BLOCK-VAR BLOCK=C1 VARIABLE=PRES & 
   SENTENCE=P-SPEC ID1=2
DEFINE C1DP BLOCK-VAR BLOCK=C1 VARIABLE=DP-COL & 
   SENTENCE=COL-SPECS
DEFINE C2MD BLOCK-VAR BLOCK=C2C4C5 VARIABLE=MOLE-D & 
   SENTENCE=COL-SPECS
DEFINE C2SC BLOCK-VAR BLOCK=C2C4C5 VARIABLE=T1 & 
   SENTENCE=COL-SPECS
DEFINE C2P1 BLOCK-VAR BLOCK=C2C4C5 Variable=PRES & 
   SENTENCE=P-SPEC ID1=1
DEFINE C2P2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=PRES & 
   SENTENCE=P-SPEC ID1=2
DEFINE C2DP BLOCK-VAR BLOCK=C2C4C5 VARIABLE=DP-COL & 
   SENTENCE=COL-SPECS
DEFINE C2IC1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=MOLE-DRAW & 
   SENTENCE=STRIPPER ID1=C4
DEFINE C2IC2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=MOLE-DRAW & 
   SENTENCE=STRIPPER ID1=C5
DEFINE C4QN BLOCK-VAR BLOCK=C2C4C5 VARIABLE=Q-REB & 
   SENTENCE=STRIPPER ID1=C4
DEFINE C5QN BLOCK-VAR BLOCK=C2C4C5 VARIABLE=Q-REB & 
   SENTENCE=STRIPPER ID1=C5
DEFINE C1T1 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=T-EST & 
   ID1=1
DEFINE C1T2 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=T-EST & 
   ID1=2
DEFINE C1T3 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=T-EST & 
   ID1=3
DEFINE C1T4 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=T-EST & 
   ID1=4
DEFINE C1T5 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=T-EST & 
   ID1=5
DEFINE C1T6 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=T-EST & 
   ID1=6
DEFINE C1T7 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=T-EST & 
   ID1=7
DEFINE C1T8 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=T-EST & 
   ID1=8
DEFINE C1T9 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=T-EST & 
   ID1=9
DEFINE C1T10 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP & 
   SENTENCE=T-EST ID1=10
DEFINE C1T11 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP & 
   SENTENCE=T-EST ID1=11
DEFINE C1T12 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=12
DEFINE C1T13 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=13
DEFINE C1T14 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=14
DEFINE C1T15 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=15
DEFINE C1T16 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=16
DEFINE C1T17 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=17
DEFINE C1T18 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=18
DEFINE C1T19 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=19
DEFINE C1T20 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=20
DEFINE C1T21 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=21
DEFINE C1T22 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=22
DEFINE C1T23 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=23
DEFINE C1T24 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=24
DEFINE C1T25 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=25
DEFINE C1T26 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=26
DEFINE C1T27 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=27
DEFINE C1T28 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=28
DEFINE C1T29 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=29
DEFINE C2T1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=1
DEFINE C2T2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=2
DEFINE C2T3 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=3
DEFINE C2T4 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
    SENTENCE=T-EST ID1=4
DEFINE C2T5 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=5
DEFINE C2T6 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=6
DEFINE C2T7 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=7
DEFINE C2T8 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=8
DEFINE C2T9 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=9
DEFINE C2T10 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=10
DEFINE C2T11 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=11
DEFINE C2T12 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=12
DEFINE C2T13 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=13
DEFINE C2T14 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=14
DEFINE C2T15 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=15
DEFINE C2T16 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=16
DEFINE C2T17 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=17
DEFINE C2T18 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=18
DEFINE C2T19 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=19
DEFINE C2T20 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=20
DEFINE C2T21 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=21
DEFINE C2T22 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=22
DEFINE C2T23 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=23
DEFINE C2T24 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=24
DEFINE C4T1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=STR-T-EST ID1=C4 ID2=1
DEFINE C4T2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=STR-T-EST ID1=C4 ID2=2
DEFINE C4T3 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=STR-T-EST ID1=C4 ID2=3
DEFINE C5T1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
    SENTENCE=STR-T-EST ID1=C5 ID2=1
DEFINE C5T2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
    SENTENCE=STR-T-EST ID1=C5 ID2=2
DEFINE C5T3 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
    SENTENCE=STR-T-EST ID1=C5 ID2=3
DEFINE C1L1 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=1
DEFINE C1L2 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=2
DEFINE C1L3 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=3
DEFINE C1L4 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=4
DEFINE C1L5 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=5
DEFINE C1L6 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=6
DEFINE C1L7 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=7
DEFINE C1L8 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=8
DEFINE C1L9 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=9
DEFINE C1L10 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=10
DEFINE C1L11 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=11
DEFINE C1L12 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=12
DEFINE C1L13 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=13
DEFINE C1L14 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=14
DEFINE C1L15 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=15
DEFINE C1L16 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=16
DEFINE C1L17 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=17
DEFINE C1L18 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=18
DEFINE C1L19 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=L-EST ID1=19
DEFINE C1L20 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
SENTENCE=L-EST ID1=20
DEFINE C1L21 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=21
DEFINE C1L22 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=22
DEFINE C1L23 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=23
DEFINE C1L24 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=24
DEFINE C1L25 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=25
DEFINE C1L26 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=26
DEFINE C1L27 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=27
DEFINE C1L28 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=28
DEFINE C1L29 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=29
DEFINE C1V1 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=1
DEFINE C1V2 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=2
DEFINE C1V3 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=3
DEFINE C1V4 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=4
DEFINE C1V5 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=5
DEFINE C1V6 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=6
DEFINE C1V7 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=7
DEFINE C1V8 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=8
DEFINE C1V9 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=9
DEFINE C1V10 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=10
DEFINE C1V11 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=11
DEFINE C1V12 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=12
DEFINE C1V13 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=13
SENTENCE=L-EST ID1=7
DEFINE C2L8 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=8
DEFINE C2L9 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=9
DEFINE C2L10 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=10
DEFINE C2L11 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=11
DEFINE C2L12 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=12
DEFINE C2L13 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=13
DEFINE C2L14 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=14
DEFINE C2L15 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=15
DEFINE C2L16 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=16
DEFINE C2L17 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=17
DEFINE C2L18 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=18
DEFINE C2L19 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=19
DEFINE C2L20 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=20
DEFINE C2L21 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=21
DEFINE C2L22 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=22
DEFINE C2L23 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=23
DEFINE C2L24 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=24
DEFINE C2V1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=V-EST ID1=1
DEFINE C2V2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=V-EST ID1=2
DEFINE C2V3 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=V-EST ID1=3
DEFINE C2V4 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=V-EST ID1=4
DEFINE C2V5 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=V-EST ID1=5
DEFINE C2V6 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=6
DEFINE C2V7 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=7
DEFINE C2V8 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=8
DEFINE C2V9 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=9
DEFINE C2V10 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=10
DEFINE C2V11 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=11
DEFINE C2V12 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=12
DEFINE C2V13 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=13
DEFINE C2V14 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=14
DEFINE C2V15 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=15
DEFINE C2V16 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=16
DEFINE C2V17 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=17
DEFINE C2V18 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=18
DEFINE C2V19 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=19
DEFINE C2V20 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=20
DEFINE C2V21 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=21
DEFINE C2V22 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=22
DEFINE C2V23 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=23
DEFINE C2V24 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=V-EST ID1=24
DEFINE C4L1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=STR-L-EST ID1=C4 ID2=1
DEFINE C4L2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=STR-L-EST ID1=C4 ID2=2
DEFINE C4L3 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=STR-L-EST ID1=C4 ID2=3
DEFINE C5L1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=STR-L-EST ID1=C5 ID2=1
DEFINE C5L2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=STR-L-EST ID1=C5 ID2=2
DEFINE C5L3 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=STR-L-EST ID1=C5 ID2=3
DEFINE C4V1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=STR-V-EST ID1=C4 ID2=1
DEFINE C4V2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=STR-V-EST ID1=C4 ID2=2
DEFINE C4V3 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=STR-V-EST ID1=C4 ID2=3
DEFINE C5V1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=STR-V-EST ID1=C5 ID2=1
DEFINE C5V2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=STR-V-EST ID1=C5 ID2=2
DEFINE C5V3 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
  SENTENCE=STR-V-EST ID1=C5 ID2=3
F WRITE(NTERM,*), '+++ DATA RECONCILITAITON FORTRAN STARTED +++'
C READ IN MEASURED VALUES FROM FILE
F INQUIRE (FILE='IMEAS.DAT', EXIST=THERE)
F IF (. NOT.THERE) THEN
F   WRITE(NTERM,*), '+++ ERROR: IMEAS.DAT DOES NOT EXIST +++'
F   WRITE(NRPT,*), '+++ ERROR: IMEAS.DAT WAS NOT FOUND +++'
F   WRITE(NHSTRY,*), '+++ ERROR: IMEAS.DAT DID NOT EXIST +++'
F   GO TO 50
F ENDIF
F OPEN (UNIT=63, STATUS='OLD', FILE='IMEAS.DAT')
F REWIND 63
F READ(63,100) SF01
F READ(63,100) SF11
F READ(63,100) SF12
F READ(63,100) SF13
F READ(63,100) SF21
F READ(63,100) SF22
F READ(63,100) SF31
F READ(63,100) SF32
F READ(63,100) SF41
F READ(63,100) SF42
F READ(63,100) SF51
F READ(63,100) SF52
F READ(63,100) SF61
F READ(63,100) SF62
F READ(63,100) ST01
F READ(63,100) ST12
F READ(63,100) ST13
READ(63,100) ST21
READ(63,100) ST22
READ(63,100) ST23
READ(63,100) ST31
READ(63,100) ST32
READ(63,100) ST41
READ(63,100) ST42
READ(63,100) ST51
READ(63,100) ST52
READ(63,100) ST61
READ(63,100) ST62
CLOSE (UNIT=63)
WRITE(NTERM,*) 'IMEAS.DAT READ SUCCESSFULLY'
READ VARIANCES FOR MEASURED VARIABLES FROM FILE
50 INQUIRE (FILE='IVARNC.DAT', EXIST= THERE)
IF (.NOT.THERE) THEN
   WRITE(NTERM,*) '*** ERROR: IVARNC.DAT DOES NOT EXIST ***'
   WRITE(NRPT,*) '*** ERROR: IVARNC.DAT WAS NOT FOUND ***'
   WRITE(NHSTRY,*) '*** ERROR: IVARNC.DAT DID NOT EXIST ***'
GO TO 52
ENDIF
OPEN (UNIT=63, STATUS='OLD', FILE='IVARNC.DAT')
REWRITE 63
READ(63,100) VF01
READ(63,100) VF11
READ(63,100) VF12
READ(63,100) VF13
READ(63,100) VF21
READ(63,100) VF22
READ(63,100) VF31
READ(63,100) VF32
READ(63,100) VF41
READ(63,100) VF42
READ(63,100) VF51
READ(63,100) VF52
READ(63,100) VF61
READ(63,100) VF62
READ(63,100) VT01
READ(63,100) VT12
READ(63,100) VT13
READ(63,100) VT21
READ(63,100) VT22
READ(63,100) VT23
READ(63,100) VT31
READ(63,100) VT32
READ(63,100) VT41
READ(63,100) VT42
READ(63,100) VT51
READ(63,100) VT52
READ(63,100) VT61
READ(63,100) VT62
CLOSE (UNIT=63)
WRITE(NTERM,*) 'IVARNC.DAT READ SUCCESSFULLY'
READ DATA RECONCILIATION WEIGHTS FOR EACH VARIABLE FROM FILE
52 INQUIRE (FILE='IWGHT.DAT', EXIST= THERE)
IF (.NOT. THERE) THEN
   WRITE(NTERM,*) '*** ERROR: IWGHT.DAT DOES NOT EXIST ***'
   WRITE(NRPT,*) '*** ERROR: IWGHT.DAT WAS NOT FOUND ***'
   WRITE(NHSTRY,*) '*** ERROR: IWGHT.DAT DID NOT EXIST ***'
   GO TO 54
ENDIF
OPEN (UNIT=63, STATUS='OLD', FILE='IWGHT.DAT')
REWIND 63
READ(63,100) WF01
READ(63,100) WF11
READ(63,100) WF12
READ(63,100) WF13
READ(63,100) WF21
READ(63,100) WF22
READ(63,100) WF31
READ(63,100) WF32
READ(63,100) WF41
READ(63,100) WF42
READ(63,100) WF51
READ(63,100) WF52
READ(63,100) WF61
READ(63,100) WF62
READ(63,100) WT01
READ(63,100) WT12
READ(63,100) WT13
READ(63,100) WT21
READ(63,100) WT22
READ(63,100) WT23
READ(63,100) WT31
READ(63,100) WT32
READ(63,100) WT41
READ(63,100) WT42
READ(63,100) WT51
READ(63,100) WT52
READ(63,100) WT61
READ(63,100) WT62
CLOSE (UNIT=63)
WRITE(NTERM,*) 'IDWGT.DAT READ SUCCESSFULLY'
READ DATA FREE VARIABLE BOUNDS FOR DATA RECONCILIATION

INQUIRE (FILE='IDFREE.DAT', EXIST= THERE)
IF (.NOT. THERE) THEN
  WRITE(NTERM,*) '*** ERROR: IDFREE.DAT DOES NOT EXIST ***'
  WRITE(NRPT,*) '*** ERROR: IDFREE.DAT WAS NOT FOUND ***'
  WRITE(NHSTRY,*) '*** ERROR: IDFREE.DAT DID NOT EXIST ***'
  GO TO 56
ENDIF
OPEN (UNIT=63, STATUS='OLD', FILE='IDFREE.DAT')
REWIND 63
READ(63,100) BSTABF
READ(63,100) BSTABT
READ(63,100) BC1RR
READ(63,100) BC1RDV
READ(63,100) BC1RBF
READ(63,100) BC1RBT
READ(63,100) BEIT
READ(63,100) BC2MD
READ(63,100) BC2RBF
READ(63,100) BC2RBT
READ(63,100) BC2SCT
READ(63,100) BC4QN
READ(63,100) BC5QN
READ(63,100) BC2C4F
READ(63,100) BC2C5F
CLOSE (UNIT=63)
WRITE(NTERM,*) 'IDFREE.DAT READ SUCCESSFULLY'
READ PLANT SPECIFICATIONS FROM FILE
INQUIRE (FILE='ISMST.DAT', EXIST= THERE)
IF (.NOT. THERE) THEN
  WRITE(NTERM,*) '*** ERROR: ISMST.DAT DOES NOT EXIST ***'
  WRITE(NRPT,*) '*** ERROR: ISMST.DAT WAS NOT FOUND ***'
  WRITE(NHSTRY,*) '*** ERROR: ISMST.DAT DID NOT EXIST ***'
  GO TO 58
ENDIF
OPEN (UNIT=63, STATUS='OLD', FILE='ISMST.DAT')
READ(63,100) STABF
READ(63,100) STABT
READ(63,100) STABP
READ(63,100) STBZ1
READ(63,100) STBZ2
READ(63,100) STBZ3
READ(63,100) STBZ4
READ(63,100) STBZ5
READ(63,100) STBZ6
READ(63,100) STBZ7
READ(63,100) STBZ8
READ(63,100) STBZ9
READ(63,100) STBZ10
READ(63,100) STBZ11
READ(63,100) STBZ12
READ(63,100) STBZ13
READ(63,100) STBZ14
READ(63,100) STBZ15
READ(63,100) STBZ16
READ(63,100) STBZ17
READ(63,100) STBZ18
READ(63,100) STBZ19
READ(63,100) STBZ20
READ(63,100) STBZ21
READ(63,100) STBZ22
READ(63,100) STBZ23
C  C2REBL STREAM ESTIMATIONS
READ(63,100) C2RBF1
C2RBF2 = C2RBF1
READ(63,100) C2RBT1
C2RBT2 = C2RBT1
READ(63,100) C2RBP1
C2RBP2 = C2RBP1
READ(63,100) C2RZ1
READ(63,100) C2RZ2
READ(63,100) C2RZ3
READ(63,100) C2RZ4
READ(63,100) C2RZ5
READ(63,100) C2RZ6
READ(63,100) C2RZ7
READ(63,100) C2RZ8
READ(63,100) C2RZ9
READ(63,100) C2RZ10
READ(63,100) C2RZ11
READ(63,100) C2RZ12
READ(63,100) C2RZ13
READ(63,100) C2RZ14
READ(63,100) C2RZ15
READ(63,100) C2RZ16
READ(63,100) C2RZ17
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<th>COLUMN SPECIFICATIONS</th>
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<tr>
<td>F</td>
<td>READ(63,100) C1RA</td>
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<tr>
<td>F</td>
<td>READ(63,100) C1RDV</td>
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<tr>
<td>F</td>
<td>READ(63,100) C1RBFL</td>
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<td>F</td>
<td>READ(63,100) C1RBT</td>
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<tr>
<td>F</td>
<td>READ(63,100) C1DP</td>
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<tr>
<td>F</td>
<td>READ(63,100) C1P1</td>
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<td>F</td>
<td>READ(63,100) C1P2</td>
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<td>READ(63,100) C2SC</td>
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<td>READ(63,100) C2DP</td>
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<td>READ(63,100) C2P2</td>
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<td>F</td>
<td>READ(63,100) C2IC1</td>
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C2 TEMPERATURE PROFILE

F  READ(63,100) C2T1
F  READ(63,100) C2T2
F  READ(63,100) C2T3
F  READ(63,100) C2T4
F  READ(63,100) C2T5
F  READ(63,100) C2T6
F  READ(63,100) C2T7
F  READ(63,100) C2T8
F  READ(63,100) C2T9
F  READ(63,100) C2T10
F  READ(63,100) C2T11
F  READ(63,100) C2T12
F  READ(63,100) C2T13
F  READ(63,100) C2T14
F  READ(63,100) C2T15
F  READ(63,100) C2T16
F  READ(63,100) C2T17
F  READ(63,100) C2T18
F  READ(63,100) C2T19
F  READ(63,100) C2T20
F  READ(63,100) C2T21
F  READ(63,100) C2T22
F  READ(63,100) C2T23
F  READ(63,100) C2T24

C4 TEMPERATURE PROFILE

F  READ(63,100) C4T1
F  READ(63,100) C4T2
F  READ(63,100) C4T3

C5 TEMPERATURE PROFILE

F  READ(63,100) C5T1
C1 LIQUID AND VAPOUR FLOW PROFILES

READ(63,100) C5T2
READ(63,100) C5T3
READ(63,100) C1L1
READ(63,100) C1L2
READ(63,100) C1L3
READ(63,100) C1L4
READ(63,100) C1L5
READ(63,100) C1L6
READ(63,100) C1L7
READ(63,100) C1L8
READ(63,100) C1L9
READ(63,100) C1L10
READ(63,100) C1L11
READ(63,100) C1L12
READ(63,100) C1L13
READ(63,100) C1L14
READ(63,100) C1L15
READ(63,100) C1L16
READ(63,100) C1L17
READ(63,100) C1L18
READ(63,100) C1L19
READ(63,100) C1L20
READ(63,100) C1L21
READ(63,100) C1L22
READ(63,100) C1L23
READ(63,100) C1L24
READ(63,100) C1L25
READ(63,100) C1L26
READ(63,100) C1L27
READ(63,100) C1L28
READ(63,100) C1L29
READ(63,100) C1V1
READ(63,100) C1V2
READ(63,100) C1V3
READ(63,100) C1V4
READ(63,100) C1V5
READ(63,100) C1V6
READ(63,100) C1V7
READ(63,100) C1V8
READ(63,100) C1V9
READ(63,100) C1V10
READ(63,100) C1V11
READ(63,100) C1V12
READ(63,100) C1V13
F READ(63,100) C1V14
F READ(63,100) C1V15
F READ(63,100) C1V16
F READ(63,100) C1V17
F READ(63,100) C1V18
F READ(63,100) C1V19
F READ(63,100) C1V20
F READ(63,100) C1V21
F READ(63,100) C1V22
F READ(63,100) C1V23
F READ(63,100) C1V24
F READ(63,100) C1V25
F READ(63,100) C1V26
F READ(63,100) C1V27
F READ(63,100) C1V28
F READ(63,100) C1V29
C C2 LIQUID AND VAPOUR FLOW PROFILES
F READ(63,100) C2L1
F READ(63,100) C2L2
F READ(63,100) C2L3
F READ(63,100) C2L4
F READ(63,100) C2L5
F READ(63,100) C2L6
F READ(63,100) C2L7
F READ(63,100) C2L8
F READ(63,100) C2L9
F READ(63,100) C2L10
F READ(63,100) C2L11
F READ(63,100) C2L12
F READ(63,100) C2L13
F READ(63,100) C2L14
F READ(63,100) C2L15
F READ(63,100) C2L16
F READ(63,100) C2L17
F READ(63,100) C2L18
F READ(63,100) C2L19
F READ(63,100) C2L20
F READ(63,100) C2L21
F READ(63,100) C2L22
F READ(63,100) C2L23
F READ(63,100) C2L24
F READ(63,100) C2V1
F READ(63,100) C2V2
F READ(63,100) C2V3
F READ(63,100) C2V4
READ(63,100) C2V5
READ(63,100) C2V6
READ(63,100) C2V7
READ(63,100) C2V8
READ(63,100) C2V9
READ(63,100) C2V10
READ(63,100) C2V11
READ(63,100) C2V12
READ(63,100) C2V13
READ(63,100) C2V14
READ(63,100) C2V15
READ(63,100) C2V16
READ(63,100) C2V17
READ(63,100) C2V18
READ(63,100) C2V19
READ(63,100) C2V20
READ(63,100) C2V21
READ(63,100) C2V22
READ(63,100) C2V23
READ(63,100) C2V24
C  C4 LIQUID AND VAPOUR FLOW PROFILES
READ(63,100) C4L1
READ(63,100) C4L2
READ(63,100) C4L3
READ(63,100) C4V1
READ(63,100) C4V2
READ(63,100) C4V3
READ(63,100) C5L1
READ(63,100) C5L2
READ(63,100) C5L3
READ(63,100) C5V1
READ(63,100) C5V2
READ(63,100) C5V3
CLOSE (UNIT=63)
WRITE(NTERM,*), 'ISMST.DAT READ SUCCESSFULLY'
WRITE(NTERM,*), '+++ DATA RECONCILIATION FORTRAN COMPLETE +++'
C FORMAT STATEMENTS
F 100 FORMAT(15X, E15.8)
    EXECUTE FIRST

FORTRAN OPDATA
F COMMON / USRPVL / PVAP,PDIST,PLTISO,PHISO,PLTDST,PSSFED,PVALS
F COMMON / USRCST / CSTAB,COF1,COF2
F COMMON / USRQLT / QLTISO
F LOGICAL THERE
DEFINE F01 STREAM-VAR STREAM=STAB SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F11 STREAM-PROP STREAM=VAP PROPERTY=V-STDVOL
DEFINE F11STD STREAM-VAR STREAM=VAP SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F12 STREAM-VAR STREAM=C1RFLX SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F13 STREAM-VAR STREAM=DIST-C4 SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F21 STREAM-VAR STREAM=C1REBL SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F22 STREAM-VAR STREAM=SPLTFEED SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F31 STREAM-VAR STREAM=LT-ISO SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F32 STREAM-VAR STREAM=C2RFLX SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F41 STREAM-VAR STREAM=IC1 SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F42 STREAM-VAR STREAM=HV-ISO SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F51 STREAM-VAR STREAM=IC2 SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F52 STREAM-VAR STREAM=LT-DIST SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F61 STREAM-VAR STREAM=C2REBL SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F62 STREAM-VAR STREAM=SSFEED SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE T01 STREAM-VAR STREAM=STAB SUBSTREAM=MIXED & VARIABLE=TEMP
DEFINE T11 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP & SENTENCE=PROFILE ID1=3
DEFINE T12 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP & SENTENCE=PROFILE ID1=2
DEFINE T13 STREAM-VAR STREAM=DIST-C4 SUBSTREAM=MIXED & VARIABLE=TEMP
DEFINE T21 STREAM-VAR STREAM=SPLTFEED SUBSTREAM=MIXED & VARIABLE=TEMP
DEFINE T22 STREAM-VAR STREAM=C1REBL SUBSTREAM=MIXED & VARIABLE=TEMP
DEFINE T23 STREAM-VAR STREAM=SPLT SUBSTREAM=MIXED & VARIABLE=TEMP
DEFINE T31 BLOCK-VAR BLOCK=C2C4CS VARIABLE=TEMP & SENTENCE=PROFILE ID1=2
DEFINE T32 STREAM-VAR STREAM=LT-ISO SUBSTREAM=MIXED & VARIABLE=TEMP
DEFINE T41 STREAM-VAR STREAM=IC1 SUBSTREAM=MIXED & VARIABLE=TEMP
DEFINE T42 STREAM-VAR STREAM=HV-ISO SUBSTREAM=MIXED & VARIABLE=TEMP
DEFINE T51 STREAM-VAR STREAM=IC2 SUBSTREAM=MIXED & VARIABLE=TEMP
DEFINE T52 STREAM-VAR STREAM=LT-DIST SUBSTREAM=MIXED & VARIABLE=TEMP
DEFINE T61 STREAM-VAR STREAM=SSFEED SUBSTREAM=MIXED & VARIABLE=TEMP
DEFINE T62 STREAM-VAR STREAM=C2REBL SUBSTREAM=MIXED & VARIABLE=TEMP
DEFINE P01 STREAM-VAR STREAM=STAB SUBSTREAM=MIXED & VARIABLE=PRES
DEFINE DCIC5 MOLE-FRAC STREAM=DIST-C4 SUBSTREAM=MIXED & COMPONENT=IPENTANE
DEFINE DCNC5 MOLE-FRAC STREAM=DIST-C4 SUBSTREAM=MIXED & COMPONENT=PEPTANE
DEFINE RVA31 STREAM-PROP STREAM=LT-ISO PROPERTY=RVP
DEFINE TBUB31 STREAM-PROP STREAM=LT-ISO PROPERTY=TUB
DEFINE D1A41 STREAM-PROP STREAM=HV-ISO PROPERTY=TBP-10
DEFINE D9A41 STREAM-PROP STREAM=HV-ISO PROPERTY=TBP-90
DEFINE D1A51 STREAM-PROP STREAM=LT-DIST PROPERTY=TBP-10
DEFINE D9A51 STREAM-PROP STREAM=LT-DIST PROPERTY=TBP-90
DEFINE C1QN BLOCK-VAR BLOCK=C1 VARIABLE=DUTY & SENTENCE=PA-RESULTS ID1=C1REBL
DEFINE C2QN BLOCK-VAR BLOCK=F2 VARIABLE=QCALC & SENTENCE=PARAM
DEFINE STABF STREAM-VAR STREAM=STAB SUBSTREAM=MIXED & VARIABLE=MOLE-FLOW
DEFINE STABT STREAM-VAR STREAM=STAB SUBSTREAM=MIXED & VARIABLE=TEMP
DEFINE STABP STREAM-VAR STREAM=STAB SUBSTREAM=MIXED & VARIABLE=PRES
VECTOR-DEF STABZ STREAM STAB
DEFINE C2RBLF STREAM-VAR STREAM=C2REBL SUBSTREAM=MIXED & VARIABLE=MOLE-FLOW
DEFINE C2RBLT STREAM-VAR STREAM=C2REBL SUBSTREAM=MIXED & VARIABLE=TEMP
DEFINE C2RBLP STREAM-VAR STREAM=C2REBL SUBSTREAM=MIXED & VARIABLE=PRES
VECTOR-DEF C2RBLZ STREAM C2REBL
DEFINE E1T BLOCK-VAR BLOCK=E1 VARIABLE=TEMP SENTENCE=PARAM
DEFINE E1P BLOCK-VAR BLOCK=E1 VARIABLE=PRES SENTENCE=PARAM
DEFINE C1RR BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-RR &
    SENTENCE=COL-SPECS
DEFINE C1RDV BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-RDV &
    SENTENCE=COL-SPECS
DEFINE C1RBFL BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
    SENTENCE=PUMPAROUND ID1=C1REBL
DEFINE C1RBT BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=PUMPAROUND ID1=C1REBL
DEFINE C1P1 BLOCK-VAR BLOCK=C1 VARIABLE=PRES &
    SENTENCE=P-SPEC ID1=1
DEFINE C1P2 BLOCK-VAR BLOCK=C1 VARIABLE=PRES &
    SENTENCE=P-SPEC ID1=2
DEFINE C1DP BLOCK-VAR BLOCK=C1 VARIABLE=DP-COL &
    SENTENCE=COL-SPECS
VECTOR-DEF C1TEMP PROFILE BLOCK=C1 VARIABLE=TEMP &
    SENTENCE=PROFILE
DEFINE C2MD BLOCK-VAR BLOCK=C2C4C5 VARIABLE=MOLE-D &
    SENTENCE=COL-SPECS
DEFINE C2SC BLOCK-VAR BLOCK=C2C4C5 VARIABLE=T1 &
    SENTENCE=COL-SPECS
DEFINE C2P1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=PRES &
    SENTENCE=P-SPEC ID1=1
DEFINE C2P2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=PRES &
    SENTENCE=P-SPEC ID1=2
DEFINE C2DP BLOCK-VAR BLOCK=C2C4C5 VARIABLE=DP-COL &
    SENTENCE=COL-SPECS
VECTOR-DEF C2TEMP PROFILE BLOCK=C2C4C5 VARIABLE=TEMP &
    SENTENCE=PROFILE
VECTOR-DEF C4C5T PROFILE BLOCK=C2C4C5 VARIABLE=TEMP &
    SENTENCE=ST-PROFILE
DEFINE C4QN BLOCK-VAR BLOCK=C2C4C5 VARIABLE=Q-REB &
    SENTENCE=STRIPPER ID1=C4
DEFINE C5QN BLOCK-VAR BLOCK=C2C4C5 VARIABLE=Q-REB &
    SENTENCE=STRIPPER ID1=C5
DEFINE C2IC1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=MOLE-DRAW &
    SENTENCE=STRIPPER ID1=C4
DEFINE C2IC2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=MOLE-DRAW &
    SENTENCE=STRIPPER ID1=C5
VECTOR-DEF C1EST PROFILE BLOCK=C1 VARIABLE=LRATE &
    SENTENCE=PROFILE
VECTOR-DEF C1VEST PROFILE BLOCK=C1 VARIABLE=VRATE &
    SENTENCE=PROFILE
VECTOR-DEF C2LEST PROFILE BLOCK=C2C4C5 VARIABLE=LRATE &
    SENTENCE=PROFILE
VECTOR-DEF C2VEST PROFILE BLOCK=C2C4C5 VARIABLE=VRATE & SENTENCE=PROFILE
VECTOR-DEF C4C5SE PROFILE BLOCK=C2C4C5 VARIABLE=LRATE & SENTENCE=STR-PROFILE
VECTOR-DEF C4C5SE PROFILE BLOCK=C2C4C5 VARIABLE=VRATE & SENTENCE=STR-PROFILE

F WRITE(NTERM,*) '+++ OPTIMIZATION RESULTS FORTRAN STARTED +++'
C WRITE TO FILE MEASURED VARIABLE VALUES AFTER OPTIMIZATION
F INQUIRE (FILE='ROVARS.DAT', EXIST= THERE)
F IF ( THERE) THEN
F WRITE(NTERM,*) '+++ ERROR: ROVARS.DAT ALREADY EXISTS +++'
F WRITE(NRPT,*) '+++ ERROR: ROVARS.DAT ALREADY EXISTED +++'
F WRITE(NHSTRY,*) '+++ ERROR: ROVARS.DAT ALREADY EXISTS +++'
F GO TO 50
F ENDIF
F OPEN (UNIT=63, STATUS='NEW', FILE='ROVARS.DAT')
F WRITE(63,100) 'F01', F01
F WRITE(63,100) 'F11', F11
F WRITE(63,100) 'F12', F12
F WRITE(63,100) 'F13', F13
F WRITE(63,100) 'F21', F21
F WRITE(63,100) 'F22', F22
F WRITE(63,100) 'F31', F31
F WRITE(63,100) 'F32', F32
F WRITE(63,100) 'F41', F41
F WRITE(63,100) 'F42', F42
F WRITE(63,100) 'F51', F51
F WRITE(63,100) 'F52', F52
F WRITE(63,100) 'F61', F61
F WRITE(63,100) 'F62', F62
F WRITE(63,100) 'T01', T01
F WRITE(63,100) 'T12', T12
F WRITE(63,100) 'T13', T13
F WRITE(63,100) 'T21', T21
F WRITE(63,100) 'T22', T22
F WRITE(63,100) 'T23', T23
F WRITE(63,100) 'T31', T31
F WRITE(63,100) 'T32', T32
F WRITE(63,100) 'T41', T41
F WRITE(63,100) 'T42', T42
F WRITE(63,100) 'T51', T51
F WRITE(63,100) 'T52', T52
F WRITE(63,100) 'T61', T61
F WRITE(63,100) 'T62', T62
F CLOSE (UNIT=63)
WRITE(NTERM,*),'ROVARS.DAT WRITTEN SUCCESSFULLY'
C WRITE TO FILE A CONSTRAINT VARIABLE SUMMARY
F 50 INQUIRE (FILE='ROCNST.DAT', EXIST= THERE)
F IF (THERE) THEN
F WRITE(NTERM,*),'*** ERROR: ROCNST.DAT ALREADY EXISTS ***'
F WRITE(NRPT,*),'*** ERROR: ROCNST.DAT ALREADY EXISTED ***'
F WRITE(NHSTRY,*),'*** ERROR: ROCNST.DAT ALREADY EXISTS ***'
F GO TO 52
F ENDF
F OPEN (UNIT=63, STATUS='NEW', FILE='ROCNST.DAT')
F WRITE(63,100),'F12', F12
F WRITE(63,100),'F32', F32
F WRITE(63,100),'F41', F41
F WRITE(63,100),'F51', F51
F WRITE(63,100),'T11', T11
F WRITE(63,100),'T22', T22
F WRITE(63,100),'T31', T31
F WRITE(63,100),'T62', T62
F C5A11 = DCICS + DCNC5
F WRITE(63,100),'A11 (CSS)', C5A11
F WRITE(63,100),'A31 (RVP)', RVA31
F WRITE(63,100),'A31 (TBUB)', TBUB31
F WRITE(63,100),'A41 (TBP10)', D1A41
F WRITE(63,100),'A41 (TBP90)', D9A41
F WRITE(63,100),'A51 (TBP10)', D1A51
F WRITE(63,100),'A51 (TBP90)', D9A51
F CLOSE (UNIT=63)
F WRITE(NTERM,*),'ROCNST.DAT WRITTEN SUCCESSFULLY'
C WRITE TO FILE OBJECTIVE FUNCTION SUMMARY
F 52 INQUIRE (FILE='ROOPFN.DAT', EXIST= THERE)
F IF (THERE) THEN
F WRITE(NTERM,*),'*** ERROR: ROOPFN.DAT ALREADY EXISTS ***'
F WRITE(NRPT,*),'*** ERROR: ROOPFN.DAT ALREADY EXISTED ***'
F WRITE(NHSTRY,*),'*** ERROR: ROOPFN.DAT ALREADY EXISTS ***'
F GO TO 54
F ENDF
F OPEN (UNIT=63, STATUS='NEW', FILE='ROOPFN.DAT')
F PROFIT = PVALS - CSTAB - COF1 - COF2
F UCOST = COF1 + COF2
F WRITE(63,100) 'OBFUN-PROFIT', PROFIT
F WRITE(63,100) 'TOT PROD VALS', PVALS
F WRITE(63,100) 'TOT FEED COST', CSTAB
F WRITE(63,100) 'TOT UTIL COST', UCOST
F WRITE(63,100) 'VAP SVOLFLOW', F11STD
F WRITE(63,100) 'DISTC4 SVOLFLO', F13
WRITE(63,100) 'LTISO SVOLFL', F31
WRITE(63,100) 'HVISO SVOLFL', F42
WRITE(63,100) 'LTDIST SVOLFL', F52
WRITE(63,100) 'SSFEED SVOLFL', F62
WRITE(63,100) 'STAB SVOLFLOW', F01
WRITE(63,100) 'C1 REBL DUTY', C1QN
WRITE(63,100) 'C2 REBL DUTY', C2QN
WRITE(63,100) 'LT-ISO MARG', QLTISO
WRITE(63,100) 'LT-ISO RVIP', RVA31
CLOSE (UNIT=63)
WRITE(NTERM,*) 'ROOPFN.DA! WRITTEN SUCCESSFULLY'
C WRITE TO FILE THE VARIABLES FOR SIMULATION AFTER OPTIMIZATION
F 54 INQUIRE (FILE='ROSMST.DAT', EXIST= THERE)
F IF ( THERE ) THEN
F WRITE(NTERM,*) '*** ERROR: ROSMST.DAT ALREADY EXISTS ***'
F WRITE(NRPT,*) '*** ERROR: ROSMST.DAT ALREADY EXISTED ***'
F WRITE(NHSTRY,*) '*** ERROR: ROSMST.DAT ALREADY EXISTS ***'
F GO TO 56
F ENDIF
F OPEN (UNIT=64, STATUS='NEW', FILE='ROSMST.DAT')
C STAB STREAM SPECIFICATIONS
F WRITE(64,100) 'STAB MOLEFLOW', STABF
F WRITE(64,100) 'STAB TEMP', STABT
F WRITE(64,100) 'STAB PRESS', STABP
F DO 12 I=1,23
F TEMP = STABZ(I) / STABZ(24)
F WRITE(64,105) 'STAB Z', I, TEMP
F 12 CONTINUE
C C2REBL STREAM ESTIMATIONS
F WRITE(64,100) 'C2REBL FLOW', C2RBFL
F WRITE(64,100) 'C2REBL TEMP', C2RBLT
F WRITE(64,100) 'C2REBL PRESS', C2RBLP
F DO 14 I=1,23
F TEMP = C2RBLZ(I) / C2RBLZ(24)
F WRITE(64,105) 'C2REBL Z', I, TEMP
F 14 CONTINUE
C E1 HEATER SPECIFICATIONS
F WRITE(64,100) 'E1 TEMP', E1T
F WRITE(64,100) 'E1 PRESS', E1P
C C1 COLUMN SPECIFICATIONS
F WRITE(64,100) 'C1 RFLX RATIO', C1RR
F WRITE(64,100) 'C1 VAP/DIST', C1RDV
F WRITE(64,100) 'C1 REBL FLOW', C1RBFL
F WRITE(64,100) 'C1 REBL TEMP', C1RBT
F WRITE(64,100) 'C1 COL P DROP', C1DP
C2 COLUMN SPECIFICATIONS
F WRITE(64,100) 'C2 DIST FLOW', C2MD
F WRITE(64,100) 'C2 COND SC T', C2SC
F WRITE(64,100) 'C2 COL P DROP', C2DP
F WRITE(64,100) 'C2 TOP TRAY P', C2P1
F WRITE(64,100) 'C2 2ND TRAY P', C2P2
F WRITE(64,100) 'C2-C4 IC FLOW', C2IC1
F WRITE(64,100) 'C2-C5 IC FLOW', C2IC2

C4 COLUMN SPECIFICATIONS
F WRITE(64,100) 'C4 REBL DUTY', C4QN

C5 COLUMN SPECIFICATIONS
F WRITE(64,100) 'C5 REBL DUTY', C5QN

C1 TEMPERATURE PROFILE
F DO 10 I=1,29
FWRITE(64,105) 'C1 T, TRAY', I, C1TEMP(I)
F 10 CONTINUE

C2 TEMPERATURE PROFILE
F DO 20 I=1,24
FWRITE(64,105) 'C2 T, TRAY', I, C2TEMP(I)
F 20 CONTINUE

C4 TEMPERATURE PROFILE
F DO 25 I=1,3
F J = (2*I)-1
FWRITE(64,105) 'C4 T, TRAY', I, C4CST(J)
F 25 CONTINUE

C5 TEMPERATURE PROFILE
F DO 27 I=1,3
F J = 2*I
FWRITE(64,105) 'C5 T, TRAY', I, C4CST(J)
F 27 CONTINUE

C1 LIQUID AND VAPOUR FLOW PROFILES
F DO 30 I=1,29
FWRITE(64,105) 'C1 L, TRAY', I, C1LEST(I)
F 30 CONTINUE

C1 LIQUID AND VAPOUR FLOW PROFILES
F DO 32 I=1,29
FWRITE(64,105) 'C1 V, TRAY', I, C1VEST(I)
F 32 CONTINUE

C2 LIQUID AND VAPOUR FLOW PROFILES
F DO 34 I=1,24
FWRITE(64,105) 'C2 L, TRAY', I, C2LEST(I)
F 34 CONTINUE

C2 LIQUID AND VAPOUR FLOW PROFILES
F DO 36 I=1,24
FWRITE(64,105) 'C2 V, TRAY', I, C2VEST(I)
F 36 CONTINUE
F DO 38 I=1,3
F J = (2*I)-1
F WRITE(64,105) 'C4 L, TRAY', I, C4CSLE(J)
F 38 CONTINUE
F DO 40 I=1,3
F J = (2*I)-1
F WRITE(64,105) 'C4 V, TRAY', I, C4CSVE(J)
F 40 CONTINUE
F DO 42 I=1,3
F J = 2*I
F WRITE(64,105) 'C5 L, TRAY', I, C4CSLE(J)
F 42 CONTINUE
F DO 44 I=1,3
F J = 2*I
F WRITE(64,105) 'C5 V, TRAY', I, C4CSVE(J)
F 44 CONTINUE
F CLOSE (UNIT=64)
F WRITE(NTERM,*) 'ROSMST.DAT WRITTEN SUCCESSFULLY'
C WRITE TO FILE SET POINT VALUES
F 56 INQUIRE (FILE='ROSTPT.DAT', EXIST= THERE)
F IF (THERE) THEN
F WRITE(NTERM,*) '*** ERROR: ROSTPT.DAT ALREADY EXISTS ***'
F WRITE(NRPT,*) '*** ERROR: ROSTPT.DAT ALREADY EXISTED ***'
F WRITE(NHSTRY,*) '*** ERROR: ROSTPT.DAT ALREADY EXISTS ***'
F GO TO 56
F ENDIF
F OPEN (UNIT=64, STATUS='NEW', FILE='ROSTPT.DAT')
F WRITE(64,110) 'C1 REFLUX FLOW (F12) [BBL/DAY]', F12
F WRITE(64,110) 'C1 TRAY 3 TEMPERATURE (T11) [F]', T11
F WRITE(64,110) 'DIST-C4 C5 MOLE FRACTION (A11)', C5A11
F WRITE(64,110) 'C1 REBOILER TEMPERATURE (T22) [F]', T22
F WRITE(64,110) 'C2 REFLUX FLOW (F32) [BBL/DAY]', F32
F WRITE(64,110) 'C4 FEED FLOW (F41) [BBL/DAY]', F41
F WRITE(64,110) 'C5 FEED FLOW (F51) [BBL/DAY]', F51
F WRITE(64,110) 'C2 REBOILER TEMPERATURE (T62) [F]', T62
F WRITE(64,110) 'HV-ISO 10% TBP TEMPERATURE (A41) [F]', D1A41
F WRITE(64,110) 'HV-ISO 90% TBP TEMPERATURE (A41) [F]', D9A41
F WRITE(64,110) 'LT-DIST 10% TBP TEMPERATURE (A51) [F]', D1A51
F WRITE(64,110) 'LT-DIST 90% TBP TEMPERATURE (A51) [F]', D9A51
F CLOSE (UNIT=64)
F WRITE(NTERM,*) 'ROSTPT.DAT WRITTEN SUCCESSFULLY'
F 58 WRITE(NTERM,*) '+++ OPTIMIZATION RESULTS FORTRAN COMPLETED +++'
C FORMAT STATEMENTS
F 100 FORMAT(A13, 2X, E15.8)
F 105 FORMAT(A10, X, I2, 2X, E15.8)
F 110 FORMAT(A40, 2X, E15.8)
EXECUTE LAST

FORTRAN OPSPCSET
F COMMON / USRD1 / DVAP, DDIST, DLTIS0, DHVIS0, DLTDIST, DSSFED
F COMMON / USRD2 / DSTAB, DF0
F COMMON / USRPRM / PRMRVP
F COMMON / USRSPC / SPCRVP
F COMMON / USRCNV / CNVB2M, CNVBTM, CNVBTU, CNVP2K
F COMMON / USRFPEF / F1EFF, F2EFF
F COMMON / USRCA1 / A11U, A11L, A31UR, A31LT, A41U1, A41L1
F COMMON / USRCA2 / A41U9, A41L9, A51U1, A51L1, A51U9, A51L9
F COMMON / USRCF / F12U, F12L, F32U, F41U, F51U
F COMMON / USRCEQ / EQ1, EQ2
F COMMON / USRP1 / PC1RR, PC1RDV, PC1RB, PC1RBT, PE1T, PC2MD, PC2BF
F COMMON / USRP2 / PC2RBT, PC2SCT, PC4QN, PC5QN, PC24F, PC2CSF
F LOGICAL THERE
DEFINE C1Q1 BLOCK-VAR BLOCK=C1 VARIABLE=COND-DUTY &
SENTER=RESULTS
DEFINE C2Q1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=COND-DUTY &
SENTER=RESULTS
F WRITE(NTERM,*) '+++ OPTIMIZATION FORTRAN STARTED +++'
C CONVERSIONS:
C BBL/DAY TO M3/HR
F CNVB2M = 0.006624471
C BBL TO M3
F CNVBTM = 0.1589873
C MMBTU TO LFEBBBL
F CNVBTU = 1/6.3
C PSIA TO KPA
F CNVP2K = 6.8948
C EQUALITY CONSTRAINT VALUES
F EQ1 = C1Q1
F EQ2 = C2Q1
F WRITE(NTERM,*) 'EQUALITY CONSTRAINTS SET SUCCESSFULLY'
C READ OPTIMIZATION OBJECTIVE FUNCTION PARAMETERS FROM FILE
F INQUIRE (FILE='IOBJFN.DAT', EXIST=HERE)
F IF (.NOT.HERE) THEN
F WRITE(NTERM,*) '*** ERROR: IOBJFN.DAT DOES NOT EXIST ***'
F WRITE(NRPT,*) '*** ERROR: IOBJFN.DAT WAS NOT FOUND ***'
F WRITE(NHSTRY,*) '*** ERROR: IOBJFN.DAT DID NOT EXIST ***'
F GO TO 52
F ENDF
OPEN (UNIT=63, STATUS='OLD', FILE='IOBJFN.DAT')
REWIND 63
READ(63,100) PRMRVP
READ(63,100) SPCRVP
READ(63,100) DVAP
READ(63,100) DIST
READ(63,100) DLTIISO
READ(63,100) DHVISO
READ(63,100) DLTDST
READ(63,100) DSSFED
READ(63,100) DSTAB
READ(63,100) DFO
READ(63,100) F1EFF
READ(63,100) F2EFF
CLOSE (UNIT=63)
WRITE(NTERM,*) 'IOBJFN.DAT READ SUCCESSFULLY'
C READ OPTIMIZATION CONSTRAINT BOUNDS FROM FILE
52 INQUIRE (FILE='ICNSTR.DAT', EXIST=THEIR)
IF (.NOT.THERE) THEN
WRITE(NTERM,*) '*** ERROR: ICNSTR.DAT DOES NOT EXIST ***'
WRITE(NRPT,*) '*** ERROR: ICNSTR.DAT WAS NOT FOUND ***'
WRITE(NHSTRY,*) '*** ERROR: ICNSTR.DAT DID NOT EXIST ***'
GO TO 54
ENDIF
OPEN (UNIT=63, STATUS='OLD', FILE='ICNSTR.DAT')
REWIND 63
READ(63,100) A11U
READ(63,100) A11L
READ(63,100) A31UR
READ(63,100) A31LT
READ(63,100) A41U1
READ(63,100) A41L1
READ(63,100) A41U9
READ(63,100) A41L9
READ(63,100) A51U1
READ(63,100) A51L1
READ(63,100) A51U9
READ(63,100) A51L9
READ(63,100) F12U
READ(63,100) F12L
READ(63,100) F32U
READ(63,100) F41U
READ(63,100) F51U
READ(63,100) T11U
READ(63,100) T11L
F    READ(63,100) T22U
F    READ(63,100) T22L
F    READ(63,100) T31U
F    READ(63,100) T31L
F    READ(63,100) T62U
F    READ(63,100) T62L
F    CLOSE (UNIT=63)
F  WRITE(NTERM,*) 'ICNSTR.DAT READ SUCCESSFULLY'
C    READ DATA FREE VARIABLE BOUNDS FOR DATA RECONCILIATION
F 54 INQUIRE (FILE='IOFREE.DAT', EXIST=HERE)
F  IF (.NOT.THERE) THEN
F    WRITE(NTERM,*) '*** ERROR: IOFREE.DAT DOES NOT EXIST ***'
F    WRITE(NRPT,*) '*** ERROR: IOFREE.DAT WAS NOT FOUND ***'
F    WRITE(NHSTRY,*) '*** ERROR: IOFREE.DAT DID NOT EXIST ***'
F  GO TO 56
F  ENDIF
F  OPEN (UNIT=63, STATUS='OLD', FILE='IOFREE.DAT')
F  REWIND 63
F  READ(63,100) PC1RR
F  READ(63,100) PC1RDV
F  READ(63,100) PC1RBF
F  READ(63,100) PC1RBT
F  READ(63,100) PE1T
F  READ(63,100) PC2MD
F  READ(63,100) PC2RBF
F  READ(63,100) PC2RBT
F  READ(63,100) PC2SCT
F  READ(63,100) PC4QN
F  READ(63,100) PC5QN
F  READ(63,100) PC2C4F
F  READ(63,100) PC2C5F
F  CLOSE (UNIT=63)
F  WRITE(NTERM,*) 'IOFREE.DAT READ SUCCESSFULLY'
F 56 WRITE(NTERM,*) '+++ OPTIMIZATION FORTRAN COMPLETE +++'
C    FORMAT STATEMENTS
F 100 FORMAT (15X, E15.8)
F 105 FORMAT (A13, 2X, E15.8)
    EXECUTE FIRST

CONSTRAINT C5A11L
F  COMMON / USRCA1 / A11U, A11L, A31UR, A31LT, A41U1, A41L1
    DEFINE DCIC5 MOLE-FRACTION STREAM=DIST-C4 SUBSTREAM=MIXED &
    COMPONENT=IPENTANE
    DEFINE DCNC5 MOLE-FRACTION STREAM=DIST-C4 SUBSTREAM=MIXED &
    COMPONENT=PENTANE
SPEC "DCICS + DCNC5" GE "A11L"
TOL-SPEC "0.001"

CONSTRAINT CSA11U
F COMMON / USRCA1 / A11U,A11L,A31UR,A31LT,A41U1,A41L1
DEFINE DCICS MOLE-FRAC STREAM=DIST-C4 SUBSTREAM=MIXED &
COMPONENT=IPENTANE
DEFINE DCNC5 MOLE-FRAC STREAM=DIST-C4 SUBSTREAM=MIXED &
COMPONENT=PENTANE
SPEC "DCICS + DCNC5" LE "A11U"
TOL-SPEC "0.001"

CONSTRAINT CD1A41L
F COMMON / USRCA1 / A11U,A11L,A31UR,A31LT,A41U1,A41L1
DEFINE D1A41 STREAM-PROP STREAM=HV-ISO PROPERTY=TBP-10
SPEC "D1A41" GE "A41L1"
TOL-SPEC "0.1"

CONSTRAINT CD1A41U
F COMMON / USRCA1 / A11U,A11L,A31UR,A31LT,A41U1,A41L1
DEFINE D1A41 STREAM-PROP STREAM=HV-ISO PROPERTY=TBP-10
SPEC "D1A41" LE "A41U1"
TOL-SPEC "0.1"

CONSTRAINT CD1A51L
F COMMON / USRCA2 / A41U9,A41L9,A51U1,A51L1,A51U9,A51L9
DEFINE D1A51 STREAM-PROP STREAM=LT-DIST PROPERTY=TBP-10
SPEC "D1A51" GE "A51L1"
TOL-SPEC "0.1"

CONSTRAINT CD1A51U
F COMMON / USRCA2 / A41U9,A41L9,A51U1,A51L1,A51U9,A51L9
DEFINE D1A51 STREAM-PROP STREAM=LT-DIST PROPERTY=TBP-10
SPEC "D1A51" LE "A51U1"
TOL-SPEC "0.1"

CONSTRAINT CD9A41L
F COMMON / USRCA2 / A41U9,A41L9,A51U1,A51L1,A51U9,A51L9
DEFINE D9A41 STREAM-PROP STREAM=HV-ISO PROPERTY=TBP-90
SPEC "D9A41" GE "A41L9"
TOL-SPEC "0.1"

CONSTRAINT CD9A41U
F COMMON / USRCA2 / A41U9,A41L9,A51U1,A51L1,A51U9,A51L9
DEFINE D9A41 STREAM-PROP STREAM=HV-ISO PROPERTY=TBP-90
SPEC "D9A41" LE "A41U9"
TOL-SPEC "0.1"

CONSTRAINT CD9A51L
F COMMON / USRCA2 / A41U9,A41L9,A51U1,A51L1,A51U9,A51L9
DEFINE D9A51 STREAM-PROP STREAM=LT-DIST PROPERTY=TBP-90
SPEC "D9A51" GE "A51L9"
TOL-SPEC "0.1"

CONSTRAINT CD9A51U
F COMMON / USRCA2 / A41U9,A41L9,A51U1,A51L1,A51U9,A51L9
DEFINE D9A51 STREAM-PROP STREAM=LT-DIST PROPERTY=TBP-90
SPEC "D9A51" LE "A51U9"
TOL-SPEC "0.1"

CONSTRAINT CF12L
F COMMON / USRCF / F12U,F12L,F32U,F41U,F51U
DEFINE F12 STREAM-VAR STREAM=C1RFLX SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
SPEC "F12" GE "F12L"
TOL-SPEC "1.0"

CONSTRAINT CF12U
F COMMON / USRCF / F12U,F12L,F32U,F41U,F51U
DEFINE F12 STREAM-VAR STREAM=C1RFLX SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
SPEC "F12" LE "F12U"
TOL-SPEC "1.0"

CONSTRAINT CF32U
F COMMON / USRCF / F12U,F12L,F32U,F41U,F51U
DEFINE F32 STREAM-VAR STREAM=C2RFLX SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
SPEC "F32" LE "F32U"
TOL-SPEC "1.0"

CONSTRAINT CF41U
F COMMON / USRCF / F12U,F12L,F32U,F41U,F51U
DEFINE F41 STREAM-VAR STREAM=IC1 SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
SPEC "F41" LE "F41U"
TOL-SPEC "1.0"

CONSTRAINT CF51U
F COMMON / USRCF / F12U,F12L,F32U,F41U,F51U
DEFINE F51 STREAM-VAR STREAM=IC2 SUBSTREAM=MIXED & VARIABLE=STDVOL FLOW
SPEC "F51" LE "F51U"
TOL-SPEC "1.0"

CONSTRAINT CRVPA31U
F COMMON / USRCA1 / A11U,A11L,A31UR,A31LT,A41U1,A41L1
DEFINE RVA31 STREAM-PROP STREAM=LT ISO PROPERTY=RVP
SPEC "RVA31" LE "A31UR"
TOL-SPEC "0.01"

CONSTRAINT CT11L
DEFINE T11 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP & SENTENCE=PROFILE ID1=3
SPEC "T11" GE "T11U"
TOL-SPEC "0.1"

CONSTRAINT CT11U
DEFINE T11 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP & SENTENCE=PROFILE ID1=3
SPEC "T11" LE "T11U"
TOL-SPEC "0.1"

CONSTRAINT CT22L
DEFINE T22 STREAM-VAR STREAM=C1REBL SUBSTREAM=MIXED & VARIABLE=TEMP
SPEC "T22" GE "T22L"
TOL-SPEC "0.1"

CONSTRAINT CT22U
DEFINE T22 STREAM-VAR STREAM=C1REBL SUBSTREAM=MIXED & VARIABLE=TEMP
SPEC "T22" LE "T22U"
TOL-SPEC "0.1"

CONSTRAINT CT31L
DEFINE T31 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP & SENTENCE=PROFILE ID1=2
SPEC "T31" GE "T31L"
TOL-SPEC "0.1"
CONSTRANIT CT31U
DEFINE T31 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=PROFILE ID1=2
SPEC "T31" LE "T31U"
TOL-SPEC "0.1"

CONSTRANIT CT62L
DEFINE T62 STREAM-VAR STREAM=C2REBL SUBSTREAM=MIXED &
VARIABLE=TEMP
SPEC "T62" GE "T62L"
TOL-SPEC "0.1"

CONSTRANIT CT62U
DEFINE T62 STREAM-VAR STREAM=C2REBL SUBSTREAM=MIXED &
VARIABLE=TEMP
SPEC "T62" LE "T62U"
TOL-SPEC "0.1"

CONSTRANIT CTUB31L
F COMMON / USRCA1 / A11U, A11L, A31UR, A31LT, A41U1, A41L1
DEFINE TBUB31 STREAM-PROP STREAM=LT-ISO PROPERTY=TBUB
SPEC "TBUB31" GE "A31LT"
TOL-SPEC "0.1"

CONSTRANIT EQC1Q1
F COMMON / USRCEQ / EQ1, EQ2
DEFINE C1Q1 BLOCK-VAR BLOCK=C1 VARIABLE=COND-DUTY &
SENTENCE=RESULTS
SPEC "C1Q1" EQ "EQ1"
TOL-SPEC "0.1"

CONSTRANIT EQC2Q1
F COMMON / USRCEQ / EQ1, EQ2
DEFINE C2Q1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=COND-DUTY &
SENTENCE=RESULTS
SPEC "C2Q1" EQ "EQ2"
TOL-SPEC "0.1"

OPTIMIZATION DREC
F COMMON / USRSF1 / SF01, SF11, SF12, SF13, SF21, SF22
F COMMON / USRSF2 / SF31, SF32, SF41, SF42, SF51, SF52, SF61, SF62
DEFINE F01 STREAM-VAR STREAM=STAB SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F11 STREAM-PROP STREAM=VAP PROPERTY=V-STDVOL
DEFINE F12 STREAM-VAR STREAM=C1RFLX SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F13 STREAM-VAR STREAM=DIST-C4 SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F21 STREAM-VAR STREAM=C1REBL SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F22 STREAM-VAR STREAM=SPLTFEED SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F31 STREAM-VAR STREAM=LT-ISO SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F32 STREAM-VAR STREAM=C2RFLX SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F41 STREAM-VAR STREAM=IC1 SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F42 STREAM-VAR STREAM=HV-ISO SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F51 STREAM-VAR STREAM=IC2 SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F52 STREAM-VAR STREAM=LT-DIST SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F61 STREAM-VAR STREAM=C2REBL SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F62 STREAM-VAR STREAM=SSFEED SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE T01 STREAM-VAR STREAM=STAB SUBSTREAM=MIXED &
VARIABLE=TEMP
DEFINE T12 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP & 
    SENTENCE=PROFILE ID1=2
DEFINE T13 STREAM-VAR STREAM=DIST-C4 SUBSTREAM=MIXED & 
    VARIABLE=TEMP
DEFINE T21 STREAM-VAR STREAM=SPLTFEED SUBSTREAM=MIXED & 
    VARIABLE=TEMP
DEFINE T22 STREAM-VAR STREAM=C1REBL SUBSTREAM=MIXED & 
    VARIABLE=TEMP
DEFINE T23 STREAM-VAR STREAM=SPLT SUBSTREAM=MIXED & 
    VARIABLE=TEMP
DEFINE T31 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP & 
    SENTENCE=PROFILE ID1=2
DEFINE T32 STREAM-VAR STREAM=LT-ISO SUBSTREAM=MIXED & 
    VARIABLE=TEMP
DEFINE T41 STREAM-VAR STREAM=IC1 SUBSTREAM=MIXED & 
    VARIABLE=TEMP
DEFINE T42 STREAM-VAR STREAM=HV-ISO SUBSTREAM=MIXED & 
    VARIABLE=TEMP
DEFINE T51 STREAM-VAR STREAM=IC2 SUBSTREAM=MIXED & 
    VARIABLE=TEMP
DEFINE T52 STREAM-VAR STREAM=LT-DIST SUBSTREAM=MIXED & 
    VARIABLE=TEMP
DEFINE T61 STREAM-VAR STREAM=SSFEED SUBSTREAM=MIXED & 
    VARIABLE=TEMP
DEFINE T62 STREAM-VAR STREAM=C2REBL SUBSTREAM=MIXED & 
    VARIABLE=TEMP
DEFINE C1RR BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-RR & 
    SENTENCE=COL-SPECS
DEFINE C1RDV BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-RDV & 
    SENTENCE=COL-SPECS
DEFINE C1RBFL BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & 
    SENTENCE=PUMPAROUND ID1=C1REBL
DEFINE C1RBT BLOCK-VAR BLOCK=C1 VARIABLE=TEMP & 
    SENTENCE=PUMPAROUND ID1=C1REBL
DEFINE E1T BLOCK-VAR BLOCK=E1 VARIABLE=TEMP SENTENCE=PARAM
DEFINE C2MD BLOCK-VAR BLOCK=C2C4C5 VARIABLE=MOLE-D & 
    SENTENCE=COL-SPECS
DEFINE C2RBFL BLOCK-VAR BLOCK=C2SPL1 SENTENCE=MOLE-FLOW & 
    VARIABLE=FLOW ID1=C2RBFD
DEFINE C2RBT BLOCK-VAR BLOCK=F2 VARIABLE=TEMP & 
    SENTENCE=PARAM
DEFINE C2SC BLOCK-VAR BLOCK=C2C4C5 VARIABLE=T1 & 
    SENTENCE=COL-SPECS
DEFINE C4QN BLOCK-VAR BLOCK=C2C4C5 VARIABLE=Q-REB &
SENTENCE=STRIPPER ID1=C4
DEFINE CSQN BLOCK-VAR BLOCK=C2C4C5 VARIABLE=Q-REB &
SENTENCE=STRIPPER ID1=C5
DEFINE C2IC1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=MOLE-DRAW &
SENTENCE=STRIPPER ID1=C4
DEFINE C2IC2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=MOLE-DRAW &
SENTENCE=STRIPPER ID1=C5
DEFINE STABF STREAM-VAR STREAM=STAB SUBSTREAM=MIXED &
VARIABLE=MOLE-FLOW
DEFINE STABT STREAM-VAR STREAM=STAB SUBSTREAM=MIXED &
VARIABLE=TEMP
C
CALCULATE THE WEIGHTED LEAST SQUARES ERROR TERMS
F EF01 = WF01*((F01-SF01)/VF01)**2
F EF11 = WF11*((F11-SF11)/VF11)**2
F EF12 = WF12*((F12-SF12)/VF12)**2
F EF13 = WF13*((F13-SF13)/VF13)**2
F EF21 = WF21*((F21-SF21)/VF21)**2
F EF22 = WF22*((F22-SF22)/VF22)**2
F EF31 = WF31*((F31-SF31)/VF31)**2
F EF32 = WF32*((F32-SF32)/VF32)**2
F EF41 = WF41*((F41-SF41)/VF41)**2
F EF42 = WF42*((F42-SF42)/VF42)**2
F EF51 = WF51*((F51-SF51)/VF51)**2
F EF52 = WF52*((F52-SF52)/VF52)**2
F EF61 = WF61*((F61-SF61)/VF61)**2
F EF62 = WF62*((F62-SF62)/VF62)**2
F ET01 = WT01*((T01-ST01)/VT01)**2
F ET12 = WT12*((T12-ST12)/VT12)**2
F ET13 = WT13*((T13-ST13)/VT13)**2
F ET21 = WT21*((T21-ST21)/VT21)**2
F ET22 = WT22*((T22-ST22)/VT22)**2
F ET23 = WT23*((T23-ST23)/VT23)**2
F ET31 = WT31*((T31-ST31)/VT31)**2
F ET32 = WT32*((T32-ST32)/VT32)**2
F ET41 = WT41*((T41-ST41)/VT41)**2
F ET42 = WT42*((T42-ST42)/VT42)**2
F ET51 = WT51*((T51-ST51)/VT51)**2
F ET52 = WT52*((T52-ST52)/VT52)**2
F ET61 = WT61*((T61-ST61)/VT61)**2
F ET62 = WT62*((T62-ST62)/VT62)**2
C
CALCULATE THE OVERALL OBJECTIVE FUNCTION
F DROBJ = EF01+EF11+EF12+EF13+EF21+EF22+EF31+EF32+EF41+EF42
F * +EF51+EF52+EF61+EF62+ET01+ET12+ET13+ET21+ET22+ET23
F * +ET31+ET32+ET41+ET42+ET51+ET52+ET61+ET62
MINIMIZE "DROBJ"
VARY STREAM-VAR STREAM=STAB SUBSTREAM=MIXED &
  VARIABLE=MOLE-FLOW LABEL="STAB" "STREAM" "MOLE" "FLOW"
LIMITS "STABF - BSTABF" "STABF + BSTABF"
VARY STREAM-VAR STREAM=STAB SUBSTREAM=MIXED VARIABLE=TEMP &
  LABEL="STAB" "STREAM" "TEMP"
LIMITS "STABT - BSTABT" "STABT + BSTABT"
VARY BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-RR SENTENCE=COL-SPECS &
  LABEL="C1" "REFLUX" "RATIO"
LIMITS "C1RR - BC1RR" "C1RR + BC1RR"
VARY BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-RDV SENTENCE=COL-SPECS &
  LABEL="C1" "DISTILL" "MOLE" "VAP FRAC"
LIMITS "C1RDV - BC1RDV" "C1RDV + BC1RDV"
VARY BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=PUMPAROUND ID1=C1REBL LABEL="C1" "REBOILER" "MOLE" &
  "FLOW"
LIMITS "C1RBFL - BC1RBFL" "C1RBFL + BC1RBFL"
VARY BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=PUMPAROUND &
  ID1=C1REBL LABEL="C1" "REBOILER" "OUTLET" "TEMP"
LIMITS "C1RBT - BC1RBT" "C1RBT + BC1RBT"
VARY BLOCK-VAR BLOCK=E1 VARIABLE=TEMP SENTENCE=PARAM &
  LABEL="E1" "OUTLET" "TEMP"
LIMITS "E1T - BE1T" "E1T + BE1T"
VARY BLOCK-VAR BLOCK=C2C4C5 VARIABLE=MOLE-D &
  SENTENCE=COL-SPECS LABEL="C2 TOTAL" "DISTILL" "MOLE" "FLOW"
LIMITS "C2MD - BC2MD" "C2MD + BC2MD"
VARY BLOCK-VAR BLOCK=C2SPL1 SENTENCE=MOLE-FLOW VARIABLE=FLOW &
  ID1=C2RFBD LABEL="C2RFBD" "C2RBFD" "C2RFBD" "C2RBFD"
LIMITS "C2RFBL - BC2RFBL" "C2RFBL + BC2RFBL"
VARY BLOCK-VAR BLOCK=F2 VARIABLE=TEMP SENTENCE=PARAM &
  LABEL="C2" "REBOILER" "OUTLET" "TEMP"
LIMITS "C2RBT - BC2RBT" "C2RBT + BC2RBT"
VARY BLOCK-VAR BLOCK=C2C4CS VARIABLE=T1 SENTENCE=COL-SPECS &
  LABEL="C2" "CONDENSE" "SUBCOOL" "TEMP"
LIMITS "C2SC - BC2SC" "C2SC + BC2SC"
VARY BLOCK-VAR BLOCK=C2C4C5 VARIABLE=Q-REB SENTENCE=STRIPPER &
  ID1=C4 LABEL="C4" "REBOILER" "HEAT" "DUTY"
LIMITS "C4QN - BC4QN" "C4QN + BC4QN"
VARY BLOCK-VAR BLOCK=C2C4C5 VARIABLE=Q-REB SENTENCE=STRIPPER &
  ID1=C5 LABEL="C5" "REBOILER" "HEAT" "DUTY"
LIMITS "C5QN - BC5QN" "C5QN + BC5QN"
VARY BLOCK-VAR BLOCK=C2C4C5 VARIABLE=MOLE-DRAW &
  SENTENCE=STRIPPER ID1=C4 LABEL="C2 -> C4" "CONNECT" "STREAM" &
  "MOLEFLOW"
LIMITS "C2IC1 - BC2ICF" "C2IC1 + BC2ICF"
VARY BLOCK-VAR BLOCK=C2C4C5 VARIABLE=MOLE-DRAW &
SENTENCE=STRIッPER ID1=C5 LABEL="C2 -> C5" "CONNECT" "STREAM" & "MOLEFLOW"
LIMITS "C2IC2 - BC2C5F" "C2IC2 + BC2C5F"

OPTIMIZATION OPT
F COMMON / USRD1 / DVAP,DDIST,DLTISO,DHVISO,DLTDST,DSSFED
F COMMON / USRD2 / DSTAB,DF0
F COMMON / USRPRM / PRMRVP
F COMMON / USRSPC / SPCRVP
F COMMON / USRCNV / CNVB2M,CNVBTM,CNVBU,CNVVP2K
F COMMON / USRFEE / F1EFF,F2EFF
F COMMON / USRPVL / PVAP,PDIST,PLTIISO,PHVIS0,PLTDST,PSSFED,PVALS
F COMMON / USRCST / CSTAB,COF1,COF2
F COMMON / USRQLT / QLTISO
F COMMON / USRP1 / PC1RR,PC1RDV,PC1RBF,PC1RBT,PE1T,PC2MD,PC2RBF
F COMMON / USRP2 / PC2RBT,PC2SCMT,PC4QR,PC5QR,PC2C4F,PC2C5F
DEFINE F01 STREAM-VAR STREAM=STAB SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F11STD STREAM-VAR STREAM=VAP SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F13 STREAM-VAR STREAM=DIST-C4 SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F31 STREAM-VAR STREAM=LT-IS0 SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F42 STREAM-VAR STREAM=HV-IS0 SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F52 STREAM-VAR STREAM=LT-DIST SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE F62 STREAM-VAR STREAM=SSFEED SUBSTREAM=MIXED & VARIABLE=STDVOL-FLOW
DEFINE RVA31 STREAM-PROP STREAM=LT-IS0 PROPERTY=RVP
DEFINE C1QN BLOCK-VAR BLOCK=C1 VARIABLE=DUTY & SENTENCE=PA-RESULTS ID1=C1REBL
DEFINE C2QN BLOCK-VAR BLOCK=F2 VARIABLE=QCALC & SENTENCE=PARAM
DEFINE C1RR BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-RR & SENTENCE=COL-SPECS
DEFINE C1RDRV BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-RDV & SENTENCE=COL-SPECS
DEFINE C1RBFL BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & SENTENCE=PUMPAROUND ID1=C1REBL
DEFINE C1RBT BLOCK-VAR BLOCK=C1 VARIABLE=TEMP & SENTENCE=PUMPAROUND ID1=C1REBL
DEFINE E1T BLOCK-VAR BLOCK=E1 VARIABLE=TEMP SENTENCE=PARAM
DEFINE C2MD BLOCK-VAR BLOCK=C2C4C5 VARIABLE=MOLE-D &
SENTENCE=COL-SPECS
DEFINE C2REBL BLOCK-VAR BLOCK=C2SPL1 SENTENCE=MOLE-FLOW &
VARIABLE=FLOW ID1=C2REBD
DEFINE C2REBT BLOCK-VAR BLOCK=F2 VARIABLE=TEMP &
SENTENCE=PARAM
DEFINE C2SC BLOCK-VAR BLOCK=C2C4C5 VARIABLE=T1 &
SENTENCE=COL-SPECS
DEFINE C4QN BLOCK-VAR BLOCK=C2C4C5 VARIABLE=Q-REB &
SENTENCE=STRIPPER ID1=C4
DEFINE C5QN BLOCK-VAR BLOCK=C2C4C5 VARIABLE=Q-REB &
SENTENCE=STRIPPER ID1=C5
DEFINE C2IC1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=MOLE-DRAW &
SENTENCE=STRIPPER ID1=C4
DEFINE C2IC2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=MOLE-DRAW &
SENTENCE=STRIPPER ID1=C5
C REAL TIME OPTIMIZATION OBJECTIVE FUNCTION
C PROFIT = (PRODUCT VALUES) - (FEED COST) - (UTILITY COST)
C BASIS: 1 HR
C PREMIUMS: [($/M3)∗($/M3) + ($/M3/UNIT)∗(UNIT-UNIT)]
F QLTISO = DLTISO + PRMVP∗((RVA31∗CNVP2K)−SPCRVP))
C PRODUCT VALUES: [($/HR)∗($/M3)∗(M3 DAY/HR BBL)∗(BBL/DAY)]
F PVAP = DVAP∗CNVB2M∗F11STD
F PDIST = DDIST∗CNVB2M∗F13
F PLTISO = QLTISO∗CNVB2M∗F31
F PHVIS0 = DHVIS0∗CNVB2M∗F42
F PLT5ST = DLT5ST∗CNVB2M∗F52
F PSSFED = DSSFED∗CNVB2M∗F62
F PVALS = PVAP∗PDIST∗PLTISO∗PHVIS0∗PLT5ST∗PSSFED
C FEED COST: [($/HR)∗($/M3)∗(M3 DAY/HR BBL)∗(BBL/DAY)]
F CSTAB = DSTAB∗CNVB2M∗F01
C UTILITY COSTS: [$($/HR)∗($/LFE3M)∗(LFE3/M/LFEBBL)∗(LFEBBL/MMBTU)
C ∗(MMBTU/HR)∗(1/FEFF)]
F COF1 = DFO∗CNVBTM∗CNVBTU∗C1QN∗(1/F1EFF)
F COF2 = DFO∗CNVBTM∗CNVBTU∗C2QN∗(1/F2EFF)
C PROFIT:
F PROFIT = PVALS−CSTAB−COF1−COF2
MAXIMIZE "PROFIT"
CONSTRAINTS C5A11L / C5A11U / CRVPA31U / CD1A41L / &
CD1A41U / CD1A51L / CD1A51U / CD9A41L / CD9A41U / &
CD9A51L / CD9A51U / CF12L / CF12U / CF32U / CF41U &
/ CF51U / CT11L / CT11U / CT22L / CT22U / CT31L / &
CT31U / CT62L / CT62U / CTBUB31L / EG1Q1 / EQCQ1 VARY BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-RR SENTENCE=COL-SPECS &
LABEL="C1" "MOLAR" "REFLUX" "RATIO"
LIMITS "C1RR−(C1RR+PC1RR)" "C1RR+(C1RR+PC1RR)"
VARY BLOCK=VAR BLOCK=C1 VARIABLE=MOLE-RDV SENTENCE=COL-specs &
LABEL="C1" "DISTILL" "MOLE" "VAP FRC"
LIMITS "C1RDV-(C1RDV+PC1RDV)" "C1RDV+(C1RDV+PC1RDV)"
VARY BLOCK=VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
SENTENCE=PUMPAROUND ID1=C1REBL LABEL="C1" "REBOILER" "MOLE" &
"FLOW"
LIMITS "C1RFRL-(C1RFRL+PC1RFRL)" "C1RFRL+(C1RFRL+PC1RFRL)"
VARY BLOCK=VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=PUMPAROUND &
ID1=C1REBL LABEL="C1" "REBOILER" "OUTLET" "TEMP"
LIMITS "C1RT - PC1RT" "C1RT + PC1RT"
VARY BLOCK=VAR BLOCK=E1 VARIABLE=TEMP SENTENCE=PARAM &
LABEL="E1" "OUTLET" "TEMP"
LIMITS "E1T - PE1T" "E1T + PE1T"
VARY BLOCK=VAR BLOCK=C2C4C5 VARIABLE=MOLE-D &
SENTENCE=COL-specs LABEL="C2 TOTAL" "DIST" "MOLE" "FLOW"
LIMITS "C2MD-(C2MD+PC2MD)" "C2MD+(C2MD+PC2MD)"
VARY BLOCK=VAR BLOCK=C2SP1 SENTENCE=MOLE-FLOW VARIABLE=FLOW &
ID1=C2RFBD LABEL="C2RFBD" "C2RFBD" "C2RFBD" "C2RFBD"
LIMITS "C2RFBD-(C2RFBD+PC2RFBD)" "C2RFBD+(C2RFBD+PC2RFBD)"
VARY BLOCK=VAR BLOCK=F2 VARIABLE=TEMP SENTENCE=PARAM &
LABEL="C2" "REBOILER" "OUTLET" "TEMP"
LIMITS "C2RT - PC2RT" "C2RT + PC2RT"
VARY BLOCK=VAR BLOCK=C2C4C5 VARIABLE=T1 SENTENCE=COL-specs &
LABEL="C2" "CONDENSE" "SUBCOOL" "TEMP"
LIMITS "C2SC - PC2SC" "C2SC + PC2SC"
VARY BLOCK=VAR BLOCK=C2C4C5 VARIABLE=Q-REB SENTENCE=STRIPPER &
ID1=C4 LABEL="C4" "REBOILER" "HEAT" "DUTY"
LIMITS "C4QN-(C4QN+PC4QN)" "C4QN+(C4QN+PC4QN)"
VARY BLOCK=VAR BLOCK=C2C4C5 VARIABLE=Q-REB SENTENCE=STRIPPER &
ID1=C5 LABEL="C5" "REBOILER" "HEAT" "DUTY"
LIMITS "C5QN-(C5QN+PC5QN)" "C5QN+(C5QN+PC5QN)"
VARY BLOCK=VAR BLOCK=C2C4C5 VARIABLE=MOLE-DRAW &
SENTENCE=STRIPPER ID1=C4 LABEL="C2 -> C4" "CONNECT" "STRIPE" &
"MOLEFLOW"
LIMITS "C2IC1-(C2IC1+PC2IC1F)" "C2IC1+(C2IC1+PC2IC1F)"
VARY BLOCK=VAR BLOCK=C2C4C5 VARIABLE=MOLE-DRAW &
SENTENCE=STRIPPER ID1=C5 LABEL="C2 -> C5" "CONNECT" "STRIPE" &
"MOLEFLOW"
LIMITS "C2IC2-(C2IC2+PC2IC2F)" "C2IC2+(C2IC2+PC2IC2F)"

CONV-OPTIONS
PARAM TRACEOPT=GRADUAL CHECKSEQ=YES

CONVERGENCE C2REBL WEGSTEIN
DESCRIPTION "C2 REBOILER TEAR STREAM"
BLOCK-OPTION CONV-LEVEL=3 TERM-LEVEL=2 RESTART=YES
TEAR C2REBL

CONVERGENCE DREC SQP
DESCRIPTION "SQP FOR DATA RECONCILIATION"
OPTIMIZE OPTID=DREC
PARAM MAXIT=300 MAXPASS=99998 TOL=.10 MAXLSPASS=4 &
EST-STEP=YES CONST-ITER=10 DERIV SWITCH= YES

CONVERGENCE OPT SQP
DESCRIPTION "SQP FOR OPTIMIZATION"
OPTIMIZE OPTID=OPT
PARAM MAXIT=300 MAXPASS=99998 TOL=.10 MAXLSPASS=4 &
EST-STEP=YES CONST-ITER=10 DERIV SWITCH= YES

SEQUENCE RTO DRSPCSET DREC C1 E1 C2REBL C2C4C5 C2SPL1 F2 &
(RETURN C2REBL) (RETURN DREC) DRDATA OPSPCSET OPT C1 &
E1 C2REBL C2C4C5 C2SPL1 F2 (RETURN C2REBL) (RETURN OPT) &
OPDATA

REPORT NOINSERT NOADA NOSENSITIVITY NOPROPERTY NOCOST BLOCK &
NOUNITS NOUTILITIES NOECONOMIC

BLOCK-REPORT NOSORT NOTOTBAL NOINPUT

STREAM-REPORT WIDE NOMICELFLOW MOLFRAC NOVOLFRAC NOATTR-DESC &
NOMCOMP-ATTR NOSUBS-ATTR PROPERTIES=TBP-10 TBP-90 STDVOL &
V-STDVOL VOL RVP TBUB EXCL-STREAMS=C2BOT C2RBF D

FLOWSHEET-RE NODESCRIPTIO NOTOTBAL NOCOMPBAL NOSEQUENCE &
NOFORTRAN NODESIGN-SPE NOCONSTRAINT NOOPTIMIZATI &
NOMTRANSFER
Appendix E

SPEEDUP Real Time Optimizer Code

E.1 setup

The following executable C-shell script, setup, is used to setup the SPEEDUP real time optimizer.

```csh
#!/bin/csh
#
# SPEEDUP RTO SETUP SCRIPT
#
# Sets up the SpeedUp RTO simulation and plant simulations in
# preparation for real time optimization runs.
#
# Set up plant
echo "=== SETTING UP SPEEDUP REAL TIME OPTIMIZER SIMULATIONS ==="
cd plant
if ( !-e plant6.inp ) then
    echo "=== SETUP: ERROR: plant/plant6.inp does not exist ==="
    exit
endif
if ( !-e randdata.f ) then
    echo "=== SETUP: ERROR: plant/randdata.f does not exist ==="
    exit
endif
echo "=== SETUP: Setting up ASPEN PLUS plant simulation ==="
```

355
aspen plant6 /itonly
# Set up randdata.exe
echo "=== SETUP: Setting up variable noise FORTRAN ==="
f77 randdata.f -l nag -o randdata.exe
# Set up Speedup Properties
cd ..
cd props
if ( !(e prop6.inp) ) then
  echo "=== SETUP: ERROR: props/prop6.inp does not exist ==="
  exit
endif
echo "=== SETUP: Setting up SPEEDUP properties ==="
sairun prop6 z
setenv LIBPHPR 'pwd'
# Set up Speedup Data Rec
cd ..
cd rtddr
if ( !(e model6x.speedup) ) then
  echo "=== SETUP: ERROR: rtddr/model6x.speedup does not exist ==="
  exit
endif
if ( !(e report6y.speedup) ) then
  echo "=== SETUP: ERROR: rtddr/report6y.speedup does not exist ==="
  exit
endif
if ( !(e rtddr6.f) ) then
  echo "=== SETUP: ERROR: rtddr/rtddr6.f does not exist ==="
  exit
endif
if ( !(e rtddr6.speedup) ) then
  echo "=== SETUP: ERROR: rtddr/rtddr6.speedup does not exist ==="
  exit
endif
if ( !(e rtddr6run.cmd) ) then
  echo "=== SETUP: ERROR: rtddr/rtddr6run.cmd does not exist ==="
  exit
endif
if ( !(e rtddr6setup.cmd) ) then
  echo "=== SETUP: ERROR: rtddr/rtddr6setup.cmd does not exist ==="
  exit
endif
if ( !(e speedup.include) ) then
  echo "=== SETUP: ERROR: rtddr/speedup.include does not exist ==="
  exit
endif
echo "=== SETUP: Setting up SPEEDUP RT0 data rec. simulation ==="
fortsp rtodr6.f
speedup < rtodr6setup.cmd
# Set up Speedup Optimization
cd ..
cd rtopt
if ( !(-e model6x.speedup) ) then
    echo "=== SETUP: ERROR: rtopt/model6x.speedup does not exist ==="
    exit
endif
if ( !(-e report6y.speedup) ) then
    echo "=== SETUP: ERROR: rtopt/report6y.speedup does not exist ==="
    exit
endif
if ( !(-e rtopt6.f) ) then
    echo "=== SETUP: ERROR: rtopt/rtopt6.f does not exist ==="
    exit
endif
if ( !(-e rtopt6.speedup) ) then
    echo "=== SETUP: ERROR: rtopt/rtopt6.speedup does not exist ==="
    exit
endif
if ( !(-e rtopt6run.cmd) ) then
    echo "=== SETUP: ERROR: rtopt/rtopt6run.cmd does not exist ==="
    exit
endif
if ( !(-e rtopt6setup.cmd) ) then
    echo "=== SETUP: ERROR: rtopt/rtopt6setup.cmd does not exist ==="
    exit
endif
if ( !(-e speedup.include) ) then
    echo "=== SETUP: ERROR: rtopt/speedup.include does not exist ==="
    exit
endif
echo "=== SETUP: Setting up SPEEDUP RT0 optimization simulation ==="
fortsp rtopt6.f
speedup < rtopt6setup.cmd
echo "=== SETUP: COMPLETED ==="

E.2 run

The following executable C-shell script, run, is used to run a given number of cycles of the SPEEDUP real time optimizer.
#!/bin/csh
#
# SPEEDUP RTO RUN SCRIPT
#
# Runs the SpeedUp RTO simulation and plant simulations.
#
# SYNTAX: run n
# where n = number of cycles of the real time optimizer to be run
# (default = 1 if n not given)
#
echo "=== SPEEDUP REAL TIME OPTIMIZER SIMULATION ==="
# Check number of cycles to be performed
if ( "$1" >= 1 ) then
    set MAXITN = $1
else
    set MAXITN = 1
endif
set ITN = 1
# Set Properties Environment Variable
cd props
setenv LIBPHPR 'pwd'
cd ..
# Make results directory, deleting old one first
if ( -e results ) then
    rm -r -f results
endif
mkdir results
cd results
mkdir start
cd ..
while ( $MAXITN >= $ITN )
    echo "=== REAL TIME OPTIMIZER CYCLE $ITN BEGINNING ==="
cd results
    set RESITN = "itn$ITN"
    mkdir $RESITN
cd ..
# SPEEDUP RTODR6 RUN
#
    cd rtodr
# Check if input files all exist
if ( !(-e IMEAS.DAT) ) then
    echo "=== RUN: ERROR: rtodr/IMEAS.DAT does not exist ==="
    exit
endif
if (!(-e IVARNC.DAT)) then
  echo "=== RUN: ERROR: rtodr/IVARNC.DAT does not exist ==="
  exit
eendif
if (!(-e IWGHT.DAT)) then
  echo "=== RUN: ERROR: rtodr/IWGHT.DAT does not exist ==="
  exit
eendif
if (!(-e IDFREE.DAT)) then
  echo "=== RUN: ERROR: rtodr/IDFREE.DAT does not exist ==="
  exit
eendif
if (!(-e ISET.DAT)) then
  echo "=== RUN: ERROR: rtodr/ISET.DAT does not exist ==="
  exit
eendif
if (!(-e drpreset.speedup)) then
  echo "=== RUN: ERROR: rtodr/drpreset.speedup does not exist ==="
  exit
eendif
# Remove any output files if they exist
if (!(-e RDSET.DAT)) then
  rm RDSET.DAT
endif
if (!(-e oppreset.speedup)) then
  rm oppreset.speedup
endif
if (!(-e speedup.lis)) then
  rm speedup.lis
endif
# Run SpeedUp rtodr6 job
  echo "=== RUN: Starting SPEEDUP RTO Data Reconciliation Simulation ==="
  speedup < rtodr6run.cmd
# Check if simulation ran to completion
if (!(-e RDSET.DAT)) then
  echo "=== RUN: ERROR: an error occurred running speedup rtodr6 ==="
  exit
eendif
# Copy run results to results directory
  cp RDSET.DAT ../results/$RESITN
  cp ISET.DAT ../results/$RESITN
  if ($RESITN == "itn1") then
    cp drpreset.speedup ../results/start
    cp IMEAS.DAT ../results/start
    cp ISET.DAT ../results/start
endif
    cp speedup.lis ../results/$RESITM/rtodr6.lis
# Send files to Optimization run
    cp RDSET.DAT ../rtopt/ISET.DAT
    cp oppreset.speedup ../rtopt
    cd ..
#
# SPEEDUP RTOPT6 RUN
#
    cd rtopt
# Check if input files all exist
    if ( !(-e IOBJFN.DAT) ) then
        echo "=== RUN: ERROR: rtopt/IOBJFN.DAT does not exist ==="
        exit
    endif
    if ( !(-e ICNSTR.DAT) ) then
        echo "=== RUN: ERROR: rtopt/ICNSTR.DAT does not exist ==="
        exit
    endif
    if ( !(-e IOFREE.DAT) ) then
        echo "=== RUN: ERROR: rtopt/IOFREE.DAT does not exist ==="
        exit
    endif
    if ( !(-e ISET.DAT) ) then
        echo "=== RUN: ERROR: rtopt/ISET.DAT does not exist ==="
        exit
    endif
    if ( !(-e oppreset.speedup) ) then
        echo "=== RUN: ERROR: rtopt/oppreset.speedup does not exist ==="
        exit
    endif
# Remove any output files if they exist
    if ( !-e ROSMST.DAT ) then
        rm ROSMST.DAT
    endif
    if ( !-e ROSET.DAT ) then
        rm ROSET.DAT
    endif
    if ( !-e drpreset.speedup ) then
        rm drpreset.speedup
    endif
    if ( !-e speedup.lis ) then
        rm speedup.lis
    endif
# Run SpeedUp rtopt6 job
echo "=== RUN: Starting SPEEDUP RTO Optimization Simulation ==="
speedup < rtopt6run.cmd

# Check if simulation ran to completion
if ( !(-e ROSET.DAT) ) then
    echo "=== RUN: ERROR: an error occurred running speedup rtopt6 ==="
    exit
endif

# Copy run results to results directory
cp R*.DAT ../results/$RESITN
cp speedup.lis ../results/$RESITN/rtopt6.lis

# Send files to Data Rec run, next cycle
cp ROSET.DAT ../rtodr/ISET.DAT
cp drpresp.speedup ../rtodr

# ASPEN PLANT6 RUN
#
# Set up for plant6 run
cp ROSETMST.DAT ../plant
cd ..
cd plant

# Check if input files all exist
if ( !(-e ROSETMST.DAT) ) then
    echo "=== RUN: ERROR: plant/ROSETMST.DAT does not exist ==="
    exit
endif

# Remove any output files if they exist
if ( !(-e PLVARS.DAT) ) then
    rm PLVARS.DAT
endif

# Run Aspen Plus plant6 job
echo "=== RUN: Starting ASPEN PLUS PLANT simulation ==="
aspen plant6 /sponly

# Check if simulation ran to completion
if ( !(-e PLVARS.DAT) ) then
    echo "=== RUN: ERROR: an error occurred running aspen plant6 ==="
    exit
endif

# Copy run results to results directory
cp PLVARS.DAT ../results/$RESITN

# FORTRAN RANDDATA RUN
#
# Check if input files all exist
if ( !(-e PLVARS.DAT) ) then
    echo "=== RUN: ERROR: plant/PLVARS.DAT does not exist ==="
exit
endif
if ( !(e RVARNC.DAT) ) then
  echo "=== RUN: ERROR: plant/RVARNC.DAT does not exist ==="
  exit
endif
# Remove any output files if they exist
if ( !e IMEAS.DAT ) then
  rm IMEAS.DAT
endif
# Run FORTRAN randdata.exe job
  echo "=== RUN: Starting randdata.exe ==="
  randdata.exe
# Check if simulation ran to completion
if ( !(e IMEAS.DAT) ) then
  echo "=== RUN: ERROR: an error occurred running randdata.exe ==="
  exit
endif
# Copy run results to results directory
  cp IMEAS.DAT ../results/$RESITN
# Send files to Data Rec run, next cycle
  cp IMEAS.DAT ../rtodr
cd ..
  set ITN = 'expr $ITN + 1'
end
  cp plant/plant6.rep results
  echo "=== $MAXITN REAL TIME OPTIMIZER CYCLES COMPLETED ==="

E.3 Common Code from rtodr6.speedup and rtopt6.speedup

The following sections of SPEEDUP input code appear in both rtodr6.speedup
and rtopt6.speedup. See section E.4 for the rtodr6.speedup specific code,
and section E.6 for the rtopt6.speedup specific code.

DECLARE
# Taken from the Library Declare and modified where necessary
  TYPE
  
  # ---- US UNITS OF MEASUREMENT ----
  # THE VARIABLE TYPES USED IN THIS SIMULATION:
# DEFAULT LOWER VALUE UPPER SCALING UNIT OF MEASUREMENT
# BOUND BOUND FACTOR

dens_mol_liq  2.5 : 0.01 : 7.5 : 1 UNIT= "lbmol/ft3"
dens_mol_vap  5.0E-4 : 5.0E-7 : 5 : 0.01 UNIT= "lbmol/ft3"
enth_flow  1.0 : -350 : 200 : 300 UNIT= "MMBtu/h"
enth_mol  0.050 : -1.0 : 1.0 : 1 UNIT= "MMBtu/lbmol"
enth_mol_liq  0.025 : -1.0 : 1.0 : 1 UNIT= "MMBtu/lbmol"
enth_mol_vap  0.060 : -1.0 : 1.0 : 1 UNIT= "MMBtu/lbmol"
flow_mol  1000.0 : 0.0 : 10000 : 5000 UNIT= "lbmol/h"
flow_mol_liq  1000.0 : 0.0 : 6000 : 3000 UNIT= "lbmol/h"
flow_mol_vap  1000.0 : 0.0 : 6000 : 3000 UNIT= "lbmol/h"
flow_vol  5000.0 : 0.0 : 5.0E5 : 20000 UNIT= "ft3/h"
flow_vol_liq  4000.0 : 0.0 : 5.0E5 : 15000 UNIT= "ft3/h"
flow_vol_vap  10000.0 : 0.0 : 1.0E6 : 40000 UNIT= "ft3/h"
molefraction  0.05 : 0.0 : 1.0 : 1 UNIT= "lbmol/lbmol"
pressure  14.7 : 1.0 : 1470.0 : 200 UNIT= "psia"
press_drop  164 : -300 : 300.0 : 200 UNIT= "psi"
ratio  1 : 0.0 : 100.0 : 10 UNIT= "-

temperature  100.0 : 20.0 : 800.0 : 1000 UNIT= "F"
temp_drop  5 : -200.0 : 200.0 : 200 UNIT= "F"
temp_rise  -47 : -200.0 : 200.0 : 200 UNIT= "F"
vapfraction  0.10 : 0.0 : 1.0 : 1 UNIT= "lbmol/lbmol"

# Default stream type MAINSTREAM
STREAM MAINSTREAM
SET
NOCOMP=23
TYPE
FLOW_MOL, MOLEFRACTION(NOCOMP), TEMPERATURE, PRESSURE, ENTH_MOL
COMPONENTS
H2, METHANE, ETHANE, PROPANE, IBUTANE, BUTANE,
IPENTANE, PENTANE, B4ST65, B6ST85, B8ST105, B10ST125,
B12ST145, B14ST165, B16ST185, B18ST205, B2OST235, B23ST265,
B26ST295, B29ST325, B32ST355, B35ST395, B39ST510
OPTIONS
OPSET = "PENG-ROB"
STREAM LIQUID
SET
NOCOMP=23
TYPE
FLOW_MOL_LIQ, MOLEFRACTION(NOCOMP), TEMPERATURE, PRESSURE, ENTH_MOL_LIQ
THERMO MAINSTREAM
STREAM VAPOUR
SET
NOCOMP=23
TYPE
FLOW_MOL_VAP, MOLEFRACTION(NO COMP), TEMPERATURE, PRESSURE, ENTH_MOL_VAP
THERMO MAINSTREAM
STREAM RVPMAIN
SET
NO COMP = 24
TYPE
FLOW_MOL, MOLEFRACTION(NO COMP), TEMPERATURE, PRESSURE, ENTH_MOL
COMPONENTS
H2, METHANE, ETHANE, PROPANE, IBUTANE, BUTANE,
IPENTANE, PENTANE, B45T65, B65T85, B85T105, B105T125,
B125T145, B145T165, B165T185, B185T205, B205T235, B235T265,
B265T295, B295T325, B325T355, B355T395, B395T510, AIR
OPTIONS
OP SET = "SYS0PO"
STREAM RVP LIQ
SET
NO COMP=24
TYPE
FLOW_MOL_LIQ, MOLEFRACTION(NO COMP), TEMPERATURE, PRESSURE, ENTH_MOL_LIQ
THERMO RVPMAIN
STREAM RVP VAP
SET
NO COMP=24
TYPE
FLOW_MOL_VAP, MOLEFRACTION(NO COMP), TEMPERATURE, PRESSURE, ENTH_MOL_VAP
THERMO RVPMAIN
****
FLOWSHEET
# Molar Feed to the Feed Tray of C1
STREAM STAB
OUTPUT OF MFEED IS INPUT OF F01
OUTPUT OF F01 IS INPUT 3 OF C1FT14
# Connect C1 Feed Tray to Stripping Section
OUTPUT 1 OF C1FT14 IS INPUT 1 OF C1S TYPE VAPOUR
OUTPUT 2 OF C1S IS INPUT 2 OF C1FT14 TYPE LIQUID
# Connect C1 Stripping Section to Partial Condenser and Reflux Splitter
OUTPUT 1 OF C1S IS INPUT OF C1COND TYPE VAPOUR
STREAM VAP
OUTPUT 1 OF C1COND IS INPUT OF F11 TYPE VAPOUR
OUTPUT OF F11 IS PRODUCT 1 TYPE VAPOUR
OUTPUT 2 OF C1COND IS INPUT 1 OF C1SPL1 TYPE LIQUID
STREAM DIST_C4
OUTPUT 1 OF C1SPL1 IS INPUT OF F13 TYPE LIQUID
OUTPUT OF F13 IS PRODUCT 2 TYPE LIQUID
STREAM C1RFLX
OUTPUT 2 OF C1SPL1 IS INPUT OF F12 TYPE LIQUID
OUTPUT OF F12 IS INPUT 2 OF C1S TYPE LIQUID
# Connect C1 Feed Tray to Rectifying Section
OUTPUT 2 OF C1FT14 IS INPUT 2 OF C1R TYPE LIQUID
OUTPUT 1 OF C1R IS INPUT 1 OF C1FT14 TYPE VAPOUR

# Connect C1 Rectifying Section to Reboiler
OUTPUT 2 OF C1R IS INPUT 1 OF C1BT29 TYPE LIQUID
OUTPUT 1 OF C1BT29 IS INPUT 1 OF C1R TYPE VAPOUR

STREAM SPLTFEED
OUTPUT 2 OF C1BT29 IS INPUT OF F22A TYPE LIQUID
OUTPUT 0F F22A IS INPUT OF E1 TYPE LIQUID
OUTPUT 3 OF C1BT29 IS INPUT OF C1REBL TYPE LIQUID

STREAM C1REBL
OUTPUT 0F C1REBL IS INPUT OF F21
OUTPUT 0F F21 IS INPUT OF C1TR1
OUTPUT 0F C1TR1 IS INPUT 2 OF C1BT29

# Connect SPLTFEED to E1 Heat Exchanger
STREAM SPLT
OUTPUT 0F E1 IS INPUT 0F F22
OUTPUT 0F F22 IS INPUT 3 OF C2FT21

# Connect C2 Feed Tray to Rectifying Section
OUTPUT 2 OF C2FT21 IS INPUT 2 OF C2R TYPE LIQUID
OUTPUT 1 OF C2R IS INPUT 1 OF C2FT21 TYPE VAPOUR

# Connect C2 Rectifying Section to Reboiler
OUTPUT 2 OF C2R IS INPUT 1 OF C2BT24 TYPE LIQUID
OUTPUT 1 OF C2BT24 IS INPUT 1 OF C2R TYPE VAPOUR

STREAM SSFEED
OUTPUT 2 OF C2BT24 IS INPUT OF F62 TYPE LIQUID
OUTPUT 0F F62 IS PRODUCT 6 TYPE LIQUID
OUTPUT 3 OF C2BT24 IS INPUT OF C2REBL TYPE LIQUID

STREAM C2REBL
OUTPUT 0F C2REBL IS INPUT OF F61
OUTPUT 0F F61 IS INPUT OF C2TR3
OUTPUT 0F C2TR3 IS INPUT 2 OF C2BT24

# Connect C2 Feed Tray to Stripping Section
OUTPUT 1 OF C2FT21 IS INPUT 1 OF C2S3 TYPE VAPOUR
OUTPUT 2 OF C2S3 IS INPUT 2 OF C2FT21 TYPE LIQUID

# Build C2 Stripping Section
OUTPUT 1 OF C2S3 IS INPUT 1 OF C2T18 TYPE VAPOUR
OUTPUT 1 OF C2T18 IS INPUT 1 OF C2FT17 TYPE VAPOUR
OUTPUT 2 OF C2SPL2 IS INPUT 2 OF C2S3 TYPE LIQUID

STREAM IC2
OUTPUT 1 OF C2SPL2 IS INPUT OF F51 TYPE LIQUID
OUTPUT 0F F51 IS INPUT 2 OF C5 TYPE LIQUID
OUTPUT 2 OF C2FT17 IS INPUT 2 OF C2T18 TYPE LIQUID
OUTPUT 2 OF C2T18 IS INPUT 1 OF C2SPL2 TYPE LIQUID

STREAM C5RTN1
OUTPUT 1 OF C5 IS INPUT OF C2TR2 TYPE VAPOUR

STREAM C5RTN2
OUTPUT 0F C2TR2 IS INPUT 3 OF C2FT17 TYPE VAPOUR
OUTPUT 1 OF C2FT17 IS INPUT 1 OF C2T16 TYPE VAPOUR
OUTPUT 2 OF C2T16 IS INPUT 2 OF C2FT17 TYPE LIQUID
OUTPUT 1 OF C2T16 IS INPUT 1 OF C2T15 TYPE VAPOUR
OUTPUT 2 OF C2SPL1 IS INPUT 2 OF C2T16 TYPE LIQUID

STREAM IC1
OUTPUT 1 OF C2SPL1 IS INPUT OF F41 TYPE LIQUID
OUTPUT 0F F41 IS INPUT 2 OF C4 TYPE LIQUID
OUTPUT 1 OF C2T15 IS INPUT 1 OF C2FT14 TYPE VAPOUR
OUTPUT 2 OF C2T15  IS INPUT 1 OF C2SPL1  TYPE LIQUID
OUTPUT 2 OF C2FT14 IS INPUT 2 OF C2T15  TYPE LIQUID
STREAM C4RTN1  OUTPUT 1 OF C4  IS INPUT 0 OF C2TR1  TYPE VAPOUR
STREAM C4RTN2  OUTPUT 0 OF C2TR1  IS INPUT 3 OF C2FT14  TYPE VAPOUR
OUTPUT 1 OF C2FT14 IS INPUT 1 OF C2S1  TYPE VAPOUR
OUTPUT 2 OF C2S1  IS INPUT 2 OF C2FT14  TYPE LIQUID

# Connect C2 Stripping Section to Total Condenser
OUTPUT 1 OF C2S1  IS INPUT 0 OF C2COND  TYPE VAPOUR
STREAM LT_ISO  OUTPUT 2 OF C2COND  IS INPUT 0 OF F31  TYPE LIQUID
OUTPUT 0 OF F31  IS INPUT 0 OF M2R31  TYPE LIQUID
OUTPUT 0 OF M2R31  IS INPUT 0 OF RVP31  TYPE RVPLIQ
OUTPUT 0 OF RVP31  IS PRODUCT 3  TYPE RVPLIQ
STREAM C2RFLX  OUTPUT 1 OF C2COND  IS INPUT 0 OF F32  TYPE LIQUID
OUTPUT 0 OF F32  IS INPUT 2 OF C2S1  TYPE LIQUID

# Connect C5 Reboiler
OUTPUT 2 OF C5  IS INPUT 0 OF C5REBL  TYPE LIQUID
OUTPUT 1 OF C5REBL  IS INPUT 1 OF C5  TYPE VAPOUR
STREAM HV_ISO  OUTPUT 2 OF C5REBL  IS INPUT 0 OF F52  TYPE LIQUID
OUTPUT 0 OF F52  IS PRODUCT 5  TYPE LIQUID

# Connect C4 Reboiler
OUTPUT 2 OF C4  IS INPUT 0 OF C4REBL  TYPE LIQUID
OUTPUT 1 OF C4REBL  IS INPUT 1 OF C4  TYPE VAPOUR
STREAM LT_DIST  OUTPUT 2 OF C4REBL  IS INPUT 0 OF F42  TYPE LIQUID
OUTPUT 0 OF F42  IS PRODUCT 4  TYPE LIQUID

*****
UNIT C1BT29 IS A BTRAY_SS
*****
UNIT C1COND IS A PCOND_SS
*****
UNIT C1FT14 IS A FTRAY_SS
*****
UNIT C1R IS A SECTION_SS
SET
TOP_TRAY = 15, BOTTOM_TRAY = 28
*****
UNIT C1REBL IS A HEAT_COOL
*****
UNIT C1S IS A SECTION_SS
SET
TOP_TRAY = 2, BOTTOM_TRAY = 13
*****
UNIT C1SPL1 IS A RSLIP
*****
UNIT C1TR1 IS A TEAR
*****
UNIT C2BT24 IS A BTRAY_SS
*****
UNIT C2COND IS A TCOND_SS
*****
UNIT C2FT14 IS A FTRAY_SS
*****
UNIT C2FT17 IS A FTRAY_SS
*****
UNIT C2FT21 IS A FTRAY_SS
*****
UNIT C2R IS A SECTION_SS
  SET
    TOP_TRAY = 22, BOTTOM_TRAY = 23
*****
UNIT C2REBL IS A HEAT_COOL
*****
UNIT C2S1 IS A SECTION_SS
  SET
    TOP_TRAY = 2, BOTTOM_TRAY = 13
*****
UNIT C2S3 IS A SECTION_SS
  SET
    TOP_TRAY = 19, BOTTOM_TRAY = 20
*****
UNIT C2SPL1 IS A RSLİT
*****
UNIT C2SPL2 IS A RSLİT
*****
UNIT C2T15 IS A TRAY_SS
*****
UNIT C2T16 IS A TRAY_SS
*****
UNIT C2T18 IS A TRAY_SS
*****
UNIT C2TR1 IS A TEAR
*****
UNIT C2TR2 IS A TEAR
*****
UNIT C2TR3 IS A TEAR
*****
UNIT C4 IS A SECTION_SS
  SET
    TOP_TRAY = 1, BOTTOM_TRAY = 2
*****
UNIT C4REBL IS A REBOILER_SS
****
UNIT C5 IS A SECTION_SS
  SET
    TOP_TRAY = 1, BOTTOM_TRAY = 2
****
UNIT C5REBL IS A REBOILER_SS
****
UNIT E1 IS A HEAT_COOL
****
UNIT F01 IS A VFLOW
****
UNIT F11 IS A VAP_VFLOW
****
UNIT F12 IS A LIQ_VFLOW
****
UNIT F13 IS A C5_VFLOW
****
UNIT F21 IS A VFLOW
****
UNIT F22 IS A VFLOW
****
UNIT F22A IS A LIQ_VFLOW
****
UNIT F31 IS A LIQ_VFLOW
****
UNIT F32 IS A LIQ_VFLOW
****
UNIT F41 IS A LIQ_VFLOW
****
UNIT F42 IS A TBP
****
UNIT F51 IS A LIQ_VFLOW
****
UNIT F52 IS A TBP
****
UNIT F61 IS A VFLOW
****
UNIT F62 IS A LIQ_VFLOW
****
UNIT M2R31 IS A M2R
****
UNIT MFEED IS A MOL_FEED
****
UNIT RVP31 IS A RVP
****
E.4 Additional rtdr6.speedup Code

The following SPEEDUP input code is specific to the rtdr6.speedup data reconciliation simulation. See section E.3 for the rest of the SPEEDUP input code used in rtdr6.speedup.

OPTIONS
#
# rtdr6.speedup (10/04/97)
#
  Routines NEWTON, SUPERDAE, SRQP, NL2SOL, MA28
EXECUTION
  PRINTLEVEL = 2
  TARGET = TERMINAL
  DEBUG = ON
  OPT_TOL = 1.0E-1
  SRQPGLBCON = 3
  SRQPVARINI = 1
  RESTOL = 1.0E-5
  CONVTEST = RES
  ABS_TOL = 1.0E-5
  REL_TOL = 1.0E-5
  MAXVARSTEP = 10.0
  MINNONZERO = 1.0E-8
  NONREDITER = 5
  ITERATIONS = 500
  DGLEG = ON
  RANGEFRAC = 0.1

****
GLOBAL
# DATA RECONCILIATION OF THE PLANT
# Variables to be used in the data reconciliation
VARIABLES
  *ST22, **ST23, **ST31, **ST32, **ST41, **ST42, **ST51, **ST52, **ST61,
  *VT12, **VT13, **VT21, **VT22, **VT23, **VT31, **VT32, **VT41, **VT42,
  **VT51, **VT52, **VT61, **VT62, *WF01, *WF11, *WF12,
  *CNVF2B, EF01, EF11, EF12, EF13, EF21, EF22, EF31, EF32, EF41,
EF42, EF51, EF52, EF61, EF62, ET01, ET12, ET13, ET21, ET22,
ET23, ET31, ET32, ET41, ET42, ET51, ET52, ET61, ET62

# Data Reconciliation Objective Function

MINIMIZE

EF01 + EF11 + EF12 + EF13 + EF21 + EF22 + EF31 + EF32 + EF41 +
EF42 + EF51 + EF52 + EF61 + EF62 + ET01 + ET12 + ET13 + ET21 +
ET22 + ET23 + ET31 + ET32 + ET41 + ET42 + ET51 + ET52 + ET61 +
ET62

CONSTRAINT

EF01 = WF01 * (((F01.STDVOLFL * CNVF2B) - SF01) / VF01)'2 ;
EF11 = WF11 * (((F11.STDVOLFL - SF11) / VF11)'2 ;
EF12 = WF12 * (((F12.STDVOLFL * CNVF2B) - SF12) / VF12)'2 ;
EF13 = WF13 * (((F13.STDVOLFL * CNVF2B) - SF13) / VF13)'2 ;
EF21 = WF21 * (((F21.STDVOLFL * CNVF2B) - SF21) / VF21)'2 ;
EF22 = WF22 * (((F22.STDVOLFL * CNVF2B) - SF22) / VF22)'2 ;
EF31 = WF31 * (((F31.STDVOLFL * CNVF2B) - SF31) / VF31)'2 ;
EF32 = WF32 * (((F32.STDVOLFL * CNVF2B) - SF32) / VF32)'2 ;
EF41 = WF41 * (((F41.STDVOLFL * CNVF2B) - SF41) / VF41)'2 ;
EF42 = WF42 * (((F42.STDVOLFL * CNVF2B) - SF42) / VF42)'2 ;
EF51 = WF51 * (((F51.STDVOLFL * CNVF2B) - SF51) / VF51)'2 ;
EF52 = WF52 * (((F52.STDVOLFL * CNVF2B) - SF52) / VF52)'2 ;
EF61 = WF61 * (((F61.STDVOLFL * CNVF2B) - SF61) / VF61)'2 ;
EF62 = WF62 * (((F62.STDVOLFL * CNVF2B) - SF62) / VF62)'2 ;
ET01 - WT01 = ((MFEEDE.T_OUT - ST01) / VT01)'2 ;
ET12 = WT12 * ("C1S.TRAY_SS(2)".T - ST12) / VT12)'2 ;
ET13 = WT13 * (C1COND.T - ST13) / VT13)'2 ;
ET21 = WT21 * (C1BT29.TL_OUT1 - ST21) / VT21)'2 ;
ET22 = WT22 * (C1REBL.T_OUT - ST22) / VT22)'2 ;
ET23 = WT23 * (E1.T_OUT - ST23) / VT23)'2 ;
ET31 = WT31 * ("C2S1.TRAY_SS(2)".T - ST31) / VT31)'2 ;
ET32 = WT32 * (C2COND.T - ST32) / VT32)'2 ;
ET41 = WT41 * (C2SPL1.TL_OUT1 - ST41) / VT41)'2 ;
ET42 = WT42 * (C4REBL.TL_OUT - ST42) / VT42)'2 ;
ET51 = WT51 * (C2SPL2.TL_OUT1 - ST51) / VT51)'2 ;
ET52 = WT52 * (C5REBL.TL_OUT - ST52) / VT52)'2 ;
ET61 = WT61 * (C2BT24.TL_OUT1 - ST61) / VT61)'2 ;
ET62 = WT62 * (C2REBL.T_OUT - ST62) / VT62)'2 ;

****

OPERATION

SET

# Set Feed Stream Flow, Comp, Temp and Press.

WITHIN MFEED

Z_OUT = <0.000703680, 0.0246830, 0.0473640, 0.0387240,
0.0535310, 0.0312790, 0.0351930, 0.0161490,
0.0472560, 0.0435620, 0.0496490, 0.0530710>,
P_OUT = 200.0

# Set Partial Condenser conditions in C1
WITHIN C1COND
  P = 163.0
  Q = 8.87771527360 : 1 : 50
WITHIN C1SPL1
  L_OUT1 = 114.286875754 : 10 : 1000

# Set Stripping Section Tray conditions in C1
WITHIN "C1S.TRAY_SS(2)"
  P = 167.0
  Q = 0

?REPEAT
  WITHIN "C1S.TRAY_SS(?((i)))"
    P = "C1S.TRAY_SS(2)".P + (?((i))-2)*(6/27)
    Q = 0
?WITH i = <3:13>

# Set Feed Tray conditions in C1
WITHIN C1FT14
  F_IN = 1487.17710 : 100 : 5000
  T_IN = 412.9547 : 100 : 700
  P = "C1S.TRAY_SS(2)".P + 12*(6/27)
  Q = 0

# Rectifying Section Tray conditions in C1
?REPEAT
  WITHIN "C1R.TRAY_SS(?((i)))"
    P = "C1S.TRAY_SS(2)".P + (?((i))-2)*(6/27)
    Q = 0
?WITH i = <15:28>

# Set Bottom Tray Conditions in C1
WITHIN C1BT29
  P = "C1S.TRAY_SS(2)".P + 6.0
  Q = 0
  L_OUT1 = 1199.59366066 : 100 : 3000
  L_OUT2 = 2005.69940 : 200 : 5000

# Set Reboiler Conditions in C1
WITHIN C1REBL
  P_OUT = "C1S.TRAY_SS(2)".P + 6.0

# Set Heat Exchanger Conditions in E1
WITHIN E1
  P_OUT = 34.00

# Set Partial Condenser conditions in C2
WITHIN C2COND
P = 18.95810  
Q = 38.1525304313 : 1 : 80  
T_DROP = 28.0331682663 : 5 : 200  

# Set Column Tray Conditions in C2  
WITHIN "C2S1.TRAY_SS(2)"  
P = 22.95810
Q = 0

?REPEAT  
WITHIN "C2S1.TRAY_SS(?i)"
  P = "C2S1.TRAY_SS(2)".P + (?i-2)*(12.7/22)
  Q = 0
?WITH i = <3:13>  
WITHIN C2FT14
  P = "C2S1.TRAY_SS(2)".P + 12*(12.7/22)
  Q = 0
WITHIN C2T15
  P = "C2S1.TRAY_SS(2)".P + 13*(12.7/22)
  Q = 0
WITHIN C2T16
  P = "C2S1.TRAY_SS(2)".P + 14*(12.7/22)
  Q = 0
WITHIN C2FT17
  P = "C2S1.TRAY_SS(2)".P + 15*(12.7/22)
  Q = 0
WITHIN C2T18
  P = "C2S1.TRAY_SS(2)".P + 16*(12.7/22)
  Q = 0

?REPEAT  
WITHIN "C2S3.TRAY_SS(?i)"
  P = "C2S1.TRAY_SS(2)".P + (?i-2)*(12.7/22)
  Q = 0
?WITH i = <19:20>  
WITHIN C2FT21
  T_IN = 479.6565 : 449.6565 : 509.6565
  P = "C2S1.TRAY_SS(2)".P + 19*(12.7/22)
  Q = 0

?REPEAT  
WITHIN "C2R.TRAY_SS(?i)"
  P = "C2S1.TRAY_SS(2)".P + (?i-2)*(12.7/22)
  Q = 0
?WITH i = <22:23>  

# Set Bottom Tray Conditions in C2  
WITHIN C2BT24
  P = "C2S1.TRAY_SS(2)".P + 12.7
  Q = 0
L_OUT1 = 526.158606822 : 20 : 2000
L_OUT2 = 1327.217 : 20 : 4000
# Set Reboiler Conditions in C2
WITHIN C2REBL
  P_OUT = "C2S1.TRAY_SS(2)".P + 12.7
# Set Sidedraw Splitters in C2
WITHIN C2SPL1
  L_OUT1 = 477.609398224 : 20 : 3000
WITHIN C2SPL2
  L_OUT1 = 248.210375677 : 20 : 3000
# Set C4 Tray Conditions
WITHIN "C4.TRAY_SS(1)"
  P = "C2S1.TRAY_SS(2)".P + 6.92727
  Q = 0
WITHIN "C4.TRAY_SS(2)"
  P = "C2S1.TRAY_SS(2)".P + 6.92727
  Q = 0
# Set C4 Reboiler Conditions
WITHIN C4REBL
  P = "C2S1.TRAY_SS(2)".P + 6.92727
  L_OUT = 353.870545934 : 10 : 2000
# Set C5 Tray Conditions
WITHIN "C5.TRAY_SS(1)"
  P = "C2S1.TRAY_SS(2)".P + 8.65909
  Q = 0
WITHIN "C5.TRAY_SS(2)"
  P = "C2S1.TRAY_SS(2)".P + 8.65909
  Q = 0
# Set C5 Reboiler Conditions
WITHIN C5REBL
  P = "C2S1.TRAY_SS(2)".P + 8.65909
  L_OUT = 132.989607904 : 10 : 2000
# Set Tear Stream Conditions
WITHIN C1TR1
  F_SLACK = 0.0
  T_SLACK = 0.0
  P_SLACK = 0.0
  H_SLACK = 0.0
  Z_SLACK = <0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0>
WITHIN C2TR1
  F_SLACK = 0.0
  T_SLACK = 0.0
P_SLACK = 0.0
H_SLACK = 0.0
Z_SLACK = <0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0>

WITHIN C2TR2
F_SLACK = 0.0
T_SLACK = 0.0
P_SLACK = 0.0
H_SLACK = 0.0
Z_SLACK = <0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0>

WITHIN C2TR3
F_SLACK = 0.0
T_SLACK = 0.0
P_SLACK = 0.0
H_SLACK = 0.0
Z_SLACK = <0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0>

WITHIN F01
STDTEMP = 60.0
STDRES = 14.696

WITHIN F11
STDTEMP = 60.0
STDRES = 14.696

WITHIN F12
STDTEMP = 60.0
STDRES = 14.696

WITHIN F13
STDTEMP = 60.0
STDRES = 14.696

WITHIN F21
STDTEMP = 60.0
STDRES = 14.696

WITHIN F22
STDTEMP = 60.0
STDRES = 14.696

WITHIN F22A
STDTEMP = 60.0
STDRES = 14.696
WITHIN F31
STDTEMP = 60.0
STDPRES = 14.696

WITHIN RVP31
COLDTEMP = 32.0
WARMTEMP = 100.0
STDPRES = 14.696
ZAIR = <0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1>
RHOA32 = 2.78527E-3
RHOB = 2.44686E-3

WITHIN F32
STDTEMP = 60.0
STDPRES = 14.696

WITHIN F41
STDTEMP = 60.0
STDPRES = 14.696

WITHIN F42
STDTEMP = 60.0
STDPRES = 14.696

WITHIN F51
STDTEMP = 60.0
STDPRES = 14.696

WITHIN F52
STDTEMP = 60.0
STDPRES = 14.696

WITHIN F61
STDTEMP = 60.0
STDPRES = 14.696

WITHIN F62
STDTEMP = 60.0
STDPRES = 14.696

WITHIN GLOBAL

# SET MEASURED VALUES
SF01 = 20863.014
SF11 = 75209.44167
SF12 = 7024.6257
SF13 = 884.40222
SF21 = 31955.347
SF22 = 19080.626
SF31 = 1580.2698
SF32 = 12862.473
SF41 = 5029.6623
SF42 = 3817.694
SF51 = 3264.5036
SF52 = 1847.737
SF61 = 29933.726
SF62 = 12250.671
ST01 = 412.9547
ST12 = 152.33838
ST13 = 96.372107
ST21 = 516.0132
ST22 = 586.08488
ST23 = 479.69655
ST31 = 128.35124
ST32 = 84.722528
ST41 = 240.31157
ST42 = 261.0776
ST51 = 356.19866
ST52 = 423.89816
ST61 = 623.44743
ST62 = 683.89991

# SET VARIANCES FOR MEASURED VARIABLES
VF01 = 1043.1507
VF11 = 3760.4721
VF12 = 351.23129
VF13 = 44.22011
VF21 = 1597.7674
VF22 = 954.03132
VF31 = 79.01349
VF32 = 643.12363
VF41 = 251.48312
VF42 = 190.8847
VF51 = 163.22518
VF52 = 92.386852
VF61 = 1496.6863
VF62 = 612.53556
VT01 = 20.647735
VT12 = 7.6269189
VT13 = 4.8186054
VT21 = 25.80066
VT22 = 29.304244
VT23 = 23.984827
VT31 = 6.4175619
VT32 = 4.2361264
VT41 = 12.015579
VT42 = 13.05388
VT51 = 17.809933
VT52 = 21.194908
VT61 = 31.172371
VT62 = 34.194995
#
SET WEIGHTS FOR DATA RECONCILIATION
WF01 = 2.0
WF11 = 2.0
WF12 = 2.0
WF13 = 2.0
WF21 = 2.0
WF22 = 2.0
WF31 = 2.0
WF32 = 2.0
WF41 = 2.0
WF42 = 2.0
WF51 = 2.0
WF52 = 2.0
WF61 = 2.0
WF62 = 2.0
WT01 = 2.0
WT12 = 2.0
WT13 = 2.0
WT21 = 2.0
WT22 = 2.0
WT23 = 2.0
WT31 = 2.0
WT32 = 2.0
WT41 = 2.0
WT42 = 2.0
WT51 = 2.0
WT52 = 2.0
WT61 = 2.0
WT62 = 2.0
#
SET UNIT CONVERSIONS
CNVF2B = 4.274857143  # Convet CUFT/HR to BBL/DAY
FREE
C1FT14.F_IN : 1500
C1FT14.T_IN : 420
C1SPL1.L_OUT1 : 200
C1COND.Q : 10
C1BT29.L_OUT1 : 1300
C1BT29.L_OUT2 : 2000
C2FT21.T_IN : 480
C2COND.Q : 40
C2COND.T_DROP : 40
C2BT24.L_OUT1 : 600
C2BT24.L_OUT2 : 1500
C2SPL1.L_OUT1 : 600
C4REBL.L_OUT : 450
C2SPL2.L_OUT1 : 350
C5REBL.L_OUT : 230

# Initial Guesses for Some Variables

#------------------------
# PRESET # from RESULTS
#------------------------

# The preset subsection has been omitted from this printout as it is
# preset automatically during the real time optimization

***

EXTERNAL

RECEIVE

# Read in Data Reconciliation Parameters (84 variables)
  GLOBAL.SF01, GLOBAL.SF11, GLOBAL.SF12, GLOBAL.SF13, GLOBAL.SF21,
  GLOBAL.SF22, GLOBAL.SF31, GLOBAL.SF32, GLOBAL.SF41, GLOBAL.SF42,
  GLOBAL.SF51, GLOBAL.SF52, GLOBAL.SF61, GLOBAL.SF62, GLOBAL.ST01,
  GLOBAL.ST12, GLOBAL.ST13, GLOBAL.ST21, GLOBAL.ST22, GLOBAL.ST23,
  GLOBAL.ST31, GLOBAL.ST32, GLOBAL.ST41, GLOBAL.ST42, GLOBAL.ST51,
  GLOBAL.ST52, GLOBAL.ST61, GLOBAL.ST62, GLOBAL.VF01, GLOBAL.VF11,
  GLOBAL.VF12, GLOBAL.VF13, GLOBAL.VF21, GLOBAL.VF22, GLOBAL.VF31,
  GLOBAL.VF32, GLOBAL.VF41, GLOBAL.VF42, GLOBAL.VF51, GLOBAL.VF52,
  GLOBAL.VF61, GLOBAL.VF62, GLOBAL.VT01, GLOBAL.VT12, GLOBAL.VT13,
  GLOBAL.VT21, GLOBAL.VT22, GLOBAL.VT23, GLOBAL.VT31, GLOBAL.VT32,
  GLOBAL.VT41, GLOBAL.VT42, GLOBAL.VT51, GLOBAL.VT52, GLOBAL.VT61,
  GLOBAL.VT62, GLOBAL.WF01, GLOBAL.WF11, GLOBAL.WF12, GLOBAL.WF13,
  GLOBAL.WF21, GLOBAL.WF22, GLOBAL.WF31, GLOBAL.WF32, GLOBAL.WF41,
  GLOBAL.WF42, GLOBAL.WF51, GLOBAL.WF52, GLOBAL.WF61, GLOBAL.WF62,
  GLOBAL.WT01, GLOBAL.WT12, GLOBAL.WT13, GLOBAL.WT21, GLOBAL.WT22,
  GLOBAL.WT23, GLOBAL.WT31, GLOBAL.WT32, GLOBAL.WT41, GLOBAL.WT42,
  GLOBAL.WT51, GLOBAL.WT52, GLOBAL.WT61, GLOBAL.WT62,

# Read in Simulation Set Points (43 variables)
  MFEED.Z_OUT(1), MFEED.Z_OUT(2), MFEED.Z_OUT(3), MFEED.Z_OUT(4),
  MFEED.Z_OUT(5), MFEED.Z_OUT(6), MFEED.Z_OUT(7), MFEED.Z_OUT(8),
  MFEED.Z_OUT(9), MFEED.Z_OUT(10), MFEED.Z_OUT(11), MFEED.Z_OUT(12),
  MFEED.Z_OUT(13), MFEED.Z_OUT(14), MFEED.Z_OUT(15), MFEED.Z_OUT(16),
  MFEED.Z_OUT(17), MFEED.Z_OUT(18), MFEED.Z_OUT(19), MFEED.Z_OUT(20),
  MFEED.Z_OUT(21), MFEED.Z_OUT(22), MFEED.P_OUT, C1COND.P, C1COND.Q,
  CSPL1.L_OUT1, "C1S.TRAY_SS(2)".P, C1FT14.F_IN, C1FT14.T_IN,
  C1BT29.L_OUT1, C1BT29.L_OUT2, E1.P_OUT, C2COND.P, C2COND.Q,
  C2COND.T_DROP, "C2S1.TRAY_SS(2)".P, C2FT21.T_IN, C2BT24.L_OUT1,
  C2BT24.L_OUT2, CSPL1.L_OUT1, CSPL2.L_OUT1, C4REBL.L_OUT,
  CSREBL.L_OUT,

# Read in Free variables Bounds (30 variables)
  UBOUND (C1COND.Q), LBOUND(C1COND.Q),
  UBOUND (CSPL1.L_OUT1), LBOUND (CSPL1.L_OUT1),
UBOUND (C1FT14_F_IN), LBOUND (C1FT14_F_IN),
UBOUND (C1FT14_T_IN), LBOUND (C1FT14_T_IN),
UBOUND (C1BT29_L_OUT1), LBOUND (C1BT29_L_OUT1),
UBOUND (C1BT29_L_OUT2), LBOUND (C1BT29_L_OUT2),
UBOUND (C2COND_Q), LBOUND (C2COND_Q),
UBOUND (C2COND_T_DROP), LBOUND (C2COND_T_DROP),
UBOUND (C2FT21_T_IN), LBOUND (C2FT21_T_IN),
UBOUND (C2BT24_L_OUT1), LBOUND (C2BT24_L_OUT1),
UBOUND (C2BT24_L_OUT2), LBOUND (C2BT24_L_OUT2),
UBOUND (C2SPL1_L_OUT1), LBOUND (C2SPL1_L_OUT1),
UBOUND (C2SPL2_L_OUT1), LBOUND (C2SPL2_L_OUT1),
UBOUND (C4REBL_L_OUT), LBOUND (C4REBL_L_OUT),
UBOUND (C5REBL_L_OUT), LBOUND (C5REBL_L_OUT)

TRANSMIT

# Write out Simulations Set Points after Data Rec (44 variables)
MFEED_Z_OUT(1), MFEED_Z_OUT(2), MFEED_Z_OUT(3), MFEED_Z_OUT(4),
MFEED_Z_OUT(5), MFEED_Z_OUT(6), MFEED_Z_OUT(7), MFEED_Z_OUT(8),
MFEED_Z_OUT(9), MFEED_Z_OUT(10), MFEED_Z_OUT(11), MFEED_Z_OUT(12),
MFEED_Z_OUT(13), MFEED_Z_OUT(14), MFEED_Z_OUT(15), MFEED_Z_OUT(16),
MFEED_Z_OUT(17), MFEED_Z_OUT(18), MFEED_Z_OUT(19), MFEED_Z_OUT(20),
MFEED_Z_OUT(21), MFEED_Z_OUT(22), MFEED_P_OUT, C1COND_P, C1COND_Q,
C1SPL1_L_OUT1, "C1S.TRAY_SS(2)".P, C1FT14_F_IN, C1FT14_T_IN,
C1BT29_L_OUT1, C1BT29_L_OUT2, E1_P_OUT, C2COND_P, C2COND_Q,
C2COND_T_DROP, "C2S1.TRAY_SS(2)".P, C2FT21_T_IN, C2BT24_L_OUT1,
C2BT24_L_OUT2, C2SPL1_L_OUT1, C2SPL2_L_OUT1, C4REBL_L_OUT,
C5REBL_L_OUT, F31_TL_OUT

****

E.5  rtodr6.f

The following FORTRAN input code, rtodr6.f, contains SPEEDUP EDI
(External Data Interface) subroutines used by rtodr6.speedup.

C RTODR6.SPEEDUP ROUTINES FOR EDI
C
C  **** EXTINI ****
C
C  THIS ROUTINE IS USED TO ALERT THE EXTERNAL SYSTEM
C  IFLAG=0 FOR SUCCESSFUL RUN
C
C     SUBROUTINE EXTINI(MODE,IFLAG)
     INTEGER MODE, IFLAG
C
WRITE (*,*) '>>>RTODR6: EXTINI CALLED - NOTHING DONE'
IFLAG=0
RETURN
END

C
C **** EXTGET ****
C
C THIS ROUTINE GETS THE DATA
C IFLAG=0 FOR SUCCESSFUL RUN
C
SUBROUTINE EXTGET(N,TAGNAM,X,T,TNEXT,IFLAG)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
DIMENSION X(N)
CHARACTER * 40 TAGNAM(N)
LOGICAL THERE
INTEGER FNFREE
C GET A FREE CHANNEL FOR THE FILE
ICHAN=FNFREE()
C
WRITE (*,*) '>>>RTODR6: EXTGET CALLED - READING IN DATA'
C READ IN MEASURED VALUES FROM FILE IMEAS.DAT
INQUIRE (FILE='IMEAS.DAT', EXIST=THERE)
IF (.NOT.THERE) THEN
  GO TO 915
ENDIF
OPEN (UNIT=ICHAN, STATUS='OLD', ERR=910, FILE='IMEAS.DAT')
REWRIND (UNIT=ICHAN)
DO 20 M=1,28
  READ (ICHAN,100,ERR=900,END=905) X(M)
20 CONTINUE
CLOSE (UNIT=ICHAN)
C READ IN VARIANCES FROM FILE IVARNC.DAT
INQUIRE (FILE='IVARNC.DAT', EXIST=THERE)
IF (.NOT.THERE) THEN
  GO TO 920
ENDIF
OPEN (UNIT=ICHAN, STATUS='OLD', ERR=910, FILE='IVARNC.DAT')
REWRIND (UNIT=ICHAN)
DO 25 M=29,56
  READ (ICHAN,100,ERR=900,END=905) X(M)
25 CONTINUE
CLOSE (UNIT=ICHAN)
C READ IN WEIGHTS FROM FILE IWGHT.DAT
INQUIRE (FILE='IWGHT.DAT', EXIST=THERE)
IF (.NOT.THERE) THEN
GO TO 925
ENDIF
OPEN (UNIT=ICHAN, STATUS='OLD', ERR=910, FILE='IWGHT.DAT')
REWIND (UNIT=ICHAN)
DO 30 M=57,84
   READ (ICHAN, 100, ERR=900, END=905) X(M)
30 CONTINUE
CLOSE (UNIT=ICHAN)
C READ IN SET VARIABLES FROM FILE ISET.DAT
INQUIRE (FILE='ISET.DAT', EXIST=THEIR)
IF (.NOT.THERE) THEN
   GO TO 930
ENDIF
OPEN (UNIT=ICHAN, STATUS='OLD', ERR=910, FILE='ISET.DAT')
REWIND (UNIT=ICHAN)
DO 35 M=85,127
   READ (ICHAN, 105, ERR=900, END=905) X(M)
35 CONTINUE
CLOSE (UNIT=ICHAN)
C READ IN FREE VARAIBLE BOUNDS FROM FILE IDFREE.DAT
INQUIRE (FILE='IDFREE.DAT', EXIST=THEIR)
IF (.NOT.THERE) THEN
   GO TO 935
ENDIF
OPEN (UNIT=ICHAN, STATUS='OLD', ERR=910, FILE='IDFREE.DAT')
REWIND (UNIT=ICHAN)
READ(ICHAN, 100, ERR=900, END=905) TEMP
X(128) = X(109) + TEMP
X(129) = X(109) - TEMP
READ(ICHAN, 100, ERR=900, END=905) TEMP
X(130) = X(110) + TEMP
X(131) = X(110) - TEMP
READ(ICHAN, 100, ERR=900, END=905) TEMP
X(132) = X(112) + TEMP
X(133) = X(112) - TEMP
READ(ICHAN, 100, ERR=900, END=905) TEMP
X(134) = X(113) + TEMP
X(135) = X(113) - TEMP
READ(ICHAN, 100, ERR=900, END=905) TEMP
X(136) = X(114) + TEMP
X(137) = X(114) - TEMP
READ(ICHAN, 100, ERR=900, END=905) TEMP
X(138) = X(115) + TEMP
X(139) = X(115) - TEMP
READ(ICHAN, 100, ERR=900, END=905) TEMP
X(140) = X(118) + TEMP
X(141) = X(118) - TEMP
READ(ICHAN,100,ERR=900,END=905) TEMP
X(142) = X(119) + TEMP
X(143) = X(119) - TEMP
READ(ICHAN,100,ERR=900,END=905) TEMP
X(144) = X(121) + TEMP
X(145) = X(121) - TEMP
READ(ICHAN,100,ERR=900,END=905) TEMP
X(146) = X(122) + TEMP
X(147) = X(122) - TEMP
READ(ICHAN,100,ERR=900,END=905) TEMP
X(148) = X(123) + TEMP
X(149) = X(123) - TEMP
READ(ICHAN,100,ERR=900,END=905) TEMP
X(150) = X(124) + TEMP
X(151) = X(124) - TEMP
READ(ICHAN,100,ERR=900,END=905) TEMP
X(152) = X(125) + TEMP
X(153) = X(125) - TEMP
READ(ICHAN,100,ERR=900,END=905) TEMP
X(154) = X(126) + TEMP
X(155) = X(126) - TEMP
READ(ICHAN,100,ERR=900,END=905) TEMP
X(156) = X(127) + TEMP
X(157) = X(127) - TEMP
CLOSE (UNIT=ICHAN)
WRITE (*,*) '>>RTODR6: EXTGET - DATA READ SUCCESSFULLY'
IFLAG=0
100 FORMAT(15X, E15.8)
105 FORMAT(42X, E15.8)
RETURN

C ERROR STATEMENTS
900 WRITE(*,*) 'RTODR6: EXTGET: Error reading ',TAGNAM(M)
      IFLAG = -1
RETURN
905 WRITE(*,*) 'RTODR6: EXTGET: EOF reached reading ',TAGNAM(M)
      IFLAG = -1
RETURN
910 WRITE(*,*) 'RTODR6: EXTGET: Error opening file'
      IFLAG = -1
RETURN
915 WRITE(*,*) 'RTODR6: EXTGET: IMEAS.DAT does not exist'
      IFLAG = -1
RETURN
920 WRITE(*,*) 'RTODR6: EXTGET: IVARNC.DAT does not exist'
   IFLAG = -1
   RETURN
925 WRITE(*,*) 'RTODR6: EXTGET: IWGHT.DAT does not exist'
   IFLAG = -1
   RETURN
930 WRITE(*,*) 'RTODR6: EXTGET: ISET.DAT does not exist'
   IFLAG = -1
   RETURN
935 WRITE(*,*) 'RTODR6: EXTGET: IDFREE.DAT does not exist'
   IFLAG = -1
   RETURN
END
C
C ***** EXTPUT *****
C
C THIS ROUTINE WRITES OUT THE CALCULATED VARIABLES
C IFLAG=0 FOR SUCCESSFUL RUN
C
SUBROUTINE EXTPUT(N,TAGNAM,X,T,IFLAG)
  IMPLICIT DOUBLE PRECISION (A-H,O-Z)
  DIMENSION X(N)
  CHARACTER * 40 TAGNAM(N)
  INTEGER FNFREE
  LOGICAL THERE
C GET A FREE CHANNEL FOR THE FILE
  ICHAN=FNFREE()
C
   WRITE (*,*) '>>>RTODR6: EXTPUT CALLED - WRITING OUT RESULTS'
C WRITE OUT SET VARIABLES TO FILE RDSET.DAT
   INQUIRE (FILE='RDSET.DAT', EXIST=THESE)
   IF (THESE) THEN
      GO TO 915
   ENDIF
   OPEN (UNIT=ICHAN, STATUS='NEW', ERR=910, FILE='RDSET.DAT')
   REWIND (UNIT=ICHAN)
   DO 10 M=1,44
      WRITE(ICHAN,100,ERR=900) TAGNAM(M), X(M)
   10 CONTINUE
   CLOSE (UNIT=ICHAN)
   WRITE (*,*) '>>>RTODR6: EXTPUT - DATA WRITTEN SUCCESSFULLY'
   IFLAG=0
100 FORMAT(A40, 2X, E15.8)
   RETURN
900 WRITE(*,*) 'RTODR6: EXTPUT: Error writing ', TAGNAM(M)
IFLAG = -1
RETURN
910 WRITE(*,*) 'RTODR6: EXTPUT: Error opening file'
   IFLAG = -1
RETURN
915 WRITE(*,*) 'RTODR6: EXTPUT: RDSET.DAT already exists'
   IFLAG = -1
RETURN
END

C
C ***** EXTRM *****
C
C TERMINATION PROGRAMME
C IFLAG=0 FOR SUCCESSFUL RUN
C
   SUBROUTINE EXTRM(IFLAG)
   IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
   WRITE (*,*)'>>>RTODR6: EXTINI CALLED - EDI FINISHED'
   IFLAG=0
   RETURN
END

C
C ***** EXTWAI *****
C
C WAIT PROGRAMME
C IFLAG=0 CONTINUE RUNNING
C IFLAG=-1 REQUEST TO TERMINATE
C
   SUBROUTINE EXTWAI (T,IFLAG)
   IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
   WRITE (*,*) '>>>RTODR6: EXTWAI CALLED - TERMINATING RUN'
   IFLAG =-1
   RETURN
END

C
C ***** EXTMSG *****
C
C MESSAGE PROGRAMME
C IFLAG=0 FOR SUCCESSFUL RUN
C
   SUBROUTINE EXTMSG (MESSGE, MESTYP, IFLAG)
   CHARACTER * (*) MESSGE
   INTEGER MESTYP, IFLAG
IFLAG=0
WRITE (*,*) '>>>RTODRG6: EXTMSG CALLED - WRITING MESSAGE'
WRITE (*,*) 'MESSAGE OF TYPE', MESTYP
WRITE (*,*) 'MESSAGE '
WRITE (*,*) 'RTODRG6: EXTMSG - MESSAGE HAS BEEN WRITTEN'
RETURN
END

C
C FUNCTION TO FIND A FREE TERMINAL
C
INTEGER FUNCTION FNFREE()
C
COPYRIGHT (C) ASPENTECH UK LTD, 1991
C
FNFREE FINDS THE FIRST FREE LOGICAL UNIT FOR ASSIGNING TO A FILE.
C
IT DOES THIS BY TRYING THEM ALL IN ASCENDING ORDER UNTIL ONE IS FREE.
C
RETURNS -1 IF NONE FREE.
C
IMPLICIT NONE
LOGICAL OPEND
INTEGER I
DO 100 I=1,119
INQUIRE(UNIT=I,OPEND=OPEND)
IF (.NOT.OPEND) THEN
  FNFREE=I
  RETURN
ENDIF
100 CONTINUE
FNFREE=-1
RETURN
END

E.6 Additional rtopt6.speedup Code

The following SPEEDUP input code is specific to the rtopt6.speedup optimization simulation. See section E.3 for the rest of the SPEEDUP input code used in rtopt6.speedup.

OPTIONS
#
# rtopt6.speedup (10/04/97)
#
ROUTINES NEWTON, SUPERDAE, SRQP, NL2SOL, MA28
EXECUTION

PRINTLEVEL = 2
TARGET = TERMINAL
DEBUG = ON
OPT_TOL = 1.0E-1
SRQPGLBCON = 2
SRQPVARINI = 1
RESTOL = 1.0E-5
CONVTEST = RES
ABS_TOL = 1.0E-5
REL_TOL = 1.0E-5
MAXVARSSTEP = 10.0
MINNNONZERO = 1.0E-8
NONREDITER = 5
ITERATIONS = 500
DOGLEG = ON
RANGEFRA = 0.1

*****

GLOBAL

# OPTIMISATION OF THE PLANT TO MAXIMISE PROFIT

# Variables to be used in the optimization

VARIABLES
*CNVP2K, *F1EFF, *F2EFF, PVALS, CSTAB, COF1, COF2, PVAP, PDIST,
PLTISO, PHVIS0, PLTDST, PSSFED, *CNVF2B, *WOBJ,

# Economic Objective Function
MAXIMIZE
(PVALS - CSTAB - COF1 - COF2) * WOBJ

CONSTRAINT

# Equality Constraints

# Premiums [($/$M3) = ($/$M3) + ($/$M3/UNIT) * (UNIT-UNIT)]
QLTISO = DLTISO + (PRMRVP * ((RVP31.RVP + CNVP2K) - SPCRVP)) ;

# Product Values [($/$HR) = ($/$M3) * (M3 HR/HR FT3) * (FT3/HR)]
PVAP = DVAP + CNVF2M + F11.STDVLNFL ;
PDIST = DDIST + CNVF2M + F13.STDVLNFL ;
PLTISO = QLTISO + CNVF2M + F31.STDVLNFL ;
PHVIS0 = DHVIS0 + CNVF2M + F42.STDVLNFL ;
PLTDST = DLTDST + CNVF2M + F52.STDVLNFL ;
PSSFED = DSSFED * CNVF2M * F62.STDVolFL;
PVALS = PVAP + PDIST + PLTISO + PHVIS0 + PLTDEST + PSSFED;

# Feed Cost [($/HR) = ($/M3) * (M3 HR/HR FT3) * (FT3/HR)]
CSTAB = DSTAB * CNVF2M * F01.STDVolFL;

# Utility Costs [($/HR) = ($/LMFEM3) * (LMFEM3/LFEBBL) * (LFEBBL/MMBTU)]
COF1 = DFO * CNVBMT * CNVBTU * C1REBL.Q * (1 / F1EFF);
COF2 = DFO * CNVBMT * CNVBTU * C2REBL.Q * (1 / F2EFF);

# Inequality Constraints
F13.CSS >= A11L;
F13.CSS <= A11U;
F42.TBP10 >= A41L1;
F42.TBP10 <= A41U1;
F42.TBP90 >= A41L9;
F42.TBP90 <= A41U9;
F52.TBP10 >= A51L1;
F52.TBP10 <= A51U1;
F52.TBP90 >= A51L9;
F52.TBP90 <= A51U9;
F12.STDVolFL >= F12L;
F12.STDVolFL <= F12U;
F32.STDVolFL >= F32U;
F32.STDVolFL <= F32U;
F41.STDVolFL >= F41U;
F51.STDVolFL <= F51U;
RVP31.RVP <= A31UR;
C2COND.T_BUBBLE >= A31LT;
"C1S.TRAY_SS(3).T" >= T11L;
"C1S.TRAY_SS(3).T" <= T11U;
C1REBL.T_OUT >= T22L;
C1REBL.T_OUT <= T22U;
"C2S1.TRAY_SS(2).T" >= T31L;
"C2S1.TRAY_SS(2).T" <= T31U;
C2REBL.T_OUT >= T62L;
C2REBL.T_OUT <= T62U;

# Indirect Free Variable Constraints
F13.L_OUT >= XF13L;
F13.L_OUT <= XF13U;
C1TR1.F_IN >= XF21L;
C1TR1.F_IN <= XF21U;
E1.F_IN >=XF22L;
E1.F_IN <=XF22U;
E1.T_OUT >= XT23L;
E1.T_OUT <= XT23U;
C2TR3.F_IN >= XF61L;
C2TR3.F_IN <= XF61U;
F62.L_OUT >= XF62L;
F62.L_OUT <= XF62U;
F31.TL_OUT >= XT32L;
F31.TL_OUT <= XT32U;
F42.L_OUT >= XF42L;
F42.L_OUT <= XF42U;
F52.L_OUT >= XF52L;
F52.L_OUT <= XF52U;
"C4.TRAY_SS(1)".L_IN >= XF41L;
"C4.TRAY_SS(1)".L_IN <= XF41U;
"C5.TRAY_SS(1)".L_IN >= XF51L;
"C5.TRAY_SS(1)".L_IN <= XF51U;
****
OPERATION
SET
# Set Feed Stream Flow, Comp, Temp and Press.
WITHIN MFEED
  Z_OUT = <0.000703680, 0.0246830, 0.0473640, 0.0387240,
         0.0535310, 0.0312790, 0.0351930, 0.0161490,
         0.0472560, 0.0435620, 0.0496490, 0.0530710,
         0.0523260, 0.0489630, 0.0444180, 0.041240,
         0.0607690, 0.0537820, 0.0598310, 0.0626870,
         0.056050, 0.0529210, >
  P_OUT = 200.0
# Set Partial Condenser conditions in C1
WITHIN C1COND
  P = 163.0
  Q = 10.28432
WITHIN C1SPL1
  L_OUT1 = 118.0199 : 10 : 1000
# Set Rectifying Section Tray conditions in C1
WITHIN "C1S.TRAY_SS(2)"
  P = 167.0
  Q = 0
?REPEAT
WITHIN "C1S.TRAY_SS(?(i))"
  P = "C1S.TRAY_SS(2)".P + (?(i)-2)*(6/27)
  Q = 0
?WITH i = <3:13>
# Set Feed Tray conditions in C1
WITHIN C1FT14
  F_IN = 1464.1499
  T_IN = 430.4696
  P = "C1S.TRAY_SS(2)".P + 12*(6/27)
  Q = 0
# Stripping Section Tray conditions in C1

?REPEAT
  WITHIN "C1R.TRAY_SS(?i)"
  P = "C1S.TRAY_SS(2)".P + (?i-2) *(6/27)
  Q = 0
?WITH i = <15:28>

# Set Bottom Tray Conditions in C1

WITHIN C1BT29
  P = "C1S.TRAY_SS(2)".P + 6.0
  Q = 0
  L_OUT1 = 1175.6446 : 100 : 4000
  L_OUT2 = 2004.8814 : 100 : 5000

# Set Reboiler Conditions in C1

WITHIN C1REBL
  P_OUT = 167.0 + 6.0

# Set Heat Exchanger Conditions in E1

WITHIN E1
  P_OUT = "C1S.TRAY_SS(2)".P + 6.0

# Set Partial Condenser conditions in C2

WITHIN C2COND
  P = 18.95810
  Q = 25.4106
  T_DROP = 32.9897 : 5 : 200

# Set Column Tray Conditions in C2

WITHIN "C2S1.TRAY_SS(2)"
  P = 22.95810
  Q = 0

?REPEAT
  WITHIN "C2S1.TRAY_SS(?i)"
  P = "C2S1.TRAY_SS(2)".P + (?i-2) *(12.7/22)
  Q = 0
?WITH i = <3:13>

WITHIN C2FT14
  P = "C2S1.TRAY_SS(2)".P + 12*(12.7/22)
  Q = 0

WITHIN C2T15
  P = "C2S1.TRAY_SS(2)".P + 13*(12.7/22)
  Q = 0

WITHIN C2T16
  P = "C2S1.TRAY_SS(2)".P + 14*(12.7/22)
  Q = 0

WITHIN C2FT17
  P = "C2S1.TRAY_SS(2)".P + 15*(12.7/22)
  Q = 0

WITHIN C2T18
P = "C2S1.TRAY_SS(2)".P + 16*(12.7/22)
Q = 0

?REPEAT
   WITH "C2S3.TRAY_SS(?i)"
   P = "C2S1.TRAY_SS(2)".P + (?i-2)*(12.7/22)
   Q = 0
?WITH i = <19:20>
   WITH C2FT21
   T_IN = 449.6569 : 100 : 700
   P = "C2S1.TRAY_SS(2)".P + 19*(12.7/22)
   Q = 0

?REPEAT
   WITH "C2R.TRAY_SS(?i)"
   P = "C2S1.TRAY_SS(2)".P + (?i-2)*(12.7/22)
   Q = 0
?WITH i = <22:23>
# Set Bottom Tray Conditions in C2
   WITH C2BT24
   P = "C2S1.TRAY_SS(2)".P + 12.7
   Q = 0
   L_OUT1 = 514.2549 : 50 : 4000
   L_OUT2 = 1328.1557 : 500 : 3000
# Set Reboiler Conditions in C2
   WITH C2REBL
   P_OUT = "C2S1.TRAY_SS(2)".P + 12.7
# Set Sidedraw Splitters in C2
   WITH C2SPL1
   L_OUT1 = 477.2064 : 50 : 2000
   WITH C2SPL2
   L_OUT1 = 241.6230 : 50 : 2000
# Set C4 Tray Conditions
   WITH "C4.TRAY_SS(1)"
   P = "C2S1.TRAY_SS(2)".P + 6.92727
   Q = 0
   WITH "C4.TRAY_SS(2)"
   P = "C2S1.TRAY_SS(2)".P + 6.92727
   Q = 0
# Set C4 Reboiler Conditions
   WITH C4REBL
   P = "C2S1.TRAY_SS(2)".P + 6.92727
   L_OUT = 353.7547 : 20 : 2000
# Set C5 Tray Conditions
   WITH "C5.TRAY_SS(1)"
   P = "C2S1.TRAY_SS(2)".P + 8.65909
   Q = 0
WITHIN "C5.TRAY_SS(2)"
   P = "C2S1.TRAY_SS(2)".P + 8.65909
   Q = 0
# Set C5 Reboiler Conditions
WITHIN C5REBL
   P = "C2S1.TRAY_SS(2)".P + 8.65909
   L_OUT = 131.1071 : 10 : 2000
# Set Tear Stream Conditions
WITHIN C1TR1
   F_SLACK = 0.0
   T_SLACK = 0.0
   P_SLACK = 0.0
   H_SLACK = 0.0
   Z_SLACK = <0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0>

WITHIN C2TR1
   F_SLACK = 0.0
   T_SLACK = 0.0
   P_SLACK = 0.0
   H_SLACK = 0.0
   Z_SLACK = <0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0>

WITHIN C2TR2
   F_SLACK = 0.0
   T_SLACK = 0.0
   P_SLACK = 0.0
   H_SLACK = 0.0
   Z_SLACK = <0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0>

WITHIN C2TR3
   F_SLACK = 0.0
   T_SLACK = 0.0
   P_SLACK = 0.0
   H_SLACK = 0.0
   Z_SLACK = <0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0>

WITHIN F01
STDTEMP = 60.0
STDTEMP = 60.0
WI THIN F11
STDTEMP = 60.0
STDTEM P = 14.696
STDTEM P = 14.696
WI THIN F12
STDTEMP = 60.0
STDTEM P = 14.696
STDTEM P = 14.696
WI THIN F13
STDTEMP = 60.0
STDTEM P = 14.696
STDTEM P = 14.696
WI THIN F21
STDTEMP = 60.0
STDTEM P = 14.696
STDTEM P = 14.696
WI THIN F22
STDTEMP = 60.0
STDTEM P = 14.696
STDTEM P = 14.696
WI THIN F22A
STDTEMP = 60.0
STDTEM P = 14.696
STDTEM P = 14.696
WI THIN F31
STDTEMP = 60.0
STDTEM P = 14.696
STDTEM P = 14.696
WI THIN RVP31
COLDTEM P = 32.0
WARMTEMP = 100.0
STDTEM P = 14.696
ZAIR = <0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1>
RHOA32 = 2.78527E-3
RHOB = 2.44686E-3
WI THIN F32
STDTEMP = 60.0
STDTEM P = 14.696
WI THIN F41
STDTEMP = 60.0
STDTEM P = 14.696
WI THIN F42
STDTEMP = 60.0
STDTEM P = 14.696
WI THIN F51
STDTEMP = 60.0
STDTEM P = 14.696
STDTEM P = 14.696
WI THIN F52
STDTEMP = 60.0
STDRES = 14.696
WITHIN F61
  STDTEMP = 60.0
  STDRES = 14.696
WITHIN F62
  STDTEMP = 60.0
  STDRES = 14.696

WITHIN GLOBAL

# Set Premium Values
PRMRVP = -0.18  # Premium for lower RVP in LT-ISO ($/M3/KPA)
SPCRVP = 97.0   # Specified RVP Value (KPA)

# Set Product Values ($/M3)
DVAP = 0.15
DDIST = 100.07
DLTISO = 182.69
DHVIS0 = 193.89
DLDST = 180.52
DSSFED = 158.34

# Set Feed Cost & Fuel Oil Cost ($/M3)
DSTAB = 158.34
DFO = 82.14

# Set Furnace Efficiencies
F1EFF = 0.70
F2EFF = 0.70

# Set Unit Conversions
CNVF2M = 2.831685E-2  # Convert CUFT/HR to M3/HR
CNVBMT = 0.1589873  # Convert BBL to M3
CNVBUT = 0.158730158  # Convert MMBTU to LFEBBL (= 1/6.3)
CNVP2K = 6.8948  # Convert PSI to KPA
CNVF2B = 4.274857143  # Convert CUFT/HR to BBL/DAY

# Set Objective Function Weight
WBJ = 2.0

# Set Constraint Values
A11U = 0.150
A11L = 0.005
A31UR = 14.0
A31LT = 110.0
A41U1 = 266.0
A41L1 = 176.0
A41U9 = 464.0
A41L9 = 284.0
A51U1 = 554.0
A51L1 = 302.0
A51U9 = 554.0
A51L9 = 302.0
F12U = 9000.0
F12L = 1000.0
F32U = 25000.0
F41U = 10604.0
F51U = 6000.0
T11U = 220.0
T11L = 125.0
T22U = 675.0
T22L = 530.0
T31U = 250.0
T31L = 120.0
T62U = 700.0
T62L = 550.0

# Set Indirect Free Variable Constraint Values
XF13L = 112.0199
XF13U = 124.0199
XF21L = 1904.8814
XF21U = 2104.8814
XF22L = 1115.6446
XF22U = 1235.6446
XT23L = 444.6569
XT23U = 454.6569
XF61L = 1263.1557
XF61U = 1393.1557
XF62L = 489.2549
XF62U = 539.2549
XT32L = 77.65493
XT32U = 87.65493
XF42L = 333.7547
XF42U = 373.7547
XF52L = 124.1071
XF52U = 138.1071
XF41L = 452.2064
XF41U = 502.2064
XF51L = 229.6230
XF51U = 253.6230

FREE
C1SPL1.L.OUT1 : 200
C1BT29.L.OUT1 : 1300
C1BT29.L.OUT2 : 2000
C2FT21.T_IN : 480
C2COND.T.DROP : 40
C2BT24.L.OUT1 : 600
C2BT24.L.OUT2 : 1500
C2SPL1.L.OUT1 : 600
C4REBL.L_OUT : 450
C2SPL2.L_OUT1 : 350
C5REBL.L_OUT : 230

# Initial Guesses for Some Variables

# The preset subsection has been omitted from this printout as it is
# preset automatically during the real time optimization

EXTERNAL

RECEIVE

# Read in Optimization Parameters (37 variables)
GLOBAL.PRMVNP, GLOBAL.SPCRVP, GLOBAL.DVAP, GLOBAL.DDIST,
GLOBAL.DTISQ, GLOBAL.DHVISQ, GLOBAL.DTDSQ, GLOBAL.DSSFED,
GLOBAL.DSTAB, GLOBAL.DFO, GLOBAL.FIEFF, GLOBAL.F2EFF,
GLOBAL.A11U, GLOBAL.A11L, GLOBAL.A31UR, GLOBAL.A31LT,
GLOBAL.A41U1, GLOBAL.A41L1, GLOBAL.A41U9, GLOBAL.A41L9,
GLOBAL.A51U1, GLOBAL.A51L1, GLOBAL.A51U9, GLOBAL.A51L9,
GLOBAL.F12U, GLOBAL.F12L, GLOBAL.F32U, GLOBAL.F41U,
GLOBAL.F51U, GLOBAL.T11U, GLOBAL.T11L, GLOBAL.T22U,
GLOBAL.T22L, GLOBAL.T31U, GLOBAL.T31L, GLOBAL.T62U,
GLOBAL.T62L,

# Read in Simulation Set Points (43 variables)
MFEED.Z_OUT(1), MFEED.Z_OUT(2), MFEED.Z_OUT(3), MFEED.Z_OUT(4),
MFEED.Z_OUT(5), MFEED.Z_OUT(6), MFEED.Z_OUT(7), MFEED.Z_OUT(8),
MFEED.Z_OUT(9), MFEED.Z_OUT(10), MFEED.Z_OUT(11), MFEED.Z_OUT(12),
MFEED.Z_OUT(13), MFEED.Z_OUT(14), MFEED.Z_OUT(15), MFEED.Z_OUT(16),
MFEED.Z_OUT(17), MFEED.Z_OUT(18), MFEED.Z_OUT(19), MFEED.Z_OUT(20),
MFEED.Z_OUT(21), MFEED.Z_OUT(22), MFEED.P_OUT, C1COND.P, C1COND.Q,
C1SPL1.L_OUT1, "C1S.TRAY_SS(2)".P, C1FT14.F_IN, C1FT14.T_IN,
C1BT29.L_OUT1, C1BT29.L_OUT2, E1.P_OUT, C2COND.P, C2COND.Q,
C2COND.T_DROP, "C2S1.TRAY_SS(2)".P, C2FT21.T_IN, C2BT24.L_OUT1,
C2BT24.L_OUT2, C2SPL1.L_OUT1, C2SPL2.L_OUT1, C4REBL.L_OUT,
C5REBL.L_OUT,

# Read in Indirect Free variable constraint values (22 variables)
GLOBAL.XF13U, GLOBAL.XF13L, GLOBAL.XF22U, GLOBAL.XF22L, GLOBAL.XF21U,
GLOBAL.XF21L, GLOBAL.XT32U, GLOBAL.XT32L, GLOBAL.XT23U, GLOBAL.XT23L,
GLOBAL.XF62U, GLOBAL.XF62L, GLOBAL.XF61U, GLOBAL.XF61L, GLOBAL.XF41U,
GLOBAL.XF41L, GLOBAL.XF51U, GLOBAL.XF51L, GLOBAL.XF42U, GLOBAL.XF42L,
GLOBAL.XF52U, GLOBAL.XF52L,

# Read in Free variables Bounds (22 variables)
UBOUND (C1SPL1.L_OUT1), LBOUND (C1SPL1.L_OUT1),
UBOUND (C1BT29.L_OUT1), LBOUND (C1BT29.L_OUT1),
UBOUND (C1BT29.L_OUT2), LBOUND (C1BT29.L_OUT2),
UBOUND (C2COND.T_DROP), LBOUND (C2COND.T_DROP),
UBOUND (C2FT21.T_IN), LBOUND (C2FT21.T_IN),
UBOUND (C2BT24.L_OUT1), LBOUND (C2BT24.L_OUT1),
UBOUND (C2BT24.L_OUT2), LBOUND (C2BT24.L_OUT2),
UBOUND (C2SPL1.L_OUT1), LBOUND (C2SPL1.L_OUT1),
UBOUND (C2SPL2.L_OUT1), LBOUND (C2SPL2.L_OUT1),
UBOUND (C4REBL.L_OUT), LBOUND (C4REBL.L_OUT),
UBOUND (C5REBL.L_OUT), LBOUND (C5REBL.L_OUT),
# Read in Indirect Free variable bounds (22 variables)
UBOUND (F13.L_OUT), LBOUND (F13.L_OUT),
UBOUND (E1.F_IN), LBOUND (E1.F_IN),
UBOUND (C1TR1.F_IN), LBOUND (C1TR1.F_IN),
UBOUND (C2COND.T), LBOUND (C2COND.T),
UBOUND (E1.T_OUT), LBOUND (E1.T_OUT),
UBOUND (F62.L_OUT), LBOUND (F62.L_OUT),
UBOUND (C2TR3.F_IN), LBOUND (C2TR3.F_IN),
UBOUND ("C4.TRAY_SS(1)".L_IN), LBOUND ("C4.TRAY_SS(1)".L_IN),
UBOUND ("C5.TRAY_SS(1)".L_IN), LBOUND ("C5.TRAY_SS(1)".L_IN),
UBOUND (F42.L_OUT), LBOUND (F42.L_OUT),
UBOUND (F52.L_OUT), LBOUND (F52.L_OUT),
# Read in Objective Function Weight (1 variable)
GLOBAL.WOBJ
TRANSMIT
# Write out Simulations Set Points after Data Rec (44 variables)
MFEED.Z_OUT(1), MFEED.Z_OUT(2), MFEED.Z_OUT(3), MFEED.Z_OUT(4),
MFEED.Z_OUT(5), MFEED.Z_OUT(6), MFEED.Z_OUT(7), MFEED.Z_OUT(8),
MFEED.Z_OUT(9), MFEED.Z_OUT(10), MFEED.Z_OUT(11), MFEED.Z_OUT(12),
MFEED.Z_OUT(13), MFEED.Z_OUT(14), MFEED.Z_OUT(15), MFEED.Z_OUT(16),
MFEED.Z_OUT(17), MFEED.Z_OUT(18), MFEED.Z_OUT(19), MFEED.Z_OUT(20),
MFEED.Z_OUT(21), MFEED.Z_OUT(22), MFEED.P_OUT, C1COND.P, C1COND.Q,
C1SPL1.L_OUT1, "C1S.TRAY_SS(2)".P, C1FT14.F_IN, C1FT14.T_IN,
C1BT29.L_OUT1, C1BT29.L_OUT2, E1.P_OUT, C2COND.P, C2COND.Q,
C2COND.T_DROP, "C2S1.TRAY_SS(2)".P, C2FT21.T_IN, C2BT24.L_OUT1,
C2BT24.L_OUT2, C2SPL1.L_OUT1, C2SPL2.L_OUT1, C4REBL.L_OUT,
C5REBL.L_OUT, F31.TL_OUT,
# Write out Aspen Simulation Setting after Optimization (208 variables)
MFEED.Z_OUT(23), C2REBL.T_OUT, C2REBL.P_OUT, C2REBL.Z_OUT(1),
C2REBL.Z_OUT(2), C2REBL.Z_OUT(3), C2REBL.Z_OUT(4), C2REBL.Z_OUT(5),
C2REBL.Z_OUT(6), C2REBL.Z_OUT(7), C2REBL.Z_OUT(8), C2REBL.Z_OUT(9),
C2REBL.Z_OUT(10), C2REBL.Z_OUT(11), C2REBL.Z_OUT(12), C2REBL.Z_OUT(13),
C2REBL.Z_OUT(14), C2REBL.Z_OUT(15), C2REBL.Z_OUT(16), C2REBL.Z_OUT(17),
C2REBL.Z_OUT(18), C2REBL.Z_OUT(19), C2REBL.Z_OUT(20), C2REBL.Z_OUT(21),
C2REBL.Z_OUT(22), C2REBL.Z_OUT(23), F11.V_OUT, F12.L_OUT,
C1REBL.T_OUT, C1BT29.P, C2COND.L_OUT2, C2BT24.P,
C4REBL.Q, C5REBL.Q, C1COND.T, "C1S.TRAY_SS(2)".T,
E.7 rtopt6.f

The following FORTRAN input code, rtopt6.f, contains SPEEDUP EDI (External Data Interface) subroutines used by rtopt6.speedup.

C RTOPT6.SPEEDUP Routines FOR EDI
C
C ***** EXTIINIT ****
C
C THIS ROUTINE IS USED TO ALERT THE EXTERNAL SYSTEM
C IFLAG=0 FOR SUCCESSFUL RUN
C
SUBROUTINE EXTIINIT(MODE,IFLAG)
INTEGER MODE, IFLAG

WRITE (*,*) '>>>RTOPT6: EXTIINIT CALLED - NOTHING DONE'
IFLAG=0
RETURN
END

C ***** EXTIGET ****
C
C THIS ROUTINE GETS THE DATA
C IFLAG=0 FOR SUCCESSFUL RUN
C
SUBROUTINE EXTIGET(N,TAGNAM,X,T,TNEXT,IFLAG)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
DIMENSION X(N)
CHARACTER = 40 TGNAM(N)
LOGICAL THERE
INTEGER FNFREE

C GET A FREE CHANNEL FOR THE FILE
ICHAN=FNFREE()

C
WRITE (*,*) '>>RTOPT6: EXTGET CALLED - READING IN DATA'

C READ IN MEASURED VALUES FROM FILE IOBJFN.DAT
   INQUIRE (FILE='IOBJFN.DAT', EXIST=THERE)
   IF (.NOT.THERE) THEN
       GO TO 915
   ENDIF
   OPEN (UNIT=ICHAN, STATUS='OLD', ERR=910, FILE='IOBJFN.DAT')
   REWIND (UNIT=ICHAN)
   DO 20 M=1,12
       READ (ICHAN,100,ERR=900,END=905) X(M)
   20 CONTINUE

C READ IN OBJECTIVE FUNCTION WEIGHT
   READ (ICHAN,100,ERR=900,END=905) X(147)
   CLOSE (UNIT=ICHAN)

C READ IN VARIANCES FROM FILE ICNSTR.DAT
   INQUIRE (FILE='ICNSTR.DAT', EXIST=THERE)
   IF (.NOT.THERE) THEN
       GO TO 920
   ENDIF
   OPEN (UNIT=ICHAN, STATUS='OLD', ERR=910, FILE='ICNSTR.DAT')
   REWIND (UNIT=ICHAN)
   DO 25 M=13,37
       READ (ICHAN,100,ERR=900,END=905) X(M)
   25 CONTINUE
   CLOSE (UNIT=ICHAN)

C READ IN SET VARAIBLES FROM FILE ISET.DAT
   INQUIRE (FILE='ISET.DAT', EXIST=THERE)
   IF (.NOT.THERE) THEN
       GO TO 930
   ENDIF
   OPEN (UNIT=ICHAN, STATUS='OLD', ERR=910, FILE='ISET.DAT')
   REWIND (UNIT=ICHAN)
   DO 35 M=38,80
       READ(ICHAN,105,ERR=900,END=905) YF31T
   35 CONTINUE
   READ(ICHAN,105,ERR=900,END=905) YF31T
   CLOSE (UNIT=ICHAN)

C READ IN FREE VARAIBLE BOUNDS FROM FILE IOFREE.DAT
INQUIRE (FILE='IOFREE.DAT', EXIST= THERE)
IF (.NOT. THERE) THEN
    GO TO 935
ENDIF
OPEN (UNIT=ICHAN, STATUS='OLD', ERR=910, FILE='IOFREE.DAT')
REWIND (UNIT=ICHAN)
READ (ICHAN, 100, ERR=900, END=905) TEMP
X(81) = X(63) + (X(63) * TEMP)
X(82) = X(63) - (X(63) * TEMP)
X(103) = X(63) + (X(63) * TEMP * 1.5)
X(104) = X(63) - (X(63) * TEMP * 1.5)
X(125) = X(63) + (X(63) * TEMP)
X(126) = X(63) - (X(63) * TEMP)
READ (ICHAN, 100, ERR=900, END=905) TEMP
X(83) = X(67) + (X(67) * TEMP)
X(84) = X(67) - (X(67) * TEMP)
X(105) = X(67) + (X(67) * TEMP * 1.5)
X(106) = X(67) - (X(67) * TEMP * 1.5)
X(127) = X(67) + (X(67) * TEMP)
X(128) = X(67) - (X(67) * TEMP)
READ (ICHAN, 100, ERR=900, END=905) TEMP
X(85) = X(68) + (X(68) * TEMP)
X(86) = X(68) - (X(68) * TEMP)
X(107) = X(68) + (X(68) * TEMP * 1.5)
X(108) = X(68) - (X(68) * TEMP * 1.5)
X(129) = X(68) + (X(68) * TEMP)
X(130) = X(68) - (X(68) * TEMP)
READ (ICHAN, 100, ERR=900, END=905) TEMP
X(87) = YF31T + TEMP
X(88) = YF31T - TEMP
X(109) = X(72) + (TEMP * 1.5)
X(110) = X(72) - (TEMP * 1.5)
X(131) = YF31T + TEMP
X(132) = YF31T - TEMP
READ (ICHAN, 100, ERR=900, END=905) TEMP
X(89) = X(74) + TEMP
X(90) = X(74) - TEMP
X(111) = X(74) + (TEMP * 1.5)
X(112) = X(74) - (TEMP * 1.5)
X(133) = X(74) + TEMP
X(134) = X(74) - TEMP
READ (ICHAN, 100, ERR=900, END=905) TEMP
X(91) = X(75) + (X(75) * TEMP)
X(92) = X(75) - (X(75) * TEMP)
X(113) = X(75) + (X(75) * TEMP * 1.5)
X(114) = X(75) - (X(75) * TEMP = 1.5)
X(135) = X(75) + (X(75) * TEMP)
X(136) = X(75) - (X(75) * TEMP)
READ(ICHAN,100,ERR=900,END=905) TEMP
X(93) = X(76) + (X(76) * TEMP)
X(94) = X(76) - (X(76) * TEMP)
X(115) = X(76) + (X(76) * TEMP = 1.5)
X(116) = X(76) - (X(76) * TEMP = 1.5)
X(137) = X(76) + (X(76) * TEMP)
X(138) = X(76) - (X(76) * TEMP)
READ(ICHAN,100,ERR=900,END=905) TEMP
X(95) = X(77) + (X(77) * TEMP)
X(96) = X(77) - (X(77) * TEMP)
X(117) = X(77) + (X(77) * TEMP = 1.5)
X(118) = X(77) - (X(77) * TEMP = 1.5)
X(139) = X(77) + (X(77) * TEMP)
X(140) = X(77) - (X(77) * TEMP)
READ(ICHAN,100,ERR=900,END=905) TEMP
X(97) = X(78) + (X(78) * TEMP)
X(98) = X(78) - (X(78) * TEMP)
X(119) = X(78) + (X(78) * TEMP = 1.5)
X(120) = X(78) - (X(78) * TEMP = 1.5)
X(141) = X(78) + (X(78) * TEMP)
X(142) = X(78) - (X(78) * TEMP)
READ(ICHAN,100,ERR=900,END=905) TEMP
X(99) = X(79) + (X(79) * TEMP)
X(100) = X(79) - (X(79) * TEMP)
X(121) = X(79) + (X(79) * TEMP = 1.5)
X(122) = X(79) - (X(79) * TEMP = 1.5)
X(143) = X(79) + (X(79) * TEMP)
X(144) = X(79) - (X(79) * TEMP)
READ(ICHAN,100,ERR=900,END=905) TEMP
X(101) = X(80) + (X(80) * TEMP)
X(102) = X(80) - (X(80) * TEMP)
X(123) = X(80) + (X(80) * TEMP = 1.5)
X(124) = X(80) - (X(80) * TEMP = 1.5)
X(145) = X(80) + (X(80) * TEMP)
X(146) = X(80) - (X(80) * TEMP)
CLOSE (UNIT=ICHAN)
WRITE (*,*) '>>>RIOPT6: EXTGET - DATA READ SUCCESSFULLY'
IFLAG=0
100 FORMAT(15X, E15.8)
105 FORMAT(42X, E15.8)
RETURN
C ERROR STATEMENTS
900 WRITE(*,*) 'RTOPT6: EXTGET: Error reading ', TTAGNAM(M)
     IFLAG = -1
     RETURN
905 WRITE(*,*) 'RTOPT6: EXTGET: EOF reached reading ', TTAGNAM(M)
     IFLAG = -1
     RETURN
910 WRITE(*,*) 'RTOPT6: EXTGET: Error opening file'
     IFLAG = -1
     RETURN
915 WRITE(*,*) 'RTOPT6: EXTGET: IOBJFN.DAT does not exist'
     IFLAG = -1
     RETURN
920 WRITE(*,*) 'RTOPT6: EXTGET: ICNSTR.DAT does not exist'
     IFLAG = -1
     RETURN
930 WRITE(*,*) 'RTOPT6: EXTGET: ISET.DAT does not exist'
     IFLAG = -1
     RETURN
935 WRITE(*,*) 'RTOPT6: EXTGET: IOFREE.DAT does not exist'
     IFLAG = -1
     RETURN
END

C **** EXTPUT ****
C
C THIS ROUTINE WRITES OUT THE CALCULATED VARIABLES
C IFLAG=0 FOR SUCCESSFUL RUN
C
SUBROUTINE EXTPUT(N,TTAGNAM,X,T,IFLAG)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
DIMENSION X(N)
CHARACTER * 40 TTAGNAM(N)
INTEGER FNFREE
LOGICAL THERE
C GET A FREE CHANNEL FOR THE FILE
ICHAN=FNFREE()
C
WRITE (*,*) '>>>>RTOPT6: EXTPUT CALLED - WRITING OUT RESULTS'
C
WRITE OUT SET VARIABLES TO FILE ROSET.DAT
INQUIRE (FILE='ROSET.DAT', EXIST=THEAR)
IF (THEAR) THEN
   GO TO 915
ENDIF
OPEN (UNIT=ICHAN, STATUS='NEW', ERR=910, FILE='ROSET.DAT')
DO 10 M=1,44
WRITE(ICHAN,100,ERR=900) TAGAIN(M), X(M)
10 CONTINUE
CLOSE (UNIT=ICHAN)
C WRITE TO FILE THE VARIABLES FOR ASPEN SIMULATION
INQUIRE (FILE='ROSMST.DAT', EXIST=THEIR)
IF (THEIR) THEN
GO TO 920
ENDIF
OPEN (UNIT=ICHAN, STATUS='NEW', ERR=910, FILE='ROSMST.DAT')
C STAB STREAM SPECIFICATIONS
WRITE(ICHAN,105,ERR=900) 'STAB MOLEFLOW', X(28)
WRITE(ICHAN,105,ERR=900) 'STAB TEMP ', X(29)
WRITE(ICHAN,105,ERR=900) 'STAB PRESS ', X(23)
DO 12 I=1,22
  WRITE(ICHAN,110,ERR=900) 'STAB Z', I, X(I)
12 CONTINUE
I = 23
WRITE(ICHAN,110,ERR=900) 'STAB Z', I, X(45)
C C2REBL STREAM ESTIMATIONS
WRITE(ICHAN,105,ERR=900) 'C2REBL FLOW ', X(39)
WRITE(ICHAN,105,ERR=900) 'C2REBL TEMP ', X(46)
WRITE(ICHAN,105,ERR=900) 'C2REBL PRESS ', X(47)
DO 14 I=48,70
  J = I - 47
  WRITE(ICHAN,110,ERR=900) 'C2REBL Z', J, X(I)
14 CONTINUE
C E1 HEATER SPECIFICATIONS
WRITE(ICHAN,105,ERR=900) 'E1 TEMP ', X(37)
WRITE(ICHAN,105,ERR=900) 'E1 PRESS ', X(32)
C C1 COLUMN SPECIFICATIONS
C1RR = X(72) / (X(26) + X(71))
C1RDV = X(71) / (X(26) + X(71))
C1CDP = X(74) - X(27)
WRITE(ICHAN,105,ERR=900) 'C1 RFLX RATIO', C1RR
WRITE(ICHAN,105,ERR=900) 'C1 VAP/DIST', C1RDV
WRITE(ICHAN,105,ERR=900) 'C1 REBL FLOW ', X(31)
WRITE(ICHAN,105,ERR=900) 'C1 REBL TEMP ', X(73)
WRITE(ICHAN,105,ERR=900) 'C1 COL P DROP', C1CDP
WRITE(ICHAN,105,ERR=900) 'C1 TOP TRAY P', X(24)
WRITE(ICHAN,105,ERR=900) 'C1 2ND TRAY P', X(27)
C C2 COLUMN SPECIFICATIONS
C2CDP = X(76) - X(36)
WRITE(ICHAN,105,ERR=900) 'C2 DIST FLOW ', X(75)
WRITE(ICHAN,105,ERR=900) 'C2 COND SC T', X(44)
WRITE(ICHAN,105,ERR=900) 'C2 COL P DROP', C2CDP
WRITE(ICHAN,105,ERR=900) 'C2 TOP TRAY P', X(33)
WRITE(ICHAN,105,ERR=900) 'C2 2ND TRAY P', X(36)
WRITE(ICHAN,105,ERR=900) 'C2-C4 IC FLOW', X(40)
WRITE(ICHAN,105,ERR=900) 'C2-C5 IC FLOW', X(41)

C C4 COLUMN SPECIFICATIONS
WRITE(ICHAN,105,ERR=900) 'C4 REBL DUTY', X(77)

C C5 COLUMN SPECIFICATIONS
WRITE(ICHAN,105,ERR=900) 'C5 REBL DUTY', X(78)

C C1 TEMPERATURE PROFILE
DO 16 I=79,107
   J = I - 78
   WRITE(ICHAN,110,ERR=900) 'C1 T, TRAY', J, X(I)
16 CONTINUE

C C2 TEMPERATURE PROFILE
DO 18 I=108,131
   J = I - 107
   WRITE(ICHAN,110,ERR=900) 'C2 T, TRAY', J, X(I)
18 CONTINUE

C C4 TEMPERATURE PROFILE
DO 20 I=132,134
   J = I - 131
   WRITE(ICHAN,110,ERR=900) 'C4 T, TRAY', J, X(I)
20 CONTINUE

C C5 TEMPERATURE PROFILE
DO 27 I=135,137
   J = I - 134
   WRITE(ICHAN,110,ERR=900) 'C5 T, TRAY', J, X(I)
27 CONTINUE

C C1 LIQUID AND VAPOUR FLOW PROFILES
C1L29 = X(30) + X(31)
DO 30 I=138,165
   J = I - 137
   WRITE(ICHAN,110,ERR=900) 'C1 L, TRAY', J, X(I)
30 CONTINUE

   J = 29
   WRITE(ICHAN,110,ERR=900) 'C1 L, TRAY', J, C1L29
DO 32 I=166,194
   J = I - 165
   WRITE(ICHAN,110,ERR=900) 'C1 V, TRAY', J, X(I)
32 CONTINUE

C C2 LIQUID AND VAPOUR FLOW PROFILES
C2L24 = X(38) + X(39)
C2V1 = 0.0
DO 34 I=195,217
   J = I - 194
WRITE(ICHAN,110,ERR=900) 'C2 L, TRAY', J, X(I)
34 CONTINUE
   J = 29
   WRITE(ICHAN,110,ERR=900) 'C2 L, TRAY', J, C2L24
   J = 1
   WRITE(ICHAN,110,ERR=900) 'C2 V, TRAY', J, C2V1
   DO 36 I=218,240
       J = I - 216
       WRITE(ICHAN,110,ERR=900) 'C2 V, TRAY', J, X(I)
   CONTINUE
36 CONTINUE
C   C4 LIQUID AND VAPOUR FLOW PROFILES
   DO 38 I=241,243
       J = I - 240
       WRITE(ICHAN,110,ERR=900) 'C4 L, TRAY', J, X(I)
   CONTINUE
38 CONTINUE
C   C4 LIQUID AND VAPOUR FLOW PROFILES
   DO 40 I=244,246
       J = I - 243
       WRITE(ICHAN,110,ERR=900) 'C4 V, TRAY', J, X(I)
   CONTINUE
40 CONTINUE
C   C5 LIQUID AND VAPOUR FLOW PROFILES
   DO 42 I=247,249
       J = I - 246
       WRITE(ICHAN,110,ERR=900) 'C5 L, TRAY', J, X(I)
   CONTINUE
42 CONTINUE
C   C5 LIQUID AND VAPOUR FLOW PROFILES
   DO 44 I=250,252
       J = I - 249
       WRITE(ICHAN,110,ERR=900) 'C5 V, TRAY', J, X(I)
   CONTINUE
44 CONTINUE
   CLOSE (UNIT=ICHAN)
   WRITE (*,*) '>>RTOPT6: EXTPUT - DATA WRITTEN SUCCESSFULLY'
   IFLAG=0
100 FORMAT(A40, 2X, E15.8)
105 FORMAT(A13, 2X, E15.8)
110 FORMAT(A10, X, I2, 2X, E15.8)
   RETURN
900 WRITE(*,*) 'RTOPT6: EXTPUT: Error writing ', TAGNAM(M)
   IFLAG = -1
   RETURN
910 WRITE(*,*) 'RTOPT6: EXTPUT: Error opening file'
   IFLAG = -1
   RETURN
915 WRITE(*,*) 'RTOPT6: EXTPUT: ROSET.DAT already exists'
   IFLAG = -1
   RETURN
920 WRITE(*,*) 'RTOPT6: EXTPUT: ROSMST.DAT already exists'
IFLAG = -1
RETURN
END

C
C ***** EXTRM *****
C
C TERMINATION PROGRAMME
C IFLAG=0 FOR SUCCESSFUL RUN
C
SUBROUTINE EXTRM(IFLAG)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
WRITE (*,*)'>>>RTOPT6: EXTRM CALLED - EDI FINISHED'
IFLAG=0
RETURN
END

C
C ***** EXTWAI *****
C
C WAIT PROGRAMME
C IFLAG=0 CONTINUE RUNNING
C IFLAG=-1 REQUEST TO TERMINATE
C
SUBROUTINE EXTWAI(T,IFLAG)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
WRITE (*,*)'>>>RTOPT6: EXTWAI CALLED - TERMINATING RUN'
IFLAG =-1
RETURN
END

C
C ***** EXTMSG *****
C
C MESSAGE PROGRAMME
C IFLAG=0 FOR SUCCESSFUL RUN
C
SUBROUTINE EXTMSG(MESSGE, MESTYP, IFLAG)
CHARACTER *= (*) MESSGE
INTEGER MESSYP, IFLAG
IFLAG=0
WRITE (*,*)'>>>RTOPT6: EXTMSG CALLED - WRITING MESSAGE'
WRITE (*,*)'MESSAGE OF TYPE', MESTYP
WRITE (*,*) 'RTOPT6: EXTMSG - MESSAGE HAS BEEN WRITTEN'
RETURN
END

C
FUNCTION TO FIND A FREE TERMINAL
C
INTEGER FUNCTION FNFREE()
COPYRIGHT (C) ASPIRE UK LTD, 1991
C
FNFREE FINDS THE FIRST FREE LOGICAL UNIT FOR ASSIGNING TO A FILE.
C
IT DOES THIS BY TRYING THEM ALL IN ASCENDING ORDER UNTIL ONE IS FREE.
C
RETURNS -1 IF NONE FREE.

IMPLICIT NONE
LOGICAL OPEND
INTEGER I
DO 100 I=1,119
   INQUIRE(UNIT=I,OPEND=OPEND)
   IF (.NOT.OPEND) THEN
      FNFREE=I
      RETURN
   ENDIF
100 CONTINUE
   FNFREE=-1
RETURN
END

E.8  model6x.speedup

The following SPEEDUP input code, model6x.speedup, contains the user
defined models used in both rtodr6.speedup and rtopt6.speedup.

MODEL btray_ss
{
   Model Version 1.0A
   SPEEDUP Model Library
   Copyright, 1982-1995 Aspen Technology, Inc. All rights reserved.
   This copyright statement must not be deleted and must be
   included in any modification or adaptation of this Model.
}
CATEGORY Distillation

HELP
   Bottom tray model for steady state distillation modelling
   using a pumparound reboiler (same as FTRAY_SS without
a V_IN stream)

INPUT 1 : flow from tray above type LIQUID
INPUT 2 : feed to tray type MAINSTREAM
OUTPUT 1 : output from tray type VAPOUR
OUTPUT 2 : overflow from tray type LIQUID
OUTPUT 3 : Reboiler pumparound draw type LIQUID

Preferred Sets : P, Q

Parameters : nocomp

$ENDHELP

SET
nocomp # number of components

TYPE
# Input 1:
  L_in  AS  flow_mol_liq
  x_in  AS  ARRAY(nocomp) OF molefraction
  T1_in AS  temperature
  P1_in AS  pressure
  hl_in AS  enth_mol_liq

# Input 2:
  F_in  AS  flow_mol
  z_in  AS  ARRAY(nocomp) OF molefraction
  T_in  AS  temperature
  P_in  AS  pressure
  h_in  AS  enth_mol

# Output 1:
  V_out AS  flow_mol_vap
  y_out AS  ARRAY(nocomp) OF molefraction
  T_v_out AS  temperature
  P_y_out AS  pressure
  h_v_out AS  enth_mol_vap

# Output 2:
  L_out1 AS  flow_mol_liq
  x_out1 AS  ARRAY(nocomp) OF molefraction
  T1_out1 AS  temperature
  P1_out1 AS  pressure
  h1_out1 AS  enth_mol_liq

# Output 3:
  L_out2 AS  flow_mol_liq
  x_out2 AS  ARRAY(nocomp) OF molefraction
  T1_out2 AS  temperature
P1_out2  AS  pressure
hl_out2  AS  enthal_mol_liq

# Internal:
F  AS  flow_mol  # mixture flowrate
H  AS  enthflow  # enthalpy of mixture
P  AS  pressure  # tray pressure
Q  AS  enthflow  # tray heat load
T  AS  temperature  # tray temperature
vf  AS  vapfraction  # vapfraction
z  AS  ARRAY(nocomp) OF molefraction  # mixture composition

STREAM
INPUT 1  L_in, x_in, T1_in, P1_in, hl_in  # liquid from tray above
INPUT 2  F_in, z_in, T_in, P_in, h_in  # mixed phase tray feed
OUTPUT 1  V_out, y_out, TV_out, PV_out, hv_out  # vapour leaving tray
OUTPUT 2  L_out1, x_out1, T1_out1, P1_out1, hl_out1  # liquid overflow
OUTPUT 3  L_out2, x_out2, T1_out2, P1_out2, hl_out2  # pumparound draw

EQUATION

# Material balance
  F  =  F_in  +  L_in  ;
  P*z  =  F_in*z_in  +  L_in*x_in  ;
  F  =  V_out  +  L_out1  +  L_out2  ;
  V_out  =  vf*F  ;
  x_out2  =  x_out1  ;

# Energy balance
  H  =  F_in*h_in  +  L_in*hl_in  +  Q  ;
  H  =  V_out*hv_out  +  L_out1*hl_out1  +  L_out2*hl_out1  ;
  hl_out2  =  hl_out1  ;

# Temperature and Pressure Equations
  T  =  TV_out  =  T1_out1  =  T1_out2  ;
P  =  PV_out  =  P1_out1  =  P1_out2  ;

PROCEDURE
  ( y_out, x_out1, vf, hv_out, hl_out1 ) flash ( T, P, z ) INPUT 1
****
MODEL liq_vflow
HELP
INPUT 1 : Stream type LIQUID
OUTPUT 1 : Same Stream type LIQUID

Preferred Sets : STDTEMP (Standard Temperature, usually 60F)
STDTEMP (Standard Pressure, usually 14.696psia)

Result Variables : RHOL = Liquid Density at Stream Conditions
VOLFL = Liquid Volume Flow
STDRHOL = Liquid Density at Std Conditions
STDVOLFL = Standard Liquid Volume Flow

Parameters : nocomp

SET

nocomp # number of components

TYPE

# Input:
L_in AS flow_mol_liq
x_in AS ARRAY(nocomp) OF molefraction
Tl_in AS temperature
P1_in AS pressure
hl_in AS enth_mol_liq

# Output:
L_out AS flow_mol_liq
x_out AS ARRAY(nocomp) OF molefraction
Tl_out AS temperature
P1_out AS pressure
hl_out AS enth_mol_liq

# Internal:
VOLFL AS flow_vol_liq # vol flowrate liquid
RHOL AS dens_mol_liq # liq molar density
STDVOLFL AS flow_vol_liq # std vol flow liq
STDRHOL AS dens_mol_liq # std liq mol density
*STDTEMP AS temperature # std temperature
*STDTEMP AS pressure # std pressure

STREAM

INPUT 1 L_in, x_in, Tl_in, P1_in, hl_in
OUTPUT 1 L_out, x_out, Tl_out, P1_out, hl_out

EQUATION

# Match Input to Output
L_in = L_out ;
x_in = x_out ;
Tl_in = Tl_out ;
P1_in = P1_out ;
hl_in = hl_out ;
# Calculate the Volume Flow of the Stream
L_in = VOLFL * RH01;

# Calculate the Standard Volume Flow of the Stream
L_in = STDVOLFL * STDRH01;

PROCEDURE
( RH01 ) dens_mol_liq ( T1_in, P1_in, x_in ) INPUT 1
( STDRH01 ) dens_mol_liq ( STDTEMP, STDPRESS, x_in ) INPUT 1

****
MODEL vap_vflow
HELP
Calculation of the Volume Flow, Standard Liquid Volume Flow
and Standard Vapour Flow of a Vapour Stream.

INPUT 1 : Stream type VAPOUR
OUTPUT 1 : Same Stream type VAPOUR

Preferred Sets : STDTEMP (Standard Temperature, usually 60F)
STDPRESS (Standard Pressure, usually 14.696psia)

Result Variables : RH0V = Vapour Density at Stream Conditions
VOLPV = Vapour Volume Flow
STDRH0L = Liquid Density at Std Conditions
STDVOLFL = Standard Liquid Volume Flow
STDVOLFV = Standard Vapour Volume Flow

Parameters : nocomp

$ENDHELP
SET
nocomp # number of components

TYPE

# Input:
V_in AS flow_mol_vap
y_in AS ARRAY(nocomp) OF molefraction
Tv_in AS temperature
Pv_in AS pressure
hv_in AS enth_mol_vap

# Output:
V_out AS flow_mol_vap
y_out AS ARRAY(nocomp) OF molefraction
Tv_out AS temperature
Pv_out AS pressure
hv_out AS enth_mol_vap

# Internal:
VOLPV AS flow_vol_vap # vol flowrate vapour
RHOV AS dens_mol_vap # vapour molar density
STDVOLFL AS flow_vol_liq  # std vol flow liq
STDROHL AS dens_mol_liq  # std liq mol density
STDVOLFv AS flow_vol_vap  # std vol flow vap
STDROHv AS dens_mol_vap  # std vap mol density
*STDTMP AS temperature  # std temperature
*STDPRES AS pressure  # std pressure

STREAM
INPUT 1  V_in,  y_in,  Tv_in,  Pv_in,  hv_in
OUTPUT 1  V_out,  y_out,  T_out,  P_out,  hv_out

EQUATION
# Match Input to Output
V_in = V_out ;
y_in = y_out ;
Tv_in = T_out ;
Pv_in = P_out ;
hv_in = hv_out ;

# Calculate the Volume Flow of the Stream
V_in = VOLFv * RH0v ;

# Calculate the Standard Liquid Volume Flow of the Stream
V_in = STDVOLFL * STDROHL ;

# Calculate the Standard Vapour Volume Flow of the Stream
V_in = STDVOLFv * STDROHv ;

PROCEDURE
( RH0v )  dens_mol_vap ( Tv_in,  Pv_in,  y_in )  INPUT 1
( STDROHL )  dens_mol_liq ( STDTMP,  STDPRES,  y_in )  INPUT 1
( STDROHv )  dens_mol_vap ( STDTMP,  STDPRES,  y_in )  INPUT 1

****
MODEL vflow
HELP

INPUT 1  :  Stream  type MAINSTREAM
OUTPUT 1  :  Same Stream  type MAINSTREAM

Preferred Sets  :  STDTMP (Standard Temperature, usually 60F)
STDROHL (Standard Pressure, usually 1.4696psia)

Result Variables  :  RH0V  =  Vapour Phase Density at Stream Conditions
VOLFV  =  Vapour Phase Volume Flow
RH0L  =  Liquid Phase Density at Stream Conditions
VOLFL  =  Liquid Phase Volume Flow
VOLF  =  Total Stream Volume Flow
STDROHL  =  Liquid Density at Std Conditions
STDVOLFL = Standard Liquid Volume Flow
Parameters : nocomp

SENDHELP

SET

nocomp

# number of components

TYPE

# Input:

F_in AS flow_mol
z_in AS ARRAY(nocomp) OF molefraction
T_in AS temperature
P_in AS pressure
h_in AS enth_mol

# Output:

F_out AS flow_mol
z_out AS ARRAY(nocomp) OF molefraction
T_out AS temperature
P_out AS pressure
h_out AS enth_mol

# Internal:

VOLFv AS flow_vol_vap # vol flowrate vapour
RHOv AS dens_mol_vap # vapour molar density
VOLF1 AS flow_vol_liq # vol flowrate liquid
RH01 AS dens_mol_liq # liquid molar density
VOLF AS flow_vol # vol flowrate total
STDVOLF1 AS flow_vol_liq # std vol flow liq
STDH01 AS dens_mol_liq # std liq mol density
*STDTEMP AS temperature # std temperature
*STDRES AS pressure # std pressure
x AS ARRAY(nocomp) OF molefraction # liquid composition
y AS ARRAY(nocomp) OF molefraction # vapour composition
vf AS vapfraction # vapour fraction
hl AS enth_mol_liq # liq spec. enthalpy
hv AS enth_mol_vap # vap spec. enthalpy
V AS flow_mol_vap # vap mole flow
L AS flow_mol_liq # liq mole flow

STREAM

INPUT 1 F_in, z_in, T_in, P_in, h_in
OUTPUT 1 F_out, z_out, T_out, P_out, h_out

EQUATION

# Match Input to Output

F_in = F_out;
z_in = z_out;
T_in = T_out;
P_in = P_out;
h_in = h_out;
# Calculate the Volume Flow of the Stream
V = F_in * vf;
F_in = L + V;
V = VOLFv * RH0v;
L = VOLF1 * RH01;
VOLF = VOLFv + VOLF1;
# Calculate the Standard Volume Flow of the Stream
F_in = STDVOLF1 * STDRH01;

PROCEDURE
( y, x, vf, hv, hl ) flash ( T_in, P_in, z_in ) INPUT 1
( RH0v ) dens_mol_vap ( T_in, P_in, y ) INPUT 1
( RH01 ) dens_mol_liq ( T_in, P_in, x ) INPUT 1
( STDRH01 ) dens_mol_liq ( STDTEMP, STDPRES, z_in ) INPUT 1

*****
MODEL C5_vflow
HELP
Calculation of the Volume Flow and Standard Liquid Volume Flow
of a Liquid Stream and C5 COMPOSITION.

INPUT 1 : Stream type LIQUID
OUTPUT 1 : Same Stream type LIQUID

Preferred Sets : STDTEMP (Standard Temperature, usually 60F)
                 STDPRES (Standard Pressure, usually 14.696psia)

Result Variables : RHOL     = Liquid Density at Stream Conditions
                   VOLFL    = Liquid Volume Flow
                   STDRHOL   = Liquid Density at Std Conditions
                   STDVOLF1 = Standard Liquid Volume Flow

Parameters       : nocomp

$SENDHELP
SET
    nocomp                        # number of components
    TYPE

# Input:
    L_in  AS        flow_mol_liq
    x_in  AS ARRAY(nocomp) OF molefraction
    T1_in AS        temperature
    P1_in AS        pressure
    hl_in AS        enth_mol_liq

# Output:
    L_out AS        flow_mol_liq
    x_out AS ARRAY(nocomp) OF molefraction
T1_out AS temperature
Pl_out AS pressure
hl_out AS enth_mol_liq

# Internal:
VOLF1 AS flow_vol_liq # vol flowrate liquid
RHO1 AS dens_mol_liq # liq molar density
STDVOLF1 AS flow_vol_liq # std vol flow liq
STDRHO1 AS dens_mol_liq # std liq mol density
*STDTEMP AS temperature # std temperature
*STDPRES AS pressure # std pressure
C55 AS molefraction # C5's in stream

STREAM
INPUT 1 L_in, x_in, T1_in, Pl_in, hl_in
OUTPUT 1 L_out, x_out, T1_out, Pl_out, hl_out

EQUATION
# Match Input to Output
L_in = L_out;
x_in = x_out;
T1_in = T1_out;
Pl_in = Pl_out;
hl_in = hl_out;

# Calculate the Volume Flow of the Stream
L_in = VOLF1 * RHO1;

# Calculate the Standard Volume Flow of the Stream
L_in = STDVOLF1 * STDRHO1;

# Calculate C5's in Stream
C55 = X_IN(7) + X_IN(8);

PROCEDURE
(RHO1) dens_mol_liq (T1_in, Pl_in, x_in) INPUT 1
(STDRHO1) dens_mol_liq (STDTEMP, STDPRES, x_in) INPUT 1

****
MODEL M2R
HELP
Convert stream type from LIQUID to RVPLIQ

INPUT 1 : Stream type LIQUID
OUTPUT 1 : Same Stream type RVPLIQ

$ENDHELP
SET
mainnc = 23 # number of components
rvpnc = 24

TYPE
# Input:
F_in AS flow_mol
STREAM

INPUT 1 F_in, z_in, T_in, P_in, h_in
OUTPUT 1 F_out, z_out, T_out, P_out, h_out

EQUATION

# Match Input to Output
F_in = F_out;
z_in = z_out(1:mainnc);
z_out(rvpnc) = 0;
T_in = T_out;
P_in = P_out;
h_in = h_out;

****

MODEL RVP

Calculation of RVP (Reid Vapour Pressure) of a stream.

HELP

Calculation of RVP (Reid Vapour Pressure) of a stream.

INPUT 1 : Stream type RVPLIQ
OUTPUT 1 : Same Stream type RVPLIQ

Preferred Sets:
COLDTEMP (Cold Temperature, usually 32F)
WARMTEMP ( Warm Temperature, usually 100F)
STDPRS (Standard Pressure, usually 14.696psia)
ZAIR (composition of Air stream)

Result Variables: RVP = Reid Vapour Pressure

$ENDHELP

SET
rvpnc = 24 # number of components

TYPE

# Input:
F_in AS flow_mol_liq
z_in AS ARRAY(rvpnc) OF molefraction
T_in AS temperature
P_in AS pressure
h_in AS enth_mol_liq
# Output:
F_out AS flow_mol_liq
z_out AS ARRAY(rvpcn) OF molefraction
T_out AS temperature
P_out AS pressure
h_out AS enth_mol_liq

# Internal:
RVP AS pressure
*STDPRES AS pressure
*COLDTEMP AS temperature
*WARMTEMP AS temperature
*ZAIR AS ARRAY(rvpcn) OF molefraction
RH032 AS dens_mol_liq
VOL32 AS flow_vol_liq
*RHOA32 AS dens_mol_vap
VOLA32 AS flow_vol_vap
FA32 AS flow_mol_vap
FMIX1 AS flow_mol
ZMIX1 AS ARRAY(rvpcn) OF molefraction
VFMIX1 AS vapfraction
VOLMIX1 AS flow_vol
PMIX1 AS pressure
YW32 AS ARRAY(rvpcn) OF molefraction
XST32 AS ARRAY(rvpcn) OF molefraction
hW32 AS enth_mol_vap
h1ST32 AS enth_mol_liq
RHOST32 AS dens_mol_liq
VOLST32 AS flow_vol_liq
RHOW32 AS dens_mol_vap
VOLW32 AS flow_vol_vap
FSAT32 AS flow_mol_liq
FW32 AS flow_mol_vap
*RHOB AS dens_mol_vap
VOLB AS flow_vol_vap
FB AS flow_mol_vap
FMIX2 AS flow_mol
ZMIX2 AS ARRAY(rvpcn) OF molefraction
VFMIX2 AS vapfraction
VOLMIX2 AS flow_vol
PMIX2 AS pressure
YVP AS ARRAY(rvpcn) OF molefraction
XLQ AS ARRAY(rvpcn) OF molefraction
hvVP AS enth_mol_vap
h1LQ AS enth_mol_liq
RHOLQ AS dens_mol_liq
VOLLQ  AS  flow_vol_liq
RHVLP  AS  dens_mol_vap
VOLVLP AS  flow_vol_vap
FLQ  AS  flow_mol_liq
FVP  AS  flow_mol_vap

STREAM
INPUT 1  F_in,  z_in,  T_in,  P_in,  h_in
OUTPUT 1  F_out,  z_out,  T_out,  P_out,  h_out

EQUATION
# Match Input to Output
F_in  =  F_out ;
z_in  =  z_out ;
T_in  =  T_out ;
P_in  =  P_out ;
h_in  =  h_out ;

# Calculate Air Stream volume at 32F to be 25% of RVP stream volume at 32F
F_in  =  VOL32  *  RH032 ;
VOLA32  =  VOL32  *  0.25 ;
FA32  =  VOLA32  *  RHOA32 ;

# Mix Air and RVP streams at 32F
FMIX1  =  FA32  +  F_in ;
FMIX1*ZMIX1  =  FA32*ZAIR  +  F_in*Z_in ;
VOLMIX1  =  VOLA32  +  VOL32 ;

# Constant Volume Flash of Mixed stream
FMIX1  =  FSAT32  +  FW32 ;
FW32  =  FMIX1  *  VFMI1 ;
FW32  =  VOLW32  *  RHOW32 ;
FSAT32  =  VOLST32  *  RHGST32 ;
VOLMIX1  =  VOLST32  +  VOLW32 ;

# Mix Air and SAT streams at 32F (Air to be 400% of SAT stream)
VOLB  =  VOLST32  *  4.0 ;
FB  =  VOLB  *  RHOB ;
FMIX2  =  FB  +  FSAT32 ;
FMIX2*ZMIX2  =  FB*ZAIR  +  FSAT32*XST32 ;
VOLMIX2  =  VOLB  +  VOLST32 ;

# Constant Volume Flash of Mixed stream
FMIX2  =  FLQ  +  FVP ;
FVP  =  FMIX2  *  VFMI2 ;
FVP  =  VOLVP  *  RHVLP ;
FLQ  =  VOLLQ  *  RholQ ;
VOLMIX2  =  VOLLQ  +  VOLVP ;

# Calculate Reid Vapour Pressure
RVP  =  FMIX2  -  STDPRES ;

PROCEDURE
( RH032 )  dens_mol_liq ( COLDTEMP, STDPRES, z_in ) INPUT 1
MODEL TBP
HELP
Calculation of TBP (True Boiling Point) Temperature for both
10% and 90% standard liquid volume distilled, as well as
liquid stream volume and standard volume flows.

INPUT 1 : Stream type LIQUID
OUTPUT 1 : Same Stream type LIQUID

Preferred Sets : STDTEMP (Standard Temperature, usually 60°F)
STDVPRES (Standard Pressure, usually 14.696 psia)

Result Variables : RHOL = Liquid Phase Density at Stream Conditions
VOLFL = Liquid Phase Volume Flow
STDRHOL = Liquid Density at Std Conditions
STDVOLFL = Standard Liquid Volume Flow
TBP10 = TBP Temperature at 10% Std Vol Distilled
TBP90 = TBP Temperature at 90% Std Vol Distilled

Parameters : nocomp

$ENDHELP
SET
nocomp # number of components
TYPE

# Input:
  L_in AS flow_mol_liq
  x_in AS ARRAY(nocomp) OF molefraction
  Tl_in AS temperature
  Pl_in AS pressure
  hl_in AS enth_mol_liq

# Output:
  L_out AS flow_mol_liq
  x_out AS ARRAY(nocomp) OF molefraction
  Tl_out AS temperature
  Pl_out AS pressure
  hl_out AS enth_mol_liq

# Internal:
  VOLFL AS flow_vol_liq # vol flowrate liquid
# liq molar density
flow_vol_liq # std vol flow liq
dens_mol_liq # std liq mol density
temperature # TBP-10% Temp
temperature # TBP-90% Temp
temperature # std temperature
pressure # std pressure

STREAM
INPUT 1 L_in, x_in, Tl_in, P1_in, hl_in
OUTPUT 1 L_out, x_out, Tl_out, P1_out, hl_out

EQUATION
# Match Input to Output
L_in = L_out ;
x_in = x_out ;
Tl_in = Tl_out ;
P1_in = P1_out ;
hl_in = hl_out ;

# Calculate the Volume Flow of the Stream
L_in = VOLFL * RH01 ;

# Calculate the Standard Volume Flow of the Stream
L_in = STDVOLFL * STDRH01 ;

PROCEDURE
( RH01 ) dens_mol_liq ( Tl_in, P1_in, x_in ) INPUT 1
( STDRH01 ) dens_mol_liq ( STDTTEMP, STDPRES, x_in ) INPUT 1
( TBP10, TBP90 ) TBP ( x_in, L_in )

****
PROCEDURE TBP
HELP
Calculation of TBP (True Boiling Point) Temperature for both
10% and 90% standard liquid volume distilled.

INPUT : X = Mole Fractions of Stream
         F = Mole Flow of Stream

OUTPUT : TBP10 = TBP Temperature at 10% Std Vol Distilled
          TBP90 = TBP Temperature at 90% Std Vol Distilled

PARAMETERS : nocomp = number of componetns

**** THIS PROCEDURE IS MEANT FOR USE WITH prop6.inp PROPERTIES ****
$ENDHELP
INPUT
molefraction(nocomp), flow_mol_liq
OUTPUT
temperature, temperature
CODE

SUBROUTINE TBP(X, NOCOMP, F, TBP10, TBP90, IFL)
C FORTRAN SUBROUTINE TO DETERMINE 10% AND 90% VOLUME DISTILLED TBP TEMPERATURES
C ------- FOR USE ONLY WITH PROP6.INP PROPERTIES -------
C
C DECLARATIONS
C F = MOLEFLOW, TBP10 = TBP AT 10% VOL DISTILL,
C TBP90 = TBP AT 90% DISTILL, NOCOMP = NO COMPS,
C SVOLF = STANDARD VOLUME FLOW OF PSUEDO-COMPS ONLY
C IFL = SPEEDUP INTEGER FAIL FLAG, M10D = TBP10 CALCULATED,
C M90D = TBP90 CALCULATED, X = MOLEFRACTIONS, DENS = MOLAR DENSITIES,
C T = UPPER TBP TEMPS OF PSEUDO-COMP, VF = CUMULATIVE STD VOL FRACTIONS.
DOUBLE PRECISION F, SVOLF, TBP10, TBP90
INTEGER NOCOMP, IFL, M10D, M90D, I
DOUBLE PRECISION X(23), DENS(23), T(23), VF(23)
IFL = 3
I = NOCOMP
C SETUP DENSITY AND PSEUDO-COMPONENT TBP ARRAYS
DO 100 I = 1, 8
   DENS(I) = 0
   T(I) = 1
   VF(I) = 0
100 CONTINUE
DENS(9) = 0.469804
DENS(10) = 0.482586
DENS(11) = 0.445019
DENS(12) = 0.41361
DENS(13) = 0.386685
DENS(14) = 0.359787
DENS(15) = 0.333838
DENS(16) = 0.304117
DENS(17) = 0.276475
DENS(18) = 0.248479
DENS(19) = 0.217059
DENS(20) = 0.189902
DENS(21) = 0.168425
DENS(22) = 0.147276
DENS(23) = 0.127239
T(8) = 113
T(9) = 149
T(10) = 185
T(11) = 221
T(12) = 257
T(13) = 293
T(14) = 329
T(15) = 365  
T(16) = 401  
T(17) = 455  
T(18) = 509  
T(19) = 563  
T(20) = 617  
T(21) = 671  
T(22) = 743  
T(23) = 950  

C  CALCULATE SVOLF  
   SVOLF = (X(9) * F) / DENS(9)  
   DO 105 I = 10,23  
      SVOLF = SVOLF + (X(I) * F) / DENS(I)  
   105 CONTINUE  

C  CALCULATE CUMULATIVE STANDARD VOLUME FRACTIONS  
   VF(9) = ((X(9) * F) / DENS(9)) / SVOLF  
   DO 110 I = 10,23  
      VF(I) = VF(I-1) + (((X(I) * F) / DENS(I)) / SVOLF)  
   110 CONTINUE  

C  CALCULATE TBP10 AND TBP90  
   TEST = 0.0  
   M1OD = 0  
   M90D = 0  
   DO 120 I = 9,23  
      IF((VF(I) .GT. 0.1) .AND. (M1OD .EQ. 0)) THEN  
         TBP10 = T(I-1)+(((0.1-VF(I-1))/VF(I)-VF(I-1)))*(T(I)-T(I-1))  
         M1OD = 1  
      ENDIF  
      IF((VF(I) .GT. 0.9) .AND. (M90D .EQ. 0)) THEN  
         TBP90 = T(I-1)+(((0.9-VF(I-1))/VF(I)-VF(I-1)))*(T(I)-T(I-1))  
         M90D = 1  
      ENDIF  
   120 CONTINUE  
   IFL = 1  
   RETURN  
END  
$ENDCODE  

E.9  report6y.speedup  

The following SPEEDUP input code, report6y.speedup, contains the user defined reports used in both rtodr6.speedup and rtopt6.speedup.
REPORT C1
HELP
Stabilizer Column (C1) Summary Profiles. Made to look similar to the
Aspen ModelManager Output.
$ENDHELP
# Text Processor Setup
?SET strtrays=2 ?END
?SET strtrayf=13 ?END
?SET rcctrays=15 ?END
?SET rcctrayf=28 ?END
FIELDS
# Date and Time for report
&1 = DATE ;
&2 = TIME ;
&177 = DATE ;
&178 = TIME ;
# 4 Decimal Results: Page 1 Temperature, Pressure, Liq Flow, Liq and Vap Enth
# Page 2 All except Tray Vapour Fractions
DECIMALS = 4
NOBLANKS
# condenser/splitter
&3 RIGHT = C1COND.T ;
&4 RIGHT = C1COND.P ;
&5 RIGHT = C1SPL1.HL_OUT1 ;
&6 RIGHT = C1COND.HV_OUT ;
&8 RIGHT = C1SPL1.L_OUT2 ;
&179 RIGHT = C1COND.V_OUT ;
&180 RIGHT = C1SPL1.L_OUT1 ;
&181 RIGHT = C1COND.V_OUT ;
&182 RIGHT = C1COND.H ;
# stripping section
?REPEAT
&7((i*6)-3) RIGHT = "C1S.TRAY_SS(?(i))".T ;
&7((i*6)-2) RIGHT = "C1S.TRAY_SS(?(i))".P ;
&7((i*6)-1) RIGHT = "C1S.TRAY_SS(?(i))".HL_OUT ;
&7((i*6)) RIGHT = "C1S.TRAY_SS(?(i))".HV_OUT ;
&7((i*6)+2) RIGHT = "C1S.TRAY_SS(?(i))".L_OUT ;
&7((i*3)+178) RIGHT = "C1S.TRAY_SS(?(i))".V_OUT ;
&7((i*3)+180) RIGHT = "C1S.TRAY_SS(?(i))".H ;
?WITH i = <strtrays:strtrayf>
# feed tray
&81 RIGHT = C1FT14.T ;
&82 RIGHT = C1FT14.P ;
&83 RIGHT = C1FT14.HL_OUT ;
&84 RIGHT = C1FT14.HV_OUT ;
&86 RIGHT = C1FT14.L_OUT ;
&220 RIGHT = C1FT14.V_OUT ;
&221 RIGHT = C1FT14.F_IN ;
&223 RIGHT = C1FT14.H ;
# rectifying section
?REPEAT
&?((i*6)-3) RIGHT = "C1R.TRAY_SS((i))".T ;
&?((i*6)-2) RIGHT = "C1R.TRAY_SS((i))".P ;
&?((i*6)-1) RIGHT = "C1R.TRAY_SS((i))".HL_OUT ;
&?((i*6)) RIGHT = "C1R.TRAY_SS((i))".HV_OUT ;
&?((i*6)+2) RIGHT = "C1R.TRAY_SS((i))".L_OUT ;
&?((i*3)+179) RIGHT = "C1R.TRAY_SS((i))".V_OUT ;
&?((i*3)+181) RIGHT = "C1R.TRAY_SS((i))".H ;
?WITH i = <rcttrays:rcttrayf>
# bottom tray
&171 RIGHT = C1BT29.T ;
&172 RIGHT = C1BT29.P ;
&173 RIGHT = C1BT29.HL_OUT1 ;
&174 RIGHT = C1BT29.HV_OUT ;
&176 RIGHT = C1BT29.L_OUT1 + C1BT29.L_OUT2 ;
&266 RIGHT = C1BT29.V_OUT ;
&267 RIGHT = C1REBL.F_OUT ;
&268 RIGHT = C1BT29.L_OUT1 + C1BT29.L_OUT2 ;
&270 RIGHT = C1BT29.H ;
# 5 Decimal Results: Page 1 Duty
# Page 2 Tray Vapour Fraction
DECIMALS = 5
NOBLANKS
# condenser/splitter
&7 RIGHT = C1COND.Q ;
&182 RIGHT = C1COND.VF ;
# stripping section
?REPEAT
&?((i*6)+1) RIGHT = "C1S.TRAY_SS((i))".Q ;
&?((i*3)+179) RIGHT = "C1S.TRAY_SS((i))".VF ;
?WITH i = <strtrays:strtrayf>
# feed tray
&85 RIGHT = C1FT14.Q ;
&222 RIGHT = C1FT14.VF ;
# rectifying section
?REPEAT
&?((i*6)+1) RIGHT = "C1R.TRAY_SS((i))".Q ;
&?((i*3)+180) RIGHT = "C1R.TRAY_SS((i))".VF ;
?WITH i = <rcttrays:rcttrayf>
# reboiler
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* C1 COLUMN SUMMARY PROFILES *

Description: STABILIZER
**C1 COLUMN SUMMARY PROFILES**

Description: STABILIZER

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REPORT C2
HELP
Splitter Column (C2) and Sidestripper Columns (C4, C5) Summary Profiles. Made to look similar to the Aspen ModelManager Output.
$ENDHELP
# Text Processor Setup
?SET strtrays=2 END
?SET strtrayf=13 END

FIELDS
# Date and Time for report
&1 = DATE ;
&2 = TIME ;
&183 = DATE ;
&184 = TIME ;

# 4 Decimal Results: Page 1 Temperature, Pressure, Liq Flow, Liq and Vap Enth
Page 2 All except Tray Vapour Fractions

DECIMALS = 4

NOLBLANKS

# condenser
&3 RIGHT = C2COND.T ;
&4 RIGHT = C2COND.P ;
&5 RIGHT = C2COND.HL.OUT1 ;
&6 RIGHT = 0.0000 ;
&8 RIGHT = C2COND.L.OUT1 ;
&185 RIGHT = 0.0000 ;
&186 RIGHT = C2COND.L.OUT2 ;

# stripping section 1

?REPEAT
&?(i+6)-1) RIGHT = "C2S1.TRAY_SS(?i)".HL.OUT ;
&?(i+6)) RIGHT = "C2S1.TRAY_SS(?i)".HV.OUT ;
&?((i+6)-3) RIGHT = "C2S1.TRAY_SS(?i)".T ;
&?((i+6)-2) RIGHT = "C2S1.TRAY_SS(?i)".P ;
&?((i+6)+2) RIGHT = "C2S1.TRAY_SS(?i)".L_OUT ;
&?((i+3)+181) RIGHT = "C2S1.TRAY_SS(?i)".V_OUT ;
&?((i+3)+183) RIGHT = "C2S1.TRAY_SS(?i)".H ;

?WITH i = <strtrays:strtrayf>

# feed tray 14
&81 RIGHT = C2FT14.T ;
&82 RIGHT = C2FT14.P ;
&83 RIGHT = C2FT14.HL.OUT ;
&84 RIGHT = C2FT14.HV.OUT ;
&86 RIGHT = C2FT14.L_OUT ;
&223 RIGHT = C2FT14.V.OUT ;
&224 RIGHT = C2FT14.F_IN ;
&226 RIGHT = C2FT14.H ;

# stripping section 2
&87 RIGHT = C2T15.T ;
&88 RIGHT = C2T15.P ;
&92 RIGHT = C2T15.L_OUT ;
&227 RIGHT = C2T15.V_OUT ;
&228 RIGHT = C2SPL1.L_OUT1 ;
&230 RIGHT = C2T15.H ;
&89 RIGHT = C2T15.HL_OUT ;
&90 RIGHT = C2T15.HV_OUT ;
&95 RIGHT = C2T16.HL_OUT ;
&96 RIGHT = C2T16.HV_OUT ;
&93 RIGHT = C2T16.T ;
&94 RIGHT = C2T16.P ;
&98 RIGHT = C2T16.L_OUT ;
&231 RIGHT = C2T16.V_OUT ;
&233 RIGHT = C2T16.H ;

# feed tray 17
&99 RIGHT = C2FT17.T ;
&100 RIGHT = C2FT17.P ;
&101 RIGHT = C2FT17.HL_OUT ;
&102 RIGHT = C2FT17.HV_OUT ;
&104 RIGHT = C2FT17.L_OUT ;
&234 RIGHT = C2FT17.V_OUT ;
&235 RIGHT = C2FT17.F_IN ;
&237 RIGHT = C2FT17.H ;

# stripping section 3
&105 RIGHT = C2T18.T ;
&106 RIGHT = C2T18.P ;
&110 RIGHT = C2T18.L_OUT ;
&238 RIGHT = C2T18.V_OUT ;
&239 RIGHT = C2SPL2.L_OUT1 ;
&241 RIGHT = C2T18.H ;
&111 RIGHT = "C2S3.TRAY_SS(19)".T ;
&112 RIGHT = "C2S3.TRAY_SS(19)".P ;
&116 RIGHT = "C2S3.TRAY_SS(19)".L_OUT ;
&242 RIGHT = "C2S3.TRAY_SS(19)".V_OUT ;
&244 RIGHT = "C2S3.TRAY_SS(19)".H ;
&117 RIGHT = "C2S3.TRAY_SS(20)".T ;
&118 RIGHT = "C2S3.TRAY_SS(20)".P ;
&122 RIGHT = "C2S3.TRAY_SS(20)".L_OUT ;
&245 RIGHT = "C2S3.TRAY_SS(20)".V_OUT ;
&247 RIGHT = "C2S3.TRAY_SS(20)".H ;
&107 RIGHT = C2T18.HL_OUT ;
&108 RIGHT = C2T18.HV_OUT ;
&113 RIGHT = "C2S3.TRAY_SS(19)".HL_OUT ;
&114 RIGHT = "C2S3.TRAY_SS(19)".HV_OUT ;
&119 RIGHT = "C2S3.TRAY_SS(20)".HL_OUT ;
&120 RIGHT = "C2S3.TRAY_SS(20)".HV_OUT ;

# feed tray 21
&123 RIGHT = C2FT21.T ;
&124 RIGHT = C2FT21.P;
&125 RIGHT = C2FT21.HL_OUT;
&126 RIGHT = C2FT21.HV_OUT;
&128 RIGHT = C2FT21.L_OUT;
&248 RIGHT = C2FT21.V_OUT;
&249 RIGHT = C2FT21.F_IN;
&251 RIGHT = C2FT21.H;

# rectifying section
&129 RIGHT = "C2R.TRAY_SS(22)".T;
&130 RIGHT = "C2R.TRAY_SS(22)".P;
&134 RIGHT = "C2R.TRAY_SS(22)".L_OUT;
&252 RIGHT = "C2R.TRAY_SS(22)".V_OUT;
&254 RIGHT = "C2R.TRAY_SS(22)".H;
&131 RIGHT = "C2R.TRAY_SS(22)".HL_OUT;
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# bottom tray
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&258 RIGHT = C2BT24.V_OUT;
&259 RIGHT = C2REBL.F_OUT;
&262 RIGHT = C2BT24.H;

# C4
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&152 RIGHT = "C4.TRAY_SS(1)".L_OUT;
&263 RIGHT = "C4.TRAY_SS(1)".V_OUT;
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&274 RIGHT = C4REBL.H ;
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# 6 Decimal Results: Page 1 Duty
#  Page 2 Tray Vapour Fraction

DECIMALS = 6
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# condenser
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# stripping section 1
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&?(i*3)+182) RIGHT = "C2S1.TRAY_SS(?(@i))".VF ;
?WITH i = <strtrays:sttrayf>

# feed tray
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&225 RIGHT = C2FT14.VF ;

# stripping section 2
&91 RIGHT = C2T15.Q ;
&229 RIGHT = C2T15.VF ;
&97 RIGHT = C2T16.Q ;
&232 RIGHT = C2T16.VF ;

# feed tray 17
&103 RIGHT = C2FT17.Q ;
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# stripping section 3
&109 RIGHT = C2T18.Q ;
&240 RIGHT = C2T18.VF ;
&115 RIGHT = "C2S3.TRAY_SS(19)".Q ;
&243 RIGHT = "C2S3.TRAY_SS(19)".VF ;
&121 RIGHT = "C2S3.TRAY_SS(20)".Q ;
&246 RIGHT = "C2S3.TRAY_SS(20)".VF ;

# feed tray 21
&127 RIGHT = C2FT21.Q ;
&250 RIGHT = C2FT21.VF ;

# rectifying section
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&253 RIGHT = "C2R.TRAY_SS(22)".VF ;
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&256 RIGHT = "C2R.TRAY_SS(23)".VF ;

# reboiler
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&261 RIGHT = C2BTL24.VF ;

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&273 RIGHT = C4REBL.VF ;

# C5
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* C4 COLUMN SUMMARY PROFILES *

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REPORT STREAMSUM
HELP
Stream Summary for Stabilizer-Splitter Flowsheet (C1, E1, C2, C4, C5). Made to look similar to the Aspen ModelManager Output.

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?SET nocomp=23 ?END

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# Date and Time for report
&1 = DATE ;
&2 = TIME ;
&167 = DATE ;
&168 = TIME ;
&333 = DATE ;
&334 = TIME ;
# Set format for report
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&?((i+5)+1) RIGHT = F51.X_OUT(?((i)))
&?((i+5)+2) RIGHT = CSREBL.X_OUT(?((i)))
?WITH i = <1:nocomp>
# Page 1 Stream Mole Flows
&118 RIGHT = C1SPL1.L_OUT1
&119 RIGHT = C4REBL.L_OUT
&120 RIGHT = F41.L_OUT
&121 RIGHT = F51.L_OUT
&122 RIGHT = CSREBL.L_OUT
# Page 1 Stream Volume Flows (cuft/hr)
&123 RIGHT = F13.VOLFL
&124 RIGHT = F42.VOLFL
&125 RIGHT = F41.VOLFL
&126 RIGHT = F51.VOLFL
&127 RIGHT = F52.VOLFL
# Page 1 Stream Volume Flows (bbl/day)
&128 RIGHT = F13.VOLFL / 0.23394
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&130 RIGHT = F41.VOLFL / 0.23394
&131 RIGHT = F51.VOLFL / 0.23394
&132 RIGHT = F52.VOLFL / 0.23394
# Page 1 Stream Standard Liquid Volume Flow (cuft/hr)
&133 RIGHT = F13.STDVLFL
&134 RIGHT = F42.STDVLFL
&135 RIGHT = F41.STDVLFL
&136 RIGHT = F51.STDVLFL
&137 RIGHT = F52.STDVLFL
# Page 1 Stream Standard Liquid Volume Flow (bbl/day)
&138 RIGHT = F13.STDVLFL / 0.23394
&139 RIGHT = F42.STDVLFL / 0.23394
&140 RIGHT = F41.STDVLFL / 0.23394
&141 RIGHT = F51.STDVLFL / 0.23394
&142 RIGHT = F52.STDVLFL / 0.23394
# Page 1 Stream Temperatures
&143 RIGHT = C1SPL1.TL_OUT1
&144 RIGHT = C4REBL.TL_OUT
&145 RIGHT = F41.TL_OUT
&146 RIGHT = F51.TL_OUT
&147 RIGHT = CSREBL.TL_OUT
# Page 1 Stream Pressures
\&148 RIGHT = C1SPL1.PL_OUT1 ;
\&149 RIGHT = C4REBL.PL_OUT ;
\&150 RIGHT = F41.PL_OUT ;
\&151 RIGHT = F51.PL_OUT ;
\&152 RIGHT = C5REBL.PL_OUT ;

# Page 1 Stream Enthalpies
\&153 RIGHT = C1SPL1.HL_OUT1 ;
\&154 RIGHT = C4REBL.HL_OUT ;
\&155 RIGHT = F41.HL_OUT ;
\&156 RIGHT = F51.HL_OUT ;
\&157 RIGHT = C5REBL.HL_OUT ;

# Page 1 Stream Densities
\&158 RIGHT = F13.RHOL ;
\&159 RIGHT = F42.RHOL ;
\&160 RIGHT = F41.RHOL ;
\&161 RIGHT = F51.RHOL ;
\&162 RIGHT = F52.RHOL ;

# Page 1 TBP10 Temperatures
\&163 RIGHT = F42.TBP10 ;
\&164 RIGHT = F52.TBP10 ;

# Page 1 TBP90 Temperatures
\&165 RIGHT = F42.TBP90 ;
\&166 RIGHT = F52.TBP90 ;

# Page 2 Stream Component Mole Fractions
?REPEAT
\&?((i*5)+164) RIGHT = C2COND.X_OUT2(?(i)) ;
\&?((i*5)+165) RIGHT = E1.Z_OUT(?(i)) ;
\&?((i*5)+166) RIGHT = F22A.X_OUT(?(i)) ;
\&?((i*5)+167) RIGHT = F62.X_OUT(?(i)) ;
\&?((i*5)+168) RIGHT = MFEED.Z_OUT(?(i)) ;
?WITH i = <1:ncomp>

# Page 2 Stream Mole Flows
\&284 RIGHT = C2COND.L_OUT2 ;
\&285 RIGHT = E1.F_OUT ;
\&286 RIGHT = F22A.L_OUT ;
\&287 RIGHT = F62.L_OUT ;
\&288 RIGHT = MFEED.F_OUT ;

# Page 2 Stream Volume Flows (cuft/hr)
\&289 RIGHT = F31.VOLFL ;
\&290 RIGHT = F22.VOLF ;
\&291 RIGHT = F22A.VOLFL ;
\&292 RIGHT = F62.VOLFL ;
\&293 RIGHT = F01.VOLF ;

# Page 2 Stream Volume Flows (bbl/day)
&331  RIGHT = RVP31.RVP ;

# Page 2 Bubble Point Temps
&332  RIGHT = C2COND.T_BUBBLE ;

# Page 3 Stream Mole Fractions
?REPEAT
  &?((i=5)+330)  RIGHT = C1COND.Y_OUT(?(i)) ;
  &?((i=5)+331)  RIGHT = F21.Z_OUT(?(i)) ;
  &?((i=5)+332)  RIGHT = F12.X_OUT(?(i)) ;
  &?((i=5)+333)  RIGHT = F61.Z_OUT(?(i)) ;
  &?((i=5)+334)  RIGHT = F32.X_OUT(?(i)) ;
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# Page 3 Stream Component Mole Flows
&450  RIGHT = C1COND.V_OUT ;
&451  RIGHT = F21.F_OUT ;
&452  RIGHT = F12.L_OUT ;
&453  RIGHT = F61.F_OUT ;
&454  RIGHT = F32.L_OUT ;

# Page 3 Stream Volume Flows (cuft/hr)
&455  RIGHT = F11.VOLFV ;
&456  RIGHT = F21.VOLF ;
&457  RIGHT = F12.VOLFL ;
&458  RIGHT = F61.VOLF ;
&459  RIGHT = F32.VOLFL ;

# Page 3 Stream Volume Flows (bbl/day)
&460  RIGHT = F11.VOLFV / 0.23394 ;
&461  RIGHT = F21.VOLF / 0.23394 ;
&462  RIGHT = F12.VOLFL / 0.23394 ;
&463  RIGHT = F61.VOLF / 0.23394 ;
&464  RIGHT = F32.VOLFL / 0.23394 ;

# Page 3 Stream Standard Liquid Volume Flows (cuft/hr)
&465  RIGHT = F11.STDVOLFL ;
&466  RIGHT = F21.STDVOLFL ;
&467  RIGHT = F12.STDVOLFL ;
&468  RIGHT = F61.STDVOLFL ;
&469  RIGHT = F32.STDVOLFL ;

# Page 3 Stream Standard Liquid Volume Flows (bbl/day)
&470  RIGHT = F11.STDVOLFL / 0.23394 ;
&471  RIGHT = F21.STDVOLFL / 0.23394 ;
&472  RIGHT = F12.STDVOLFL / 0.23394 ;
&473  RIGHT = F61.STDVOLFL / 0.23394 ;
&474  RIGHT = F32.STDVOLFL / 0.23394 ;

# Page 3 Stream Temperatures
&475  RIGHT = C1COND.TV_OUT ;
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&477  RIGHT = F12.TL_OUT ;
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&478 RIGHT = F61.T_OUT ;
&479 RIGHT = F32.TL_OUT ;

# Page 3 Stream Pressures
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&482 RIGHT = F12.PL_OUT ;
&483 RIGHT = F61.P_OUT ;
&484 RIGHT = F32.PL_OUT ;

# Page 3 Vapour Fractions
&485 RIGHT = F21 VF ;
&486 RIGHT = F61.VF ;

# Page 3 Stream Enthalpies
&487 RIGHT = C1COND.HV_OUT ;
&488 RIGHT = F21.H_OUT ;
&489 RIGHT = F12.HL_OUT ;
&490 RIGHT = F61.H_OUT ;
&491 RIGHT = F32.HL_OUT ;

# Page 3 Stream Densities
&492 RIGHT = F11.RHOV ;
&494 RIGHT = F12.RHOL ;
&495 RIGHT = F61.F_OUT / F61.VOLF ;
&496 RIGHT = F32.RHOL ;

# Page 3 Standard Volume Flows
&497 RIGHT = F11.STDVOLFV ;

# Report Layout
DISPLAY
STABILIZER-SPLITTER REPORT CREATED BY SPEEDUP ON XXXXXXXXXX, XXXXXXXXXX
Page 1 of 3

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* STREAM SUMMARY *
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COMPONENT MOLE FRACTIONS

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METHANE

ETHANE

PROPANE

IBUTANE

BUTANE

IPENTANE
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**Stabilizer-Splitter Report Created by Speedup on XX, XX**

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**Stream Summary**

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**Component Flows [Mole Fraction]**

- **H2**: XX
- **Methane**: XX

---
| ETHANE   |               |               |               |               |               |
| PROPANE  |               |               |               |               |               |
| IBUTANE  |               |               |               |               |               |
| BUTANE   |               |               |               |               |               |
| IPENTANE |               |               |               |               |               |
| PENTANE  |               |               |               |               |               |
| BP45T65  |               |               |               |               |               |
| BP65T85  |               |               |               |               |               |
| BP85T105 |               |               |               |               |               |
| BP105T125|               |               |               |               |               |
| BP125T145|               |               |               |               |               |
| BP145T165|               |               |               |               |               |
| BP165T185|               |               |               |               |               |
| BP185T205|               |               |               |               |               |
| BP205T235|               |               |               |               |               |
| BP235T265|               |               |               |               |               |
| BP265T295|               |               |               |               |               |
| BP295T325|               |               |               |               |               |
| BP325T355|               |               |               |               |               |
| BP355T395|               |               |               |               |               |
| BP395T310|               |               |               |               |               |

MOLE FLOW [LB/MOL/HR]  
VOLUME FLOW [CUFT/HR]   
VOLUME FLOW [BBL/DAY]  
STD VOL FLOW [CUFT/HR]  
STD VOL FLOW [BBL/DAY]  
TEMPERATURE [F]        
PRESSURE [PSI]         
VAPOUR FRACTION 0.0  
ENTHALPY [MMBTU/LB/MOL]  
DENSITY [LB/MOL/CUFT]  
TBP TEMP, 0.1 VOL [F]  
IBP TEMP, 0.9 VOL [F]  
REID VAP PRESS [PSI]  
BUBBLE POINT TEMP [F]  
STD VAP FLOW [CUFT/HR]  

STABILIZER-SPLITTER REPORT CREATED BY SPEEDUP ON  

Page 3 of 3

STREAM SUMMARY

STREAM NAME: VAP C1REBL C1RLX C2REBL C2RLX
From C1
Tear Stream Report for the return streams from and Sidestripper Columns (C4, C5) to the Splitter Column (C2).

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# Text Processor Setup
?SET nocomp=23 ?END

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DECIMALS = 4
NOBLANKS

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DISPLAY
SPLITTER TEAR STREAM REPORT CREATED BY SPEEDUP ON ***************, **************
Page 1 of 2

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* C1REBL -> C1BT29 TEAR STREAM *
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METHANE  **************************** **************************** ****************************
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Mole Flow [lbmol/hr]  XXXXXXXXXX  XXXXXXXXXX  XXXXXXXXXX
Temperature [F]  XXXXXXXXXX  XXXXXXXXXX  XXXXXXXXXX
Pressure [psi]  XXXXXXXXXX  XXXXXXXXXX  XXXXXXXXXX
Enthalpy [MMBTU/lbmol] XXXXXXXXXX  XXXXXXXXXX  XXXXXXXXXX
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MOLE FLOW [LB/MOL/HR]  
TEMPERATURE [°F]  
PRESSURE [PSI]  
ENTHALPY [MMBTU/LB/MOL]
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MOLE FLOW [LB/MOL/HR] XXXXXXXXXX
TEMPERATURE [F] XXXXXXXXXX
PRESSURE [PSI] XXXXXXXXXX
ENTHALPY [MMBTU/LB/MOL] XXXXXXXXXX
**ENTHALPY [MMBTU/LBMOL]**

---

****

REPORT SIMSET

HELP

Simulation Settings to be passed onto next simulation
(Based on DRSIMSET.DAT or OPSIMSET.DAT in Aspen runs).

$ENDHELP

FIELDS

# Date and Time for report
&1 = DATE ;
&2 = TIME ;
DECIMALS = 4
NOBLANKS

# SpeedUp Variable Values
&3 = C1FT14.F_IN ;
&4 = C1FT14.T_IN ;
&5 = MFEED.P_OUT ;
&6 = C1COND.Q ;
&7 = C1SPL1.L_OUT1 ;
&8 = C1BT29.L_OUT2 ;
&9 = C1BT29.L_OUT1 ;
&10 = C1BT29.P - "C1S.TRAY_SS(2)".P ;
&11 = C1COND.P ;
&12 = "C1S.TRAY_SS(2)".P ;
&13 = C2FT21.T_IN ;
&14 = E1.P_OUT ;
&15 = C2COND.T_DROP ;
&16 = C2COND.Q ;
&17 = C2BT24.L_OUT2 ;
&18 = C2BT24.L_OUT1 ;
&19 = C2BT24.P - "C2S1.TRAY_SS(2)".P ;
&20 = C2COND.P ;
&21 = "C2S1.TRAY_SS(2)".P ;
&22 = C2SPL1.L_OUT1 ;
&23 = C2SPL2.L_OUT1 ;
&24 = C4REBL.L_OUT ;
&25 = C5REBL.L_OUT ;

# Aspen Variable Values
&26 = MFEED.F_OUT ;
&27 = MFEED.T_OUT ;
&28 = MFEED.P_OUT ;
&29 = F12.L_OUT / (F13.L_OUT + F11.V_OUT) ;
&31 = C1BT29.L_OUT2 ;
&32 = C1REBL.T_OUT ;
&33 = C1BT29.P - "C1S.TRAY_SS(2)".P ;
&34 = C1COND.P ;
&35 = "C1S.TRAY_SS(2)".P ;
&36 = E1.T_OUT ;
&37 = E1.P_OUT ;
&38 = C2COND.L_OUT2 ;
&39 = C2BT24.L_OUT2 ;
&40 = C2REBL.T_OUT ;
&41 = C2COND.T ;
&42 = C2BT24.P - "C2S1.TRAY_SS(2)".P ;
&43 = C2COND.P ;
&44 = "C2S1.TRAY_SS(2)".P ;
&45 = C2SPL1.L_OUT1 ;
&46 = C2SPL2.L_OUT1 ;
&47 = C4REBL.Q ;
&48 = C5REBL.Q ;

DISPLAY
SIMULATION SETTINGS SUMMARY REPORT CREATED BY SPEEDUP ON %%%%%%%%%%%%%%%%%, %%%%%%%%%%%%%%%%%
Page 1 of 1

*******************************************************************************
* SPEEDUP SIMULATION SETTINGS *
*******************************************************************************

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C2 2ND TRAY P [PSIA]  
C2-C4 IC FLOW [LB/MOL/HR]  
C2-C5 IC FLOW [LB/MOL/HR]  
HV-ISO FLOW [LB/MOL/HR]  
LT-DIST FLOW [LB/MOL/HR]  

******************************************************************************
* ASPEN SIMULATION SETTINGS *  
******************************************************************************

STAB MOLFLOW [LB/MOL/HR]  
STAB TEMP [°F]  
STAB PRESS [PSIA]  
C1 RFLX RATIO [MOL/MOL]  
C1 VAP/DIST [MOL/MOL]  
C1 REBL FLOW [LB/MOL/HR]  
C1 REBL TEMP [°F]  
C1 COL P DROP [PSI]  
C1 TOP TRAY P [PSIA]  
C1 2ND TRAY P [PSIA]  
E1 OUT TEMP [°F]  
E1 OUT PRESS [PSIA]  
C2 DIST FLOW [LB/MOL/HR]  
C2 REBL FLOW [LB/MOL/HR]  
C2 REBL TEMP [°F]  
C2 COND SC T [°F]  
C2 COL P DROP [PSI]  
C2 TOP TRAY P [PSIA]  
C2 2ND TRAY P [PSIA]  
C2-C4 IC FLOW [LB/MOL/HR]  
C2-C5 IC FLOW [LB/MOL/HR]  
C4 REBL DUTY [MMBTU/HR]  
C5 REBL DUTY [MMBTU/HR]  

******************************************************************************

****
REPORT DREC
HELP
Objective Function and Variable Summaries for the Data
Reconciliation Runs.
$ENDHELP
# Text Processor Setup
?SET nocomp=24 ?END
FIELDS
# Date and Time for report
&1 = DATE;
&2 = TIME;
DECIMALS = 4
NOBLANKS

# Variable Values
&3 = F01.STDVLNFL * GLOBAL.CN VF2B;
&6 = F11.STDVOLFV;
&9 = F12.STDVOLFL * GLOBAL.CN VF2B;
&12 = F13.STDVOLFL * GLOBAL.CN VF2B;
&15 = F21.STDVOLFL * GLOBAL.CN VF2B;
&18 = F22.STDVOLFL * GLOBAL.CN VF2B;
&21 = F31.STDVOLFL * GLOBAL.CN VF2B;
&24 = F32.STDVOLFL * GLOBAL.CN VF2B;
&27 = F41.STDVOLFL * GLOBAL.CN VF2B;
&30 = F42.STDVOLFL * GLOBAL.CN VF2B;
&33 = F51.STDVOLFL * GLOBAL.CN VF2B;
&36 = F52.STDVOLFL * GLOBAL.CN VF2B;
&39 = F61.STDVOLFL * GLOBAL.CN VF2B;
&42 = F62.STDVOLFL * GLOBAL.CN VF2B;
&45 = MFEED.T_OUT;
&48 = "C1S.TRAY_SS(2)".T;
&51 = C1COND.T;
&54 = C1BT29.TL_OUT1;
&57 = C1REBL.T_OUT;
&60 = E1.T_OUT;
&63 = "C2S1.TRAY_SS(2)".T;
&66 = C2COND.T;
&69 = C2SPL1.TL_OUT1;
&72 = C4REBL.TL_OUT;
&75 = C2SPL2.TL_OUT1;
&78 = C5REBL.TL_OUT;
&81 = C2BT24.TL_OUT1;
&84 = C2REBL.T_OUT;

# Offset Values
&4 = (F01.STDVLNFL * GLOBAL.CN VF2B) - GLOBAL.SF01;
&7 = F11.STDVOLFV - GLOBAL.SF11;
&10 = (F12.STDVOLFL * GLOBAL.CN VF2B) - GLOBAL.SF12;
&13 = (F13.STDVOLFL * GLOBAL.CN VF2B) - GLOBAL.SF13;
&16 = (F21.STDVOLFL * GLOBAL.CN VF2B) - GLOBAL.SF21;
&19 = (F22.STDVOLFL * GLOBAL.CN VF2B) - GLOBAL.SF22;
&22 = (F31.STDVOLFL * GLOBAL.CN VF2B) - GLOBAL.SF31;
&25 = (F32.STDVOLFL * GLOBAL.CN VF2B) - GLOBAL.SF32;
&28 = (F41.STDVOLFL * GLOBAL.CN VF2B) - GLOBAL.SF41;
&31 = (F42.STDVOLFL * GLOBAL.CN VF2B) - GLOBAL.SF42;
&34 = (F51.STDVOLFL * GLOBAL.CN VF2B) - GLOBAL.SF51;
&37 = (F52.STDVMLFL * GLOBAL.CNVF2B) - GLOBAL.SF52 ;
&40 = (F61.STDVMLFL * GLOBAL.CNVF2B) - GLOBAL.SF61 ;
&43 = (F62.STDVMLFL * GLOBAL.CNVF2B) - GLOBAL.SF62 ;
&46 = MFEED.T_OUT - GLOBAL.ST01 ;
&49 = "C1S.TRAY_SS(2)".T - GLOBAL.ST12 ;
&52 = C1COND.T - GLOBAL.ST13 ;
&55 = C1BT29.TL_OUT1 - GLOBAL.ST21 ;
&58 = C1REBL.T_OUT - GLOBAL.ST22 ;
&61 = E1.T_OUT - GLOBAL.ST23 ;
&64 = "C2S1.TRAY_SS(2)".T - GLOBAL.ST31 ;
&67 = C2COND.T - GLOBAL.ST32 ;
&70 = C2SPL1.TL_OUT1 - GLOBAL.ST41 ;
&73 = C4REBL.TL_OUT - GLOBAL.ST42 ;
&76 = C2SPL2.TL_OUT1 - GLOBAL.ST51 ;
&79 = C5REBL.TL_OUT - GLOBAL.ST52 ;
&82 = C2BT24.TL_OUT1 - GLOBAL.ST61 ;
&85 = C2REBL.T_OUT - GLOBAL.ST62 ;

# Error Values
&5 = GLOBAL.EF01 ;
&8 = GLOBAL.EF11 ;
&11 = GLOBAL.EF12 ;
&14 = GLOBAL.EF13 ;
&17 = GLOBAL.EF21 ;
&20 = GLOBAL.EF22 ;
&23 = GLOBAL.EF31 ;
&26 = GLOBAL.EF32 ;
&29 = GLOBAL.EF41 ;
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&35 = GLOBAL.EF51 ;
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&65 = GLOBAL.ET31 ;
&68 = GLOBAL.ET32 ;
&71 = GLOBAL.ET41 ;
&74 = GLOBAL.ET42 ;
&77 = GLOBAL.ET51 ;
&80 = GLOBAL.ET52 ;
&83 = GLOBAL.ET61 ;
FINAL OBJECTIVE FUNCTION VALUE = %%%%%%%%%%%%%%

Objectives and Constraint Summaries for the Optimization Simulation Run.

# Date and Time for report
&1 = DATE ;
&2 = TIME ;
&31 = DATE ;
&32 = TIME ;
&61 = DATE ;
&62 = TIME ;
DECIMALS = 6

# Flow Constraint Values
&3 = F12.STDVALFL * GLOBAL.CNRF2B ;
&4 = F32.STDVALFL * GLOBAL.CNRF2B ;
&5 = F41.STDVALFL * GLOBAL.CNRF2B ;
&6 = F51.STDVALFL * GLOBAL.CNRF2B ;

# Temperature Constraint Values
&7 = "C1S.TRAY_SS(3)".T ;
&8 = C1REBL.T.OUT ;
&9 = "C2S1.TRAY_SS(2)".T ;
&10 = C2REBL.T.OUT ;

# C5 Composition Constraint Values
&11 = F13.CSS * 100 ;

# RVP Constraint Values
&12 = RVP31.RVP ;
&13 = C2COND.T_BUBBLE ;

# TBP Constraint Values
&14 = F42.TBP10 ;
&15 = F42.TBP90 ;
&16 = F52.TBP10 ;
&17 = F52.TBP90 ;

# Objective Function Summary
&18 = GLOBAL.PVALS - GLOBAL.CSTAB - GLOBAL.COF1 - GLOBAL.COF2 ;
&19 = GLOBAL.PVALS ;
&20 = GLOBAL.CSTAB ;
&21 = GLOBAL.COF1 + GLOBAL.COF2 ;

# Stream Std-vol Flows
&22 = F01.STDVL0FL ;
&24 = F11.STDVL0FL ;
&26 = F13.STDVL0FL ;
&27 = F31.STDVL0FL ;
&28 = F42.STDVL0FL ;
&29 = F52.STDVL0FL ;
&30 = F62.STDVL0FL ;

# Reboiler Heat Duties
&23 = C1REBL.Q ;
&25 = C2REBL.Q ;

# Variable Values
&33 = F01.STDVL0FL * GLOBAL.CNVF2B ;
&34 = F11.STDVL0FV ;
&35 = F12.STDVL0FL * GLOBAL.CNVF2B ;
&36 = F13.STDVL0FL * GLOBAL.CNVF2B ;
&37 = F21.STDVL0FL * GLOBAL.CNVF2B ;
&38 = F22.STDVL0FL * GLOBAL.CNVF2B ;
&39 = F31.STDVL0FL * GLOBAL.CNVF2B ;
&40 = F32.STDVL0FL * GLOBAL.CNVF2B ;
&41 = F41.STDVL0FL * GLOBAL.CNVF2B ;
&42 = F42.STDVL0FL * GLOBAL.CNVF2B ;
&43 = F51.STDVL0FL * GLOBAL.CNVF2B ;
&44 = F52.STDVL0FL * GLOBAL.CNVF2B ;
&45 = F61.STDVL0FL * GLOBAL.CNVF2B ;
&46 = F62.STDVL0FL * GLOBAL.CNVF2B ;
&47 = MFEED.T_OUT ;
&48 = "C1S.TRAY_SS(2)".T ;
&49 = C1COND.T ;
&50 = C1BT29.TL_OUT1 ;
&51 = C1REBL.T_OUT ;
&52 = E1.T_OUT ;
&53 = "C2S1.TRAY_SS(2)".T ;
&54 = C2COND.T ;
&55 = C2SPL1.TL_OUT1 ;
&56 = C4REBL.TL_OUT ;
&57 = C2SPL2.TL_OUT1 ;
&58 = C5REBL.TL_OUT ;
&59 = C2BT24.TL_OUT1 ;
&60 = C2REBL.T_OUT ;

# Set Point Values
&63 = F12.STDVL0FL * GLOBAL.CNVF2B ;
&64 = "C1S.TRAY_SS(3)".T ;
&65 = F13.CSS ;
&66 = C1REBL.T_OUT ;
&67 = F32.STDVLFL * GLOBAL.CNVF2B ;
&68 = F41.STDVLFL * GLOBAL.CNVF2B ;
&69 = F51.STDVLFL * GLOBAL.CNVF2B ;
&70 = C2REBL.T_OUT ;
&71 = F42.TBP10 ;
&72 = F42.TBP90 ;
&73 = F52.TBP10 ;
&74 = F52.TBP90 ;

DISPLAY
OPTIMIZATION SUMMARY REPORT CREATED BY SPEEDUP ON %%%%%%%%%%%%%%%%%%%, %%%%%%%%%%%%%%%%%%%
Page 1 of 3

*****************************************************************
* CONSTRAINT VALUE SUMMARY *
*****************************************************************

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th>LOWER Bound</th>
<th>VALUE</th>
<th>UPPER Bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>F12 [BBL/DAY]</td>
<td>5500.0</td>
<td>%%%%%%%%%%%%%%%%%</td>
<td>9000.0</td>
</tr>
<tr>
<td>F32 [BBL/DAY]</td>
<td></td>
<td>%%%%%%%%%%%%%%%%%</td>
<td>25000.0</td>
</tr>
<tr>
<td>F41 [BBL/DAY]</td>
<td></td>
<td>%%%%%%%%%%%%%%%%%</td>
<td>10604.0</td>
</tr>
<tr>
<td>F51 [BBL/DAY]</td>
<td></td>
<td>%%%%%%%%%%%%%%%%%</td>
<td>6000.0</td>
</tr>
<tr>
<td>T11 [F]</td>
<td>125.0</td>
<td>%%%%%%%%%%%%%%%%%</td>
<td>220.0</td>
</tr>
<tr>
<td>T22 [F]</td>
<td>500.0</td>
<td>%%%%%%%%%%%%%%%%%</td>
<td>675.0</td>
</tr>
<tr>
<td>T31 [F]</td>
<td>120.0</td>
<td>%%%%%%%%%%%%%%%%%</td>
<td>250.0</td>
</tr>
<tr>
<td>T62 [F]</td>
<td>550.0</td>
<td>%%%%%%%%%%%%%%%%%</td>
<td>700.0</td>
</tr>
<tr>
<td>A11 [PERCENT C5's]</td>
<td>0.5</td>
<td>%%%%%%%%%%%%%%%%%</td>
<td>15.0</td>
</tr>
<tr>
<td>A31-RVP [PSI]</td>
<td></td>
<td>%%%%%%%%%%%%%%%%%</td>
<td>14.0</td>
</tr>
<tr>
<td>A31-TBubble [F]</td>
<td></td>
<td>%%%%%%%%%%%%%%%%%</td>
<td></td>
</tr>
<tr>
<td>A41-TBP @ .10 VOL [F]</td>
<td>176.0</td>
<td>%%%%%%%%%%%%%%%%%</td>
<td>266.0</td>
</tr>
<tr>
<td>A41-TBP @ .90 VOL [F]</td>
<td>284.0</td>
<td>%%%%%%%%%%%%%%%%%</td>
<td>464.0</td>
</tr>
<tr>
<td>A51-TBP @ .10 VOL [F]</td>
<td>302.0</td>
<td>%%%%%%%%%%%%%%%%%</td>
<td>554.0</td>
</tr>
<tr>
<td>A51-TBP @ .90 VOL [F]</td>
<td>302.0</td>
<td>%%%%%%%%%%%%%%%%%</td>
<td>554.0</td>
</tr>
</tbody>
</table>

*****************************************************************
* OBJECTIVE FUNCTION SUMMARY *
**FINAL OBJECTIVE FUNCTION VALUE (PROFIT) [$/HR] = $**

<table>
<thead>
<tr>
<th>STREAM</th>
<th>STD-VOL FLOWS [BBL/DAY]</th>
<th>COLUMN</th>
<th>HEAT DUTY [MMBTU/HR]</th>
</tr>
</thead>
<tbody>
<tr>
<td>STAB</td>
<td></td>
<td>C1</td>
<td></td>
</tr>
<tr>
<td>VAP</td>
<td></td>
<td>C2</td>
<td></td>
</tr>
<tr>
<td>DIST-C4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>LT-ISO</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HV-ISO</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>LT-DIST</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SSFEED</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**OPTIMIZATION SUMMARY REPORT CREATED BY SPEEDUP ON %%%%%%%%**

Page 2 of 3

***************
* VARIABLE SUMMARY *
***************

<table>
<thead>
<tr>
<th>VARIABLE</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>F01 [BBL/DAY]</td>
<td>$%</td>
</tr>
<tr>
<td>F11 [CUFT/HR]</td>
<td>$%</td>
</tr>
<tr>
<td>F12 [BBL/DAY]</td>
<td>$%</td>
</tr>
<tr>
<td>F13 [BBL/DAY]</td>
<td>$%</td>
</tr>
<tr>
<td>F21 [BBL/DAY]</td>
<td>$%</td>
</tr>
<tr>
<td>F22 [BBL/DAY]</td>
<td>$%</td>
</tr>
<tr>
<td>F31 [BBL/DAY]</td>
<td>$%</td>
</tr>
<tr>
<td>F32 [BBL/DAY]</td>
<td>$%</td>
</tr>
<tr>
<td>F41 [BBL/DAY]</td>
<td>$%</td>
</tr>
<tr>
<td>F42 [BBL/DAY]</td>
<td>$%</td>
</tr>
<tr>
<td>F51 [BBL/DAY]</td>
<td>$%</td>
</tr>
<tr>
<td>F52 [BBL/DAY]</td>
<td>$%</td>
</tr>
<tr>
<td>F61 [BBL/DAY]</td>
<td>$%</td>
</tr>
<tr>
<td>F62 [BBL/DAY]</td>
<td>$%</td>
</tr>
<tr>
<td>T01 [F]</td>
<td>$%</td>
</tr>
<tr>
<td>T12 [F]</td>
<td>$%</td>
</tr>
<tr>
<td>T13 [F]</td>
<td>$%</td>
</tr>
</tbody>
</table>
E.10 prop6.inp

The following ASPEN PLUS input code, prop6.inp, contains PROPERTIES PLUS properties information for use with both rtodr6.speedup and rtopt6.speedup.

; Input Summary created by ASPEN PLUS Rel. 9.2-1 at 11:10:58 Tue Jul 30, 1996
; Directory C:\MATT Filename C:\MATT\prop6.inp ;
PROP

TITLE 'STABILIZER-SPLITTER SIMULATION PROPERTIES (PROP6)'

IN-UNITS ENG

DIAGNOSTICS
HISTORY SYS-LEVEL=1 SIM-LEVEL=1 PROP-LEVEL=0 STREAM-LEVEL=0 &
CONV-LEVEL=0 COST-LEVEL=0 ECON-LEVEL=0

SIM-OPTIONS FREE-WATER=NO

DESCRIPTION " PROPERTIES FOR SPEEDUP RUNS STBSPL6*, DREC6*, AND OPT6* "

DATABANKS ASPENPCD / PURE856 / PURECOMP / AQUEOUS / &
SOLIDS / INORGANIC

PROP-SOURCES ASPENPCD / PURE856 / PURECOMP / AQUEOUS / &
SOLIDS / INORGANIC

COMPONENTS
H2 H2 H2 /
METHANE CH4 METHANE /
ETHANE C2H6 ETHANE /
PROPANE C3H8 PROPANE /
IBUTANE C4H10-2 IBUTANE /
BUTANE C4H10-1 BUTANE /
IPENTANE C5H12-2 IPENTANE /
PENTANE C5H12-1 PENTANE /
B45T65 * B45T65 /
B65T85 * B65T85 /
B85T105 * B85T105 /
B105T125 * B105T125 /
B125T145 * B125T145 /
B145T165 * B145T165 /
B165T185 * B165T185 /
B185T205 * B185T205 /
B205T235 * B205T235 /
B235T265 * B235T265 /
B265T295 * B265T295 /
B295T325 * B295T325 /
B325T355 * B325T355 /
B355T395 * B355T395 /
B395T510 * B395T510 /
AIR AIR AIR

PC-USER

PC-DEF API-METH B45T65 NBP=128.49380 GRAV=.64840 &
MW=85.98380
PC-DEF API-METH B65T85 NBP=167.34120 GRAV=.69060 &
MW=89.15430
PC-DEF API-METH B85T105 NBP=203.78650 GRAV=.71370 &
MW=99.91430
PC-DEF API-METH B105T125 NBP=239.16230 GRAV=.7320 &
MW=110.25780
PC-DEF API-METH B125T145 NBP=275.02460 GRAV=.74760 &
MW=120.44870
PC-DEF API-METH B145T165 NBP=310.94660 GRAV=.76280 &
MW=132.08530
PC-DEF API-METH B165T185 NBP=347.01010 GRAV=.77630 &
MW=144.87180
PC-DEF API-METH B185T205 NBP=383.08250 GRAV=.78560 &
MW=160.93490
PC-DEF API-METH B205T235 NBP=428.20310 GRAV=.79940 &
MW=180.13470
PC-DEF API-METH B235T265 NBP=482.06570 GRAV=.81410 &
MW=204.11590
PC-DEF API-METH B265T295 NBP=537.76350 GRAV=.8240 &
MW=236.50410
PC-DEF API-METH B295T325 NBP=590.42290 GRAV=.82590 &
MW=270.94860
PC-DEF API-METH B325T355 NBP=643.56240 GRAV=.83250 &
MW=307.94140
PC-DEF API-METH B355T395 NBP=704.2320 GRAV=.83780 &
MW=354.40350
PC-DEF API-METH B395T510 NBP=786.51950 GRAV=.85560 &
MW=418.92730

PROPERTIES PENG-ROB SYSOPO SOLU-WATER=2

REPORT NOCOSTBLOCK NOUNITS NOUTILITIES NOECONOMIC

PROPERTY-REP NOCOMPS NOPARAMS NOPCES
E.11 rtodr6setup.cmd

The following SPEEDUP commands, rtodr6setup.cmd, are passed to SPEEDUP when the program setup is setting up the rtodr6 data reconciliation simulation.

```
2
new rtodr
store rtodr6
store model6x
store report6y
report
noexecute
opt
run
quit
```

E.12 rtodr6run.cmd

The following SPEEDUP commands, rtodr6run.cmd, are passed to SPEEDUP when the program run is running the rtodr6 data reconciliation simulation.

```
store drpreset
opt
use
run
res drpreset
preset c*
preset e*
preset f*
preset m*
preset r*
end
save oppreset (0W)
delete result drpreset
dump oppreset (=result)
disp
file
rep drec
rep streamsum
```
rep c1
rep c2
global
term
end
quit

E.13  rtopt6setup.cmd

The following SPEEDUP commands, rtopt6setup.cmd, are passed to SPEEDUP when the program setup is setting up the rtopt6 optimization simulation.

2
new rtopt
store rtopt6
store model6x
store report6y
report
noexecute
opt
run
quit

E.14  rtopt6run.cmd

The following SPEEDUP commands, rtopt6run.cmd, are passed to SPEEDUP when the program run is setting up the rtopt6 optimization simulation.

store oppreset
opt
use
run
res oppreset
preset c*
preset e*
preset f*
preset m*
preset r*
end
save drpleset (0W)
delete result oppreset
dump drpreset (=result)
disp
file
rep opt
rep streamsum
rep c1
rep c2
global
term
end
quit
NOTE TO USERS

Page(s) missing in number only; text follows. Microfilmed as received.

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Appendix F

Plant Simulation Code

F.1 plant6.inp

The following ASPEN PLUS input code, textttplant6.inp, performs a steady state plant simulation.

; ; Input Summary created by ASPEN PLUS Rel. 9.2-1 at 13:21:06 Wed May 14, 1997
; Directory D:\ Filename plant6.inp
;
TITLE 'STABILIZER-SPLITTER PLANT SIMULATION'

IN-UNITS ENG VOLUME-FLOW='BBL/DAY' ENTHALPY-FLO='MMBTU/HR' & VOLUME=BBL HEAD=FT HEAT=MMBTU

DEF-STREAMS CONVEN ALL

DIAGNOSTICS
  HISTORY SYS-LEVEL=4 SIM-LEVEL=2 PROP-LEVEL=0 STREAM-LEVEL=1 & CONV-LEVEL=2 COST-LEVEL=0 ECON-LEVEL=0

SIM-OPTIONS
  IN-UNITS ENG
  SIM-OPTIONS FREE-WATER=NO

RUN-CONTROL MAX-TIME=1.00000E+08 MAX-ERRORS=9999 MAX-FORT-ERR=50
DESCRIPTION "
STABILIZER (C1): MODELLED BY RADFRAC WITH 29 STAGES WITH A PUMPAROUND
REBOILER.
SPLITTHER (C2, C4, C5): MODELLED BY PETROFRAC WITH A 24 STAGE MAIN
COLUMN WITH AN EXTERNAL REBOILER, AND TWO 3 STAGE REBOILED
SIDESTRIPPERS (C4 AND C5). EXTERNAL REBOILER CONSISTS OF AN FSPLIT
AND A HEATER.
PROPERTIES: 15 PSEUDO-COMPONENTS, 8 CONVENTIONAL COMPONENTS,
PENG-ROBINSON E.O.S. (N.B. WATER IS NOT USED - NO FREE WATER CALCS).
BASE: MOLE BASIS USED (LMOL/HR)"

DATABANKS ASPENPCD / PURE856 / PURECOMP / AQUEOUS / &
SOLIDS / INORGANIC

PROP-SOURCES ASPENPCD / PURE856 / PURECOMP / AQUEOUS / &
SOLIDS / INORGANIC

COMPONENTS
H2 H2 H2 /
METHANE CH4 METHANE /
ETHANE C2H6 ETHANE /
PROPANE C3H8 PROPANE /
IBUTANE C4H10-2 IBUTANE /
BUTANE C4H10-1 BUTANE /
IPENTANE C5H12-2 IPENTANE /
PENTANE C5H12-1 PENTANE /
B45T65 * B45T65 /
B65T85 * B65T85 /
B85T105 * B85T105 /
B105T125 * B105T125 /
B125T145 * B125T145 /
B145T165 * B145T165 /
B165T185 * B165T185 /
B185T205 * B185T205 /
B205T235 * B205T235 /
B235T265 * B235T265 /
B265T295 * B265T295 /
B295T325 * B295T325 /
B325T355 * B325T355 /
B355T395 * B355T395 /
B395T510 * B395T510

PC-USER
PC-DEF API-METH B45T65 NBP=128.49380 GRAV=.64840 &
MW=85.98380
PC-DEF API-METH B65T85 NBP=167.34120 GRAV=.69060 &
MW=89.15430
PC-DEF API-METH B85T105 NBP=203.78650 GRAV=.71370 &
MW=99.91430
PC-DEF API-METH B105T125 NBP=239.16230 GRAV=.7320 &
MW=110.25780
PC-DEF API-METH B125T145 NBP=275.02460 GRAV=.74760 &
MW=120.44870
PC-DEF API-METH B145T165 NBP=310.94660 GRAV=.76280 &
MW=132.08530
PC-DEF API-METH B165T185 NBP=347.01010 GRAV=.77630 &
MW=144.87180
PC-DEF API-METH B185T205 NBP=383.08250 GRAV=.78560 &
MW=160.93490
PC-DEF API-METH B205T235 NBP=428.20310 GRAV=.79940 &
MW=180.13470
PC-DEF API-METH B235T265 NBP=482.06570 GRAV=.81410 &
MW=204.11590
PC-DEF API-METH B265T295 NBP=537.76350 GRAV=.8240 &
MW=236.50410
PC-DEF API-METH B295T325 NBP=590.42290 GRAV=.82590 &
MW=270.94860
PC-DEF API-METH B325T355 NBP=643.56240 GRAV=.83250 &
MW=307.94140
PC-DEF API-METH B355T395 NBP=704.23200 GRAV=.83780 &
MW=354.40350
PC-DEF API-METH B395T510 NBP=786.51950 GRAV=.85560 &
MW=418.92730

FLOWSHEET
  BLOCK C1 IN=STAB OUT=VAP DIST=C4 SPLITFEED C1RFLX C1REBL
  BLOCK C2C4C5 IN=SPLT C2REBL OUT=LT-ISO C2BOT HV-ISO &
    LT-DIST C2RFLX IC1 IC2
  BLOCK E1 IN=SPLITFEED OUT=SPLIT
  BLOCK F2 IN=C2RBFD OUT=C2REBL
  BLOCK C2SPL1 IN=C2BOT OUT=C2RBFD SSFEED

PROPERTIES PENG-ROB SOLU-WATER=2
PROP-SET RVP REIDVP SUBSTREAM=MIXED
PROP-SET STDVOL VLSTDMX UNITS='BBL/DAY' SUBSTREAM=MIXED PHASE=T
PROP-SET TBP-10 TBPT SUBSTREAM=MIXED LVPCT=10.0
PROP-SET TBP-90 TBPT SUBSTREAM=MIXED LVPCT=90.0

PROP-SET TBUB TBUB SUBSTREAM=MIXED

PROP-SET V-STDVOL VMX UNITS='CUFT/HR' SUBSTREAM=MIXED PHASE=V &
    TEMP=60.0 PRES=14.6960

PROP-SET VOL VMX UNITS='CUFT/HR' SUBSTREAM=MIXED PHASE=T

STREAM C2REBL
    SUBSTREAM MIXED TEMP=683.899910 PRES=35.65810 &
        MOLE-FLOW=1327.2170
    MOLE-FRAC H2 0.0 / METHANE 1.3091E-18 / ETHANE &
        3.9177E-15 / PROPANE 3.4897E-11 / IBUTANE 2.3334E-08 / &
        BUTANE 5.2249E-08 / IPENTANE 1.0680E-06 / PENTANE &
        6.7323E-07 / B4ST65 5.3548E-06 / B6ST85 .000013843 / &
        B8ST105 .000042311 / B10ST125 .000123760 / B12ST145 &
        .000363910 / B14ST165 .00117030 / B16ST185 .00455110 / &
        B18ST205 .0187060 / B20ST235 .1040 / B23ST265 .14430 &
        / B26ST295 .16840 / B29ST325 .17710 / B32ST355 &
        .15840 / B35ST395 .14950 / B39ST510 .073060

STREAM STAB
    SUBSTREAM MIXED TEMP=412.954698 PRES=200.0 &
        MOLE-FLOW=1487.17710
    MOLE-FRAC H2 .000703680 / METHANE .0246830 / ETHANE &
        .0473640 / PROPANE .0387240 / IBUTANE .0535310 / &
        BUTANE .0312790 / IPENTANE .0351930 / PENTANE &
        .0161490 / B4ST65 .0472560 / B6ST85 .0435620 / &
        B8ST105 .0496490 / B10ST125 .0530710 / B12ST145 &
        .0523260 / B14ST165 .0489630 / B16ST185 .0444180 / &
        B18ST205 .041240 / B20ST235 .0607690 / B23ST265 &
        .0537820 / B26ST295 .0598310 / B29ST325 .0626870 / &
        B32ST355 .056050 / B35ST395 .0529210 / B39ST510 &
        .0258480

BLOCK C2SPL1 FSPLIT
    DESCRIPTION "C2 BOTTOMS FLOW SPLITTER"
    MOLE-FLOW C2RBFD 1327.2170

BLOCK E1 HEATER
    IN-UNITS ENG VOLUME-FLOW='BBL/DAY' ENTHALPY-FLD='MMBTU/HR'
    DESCRIPTION "E1 HEAT EXCHANGER"
    PARAM TEMP=479.65650 PRES=34.0
BLOCK F2 HEATER
DESCRIPTION "C2 REBOILER FURNACE"
PARAM TEMP=683.899910 PRES=0.0

BLOCK C1 RADFRAC
SUBOBJECTS PUMPAROUND = C1REBL
DESCRIPTION "STABILISER"
PARAM NSTAGE=29 NPA=1
PUMPAROUND C1REBL 29 29 NPHASE=2 MOLE-FLOW=2005.69940 &
TEMP=586.084880
FEEDS STAB 14 ON-STAGE
PRODUCTS VAP 1 V / DIST-C4 1 L / SPLITFEED 29 L
PSEUDO-STREA C1REBL 1 / C1REBL PA=C1REBL
P-SPEC 1 163.0 / 2 167.0
COL-SPEC QU=.0 DP-COL=6.0 MOLE-RDV=.60262460 &
MOLE-RR=3.15630830
T-EST 1 89.5350 / 2 149.040 / 3 169.260 / 4 182.040 / &
5 192.140 / 6 200.260 / 7 206.640 / 8 211.750 / &
9 216.380 / 10 221.630 / 11 229.350 / 12 243.370 / &
13 275.160 / 14 386.670 / 15 389.440 / 16 391.110 &
/ 17 392.160 / 18 392.890 / 19 393.490 / 20 &
394.060 / 21 394.670 / 22 395.410 / 23 396.360 / &
24 397.680 / 25 399.710 / 26 403.380 / 27 411.850 &
/ 28 436.50 / 29 519.830
L-EST 1 1022.0250 / 2 991.26280 / 3 985.080 / 4 &
974.47260 / 5 962.86240 / 6 955.5350 / 7 949.85040 &
/ 8 942.2590 / 9 928.30430 / 10 900.91910 / 11 &
845.60520 / 12 723.95590 / 13 413.66660 / 14 &
1449.9490 / 15 1500.8610 / 16 1531.4830 / 17 &
1550.3670 / 18 1563.3520 / 19 1573.6410 / 20 &
1583.0950 / 21 1593.0030 / 22 1604.5030 / 23 &
1618.8610 / 24 1637.8240 / 25 1664.3390 / 26 &
1703.9790 / 27 1764.4650 / 28 1818.9030 / 29 &
3205.2810
V-EST 1 173.31230 / 2 1195.3370 / 3 1278.8590 / 4 &
1276.6760 / 5 1262.0680 / 6 1250.4580 / 7 1243.1260 &
/ 8 1237.4460 / 9 1229.8550 / 10 1215.90 / 11 &
1188.5150 / 12 1133.2540 / 13 1011.5520 / 14 &
701.56250 / 15 250.3680 / 16 301.27930 / 17 &
331.90150 / 18 350.78570 / 19 363.77040 / 20 &
374.06010 / 21 383.51360 / 22 393.42180 / 23 &
404.92140 / 24 419.27950 / 25 438.24310 / 26 &
464.75790 / 27 504.39750 / 28 564.88340 / 29 &
619.32170
TRAY-REPORT TRAY-OPTION=ALL-TRAYS
REPORT NOCOMPS NOHYDRAULIC MOENTH NOSPLITS

BLOCK C2C4C5 PETROFRAC
SUBOBJECTS STRIPPER = C4 C5
DESCRIPTION "SPLITTER"
PARAM NPA=0 NSTRIP=2 NSSTRIP=6 NSTAGE=24 HYDRAULIC=NO
FEEDS SPLIT 21 ON-STAGE / C2REBL 24 ON-STAGE
PRODUCTS LT-IS0 1 L / C2B0T 24 L
COL-SPECS CONDENSER=SUBCOOLED REBOILER=NONE-BOTFEED &
   T1=84.7225280 MOLE-D=186.57490 DP-COL=12.70
P-SPEC 1 18.95810 / 2 22.95810
T-EST 1 84.7230 / 2 150.930 / 3 169.420 / 4 181.130 / &
   5 188.750 / 6 194.010 / 7 197.990 / 8 201.440 / &
   9 204.930 / 10 208.970 / 11 214.20 / 12 221.490 / &
  13 232.330 / 14 249.640 / 15 278.020 / 16 320.730 &
   / 17 358.980 / 18 388.210 / 19 415.850 / 20 &
  441.860 / 21 483.390 / 22 531.190 / 23 570.180 / &
  24 626.450
V-EST 1 0.0 / 2 2776.1290 / 3 3094.8350 / 4 3095.9990 &
   / 5 3101.710 / 6 3106.5220 / 7 3108.8040 / 8 &
  3107.4250 / 9 3100.7670 / 10 3086.2130 / 11 &
  3059.6610 / 12 3014.5630 / 13 2939.0650 / 14 &
  2809.8090 / 15 2473.5240 / 16 2206.0180 / 17 &
  2037.2320 / 18 1833.3290 / 19 1747.6360 / 20 &
  1647.220 / 21 1439.3880 / 22 772.39920 / 23 &
  965.84870 / 24 953.74740
L-EST 1 2776.1290 / 2 2908.260 / 3 2909.4240 / 4 &
   2915.1350 / 5 2919.9470 / 6 2922.2290 / 7 2920.850 &
   / 8 2914.1920 / 9 2899.6380 / 10 2873.0860 / 11 &
  2827.9890 / 12 2752.490 / 13 2623.2340 / 14 &
  2410.6880 / 15 2143.1810 / 16 1496.7840 / 17 &
  1408.0990 / 18 1322.4060 / 19 973.77810 / 20 &
  765.94590 / 21 1298.5380 / 22 1491.9880 / 23 &
  1479.8870 / 24 1853.3340
PSEUDO-STREA C2RFLEX STAGE=1
STRIPPER C4 NSTAGE=3 LDRAW=15 VRETURN=14 PRODUCT=HV-IS0 &
   MOLE-DRAW=477.61110 Q-REB=1.90090
STRIPPER C5 NSTAGE=3 LDRAW=18 VRETURN=17 PRODUCT=LT-DIST &
   MOLE-DRAW=248.21130 Q-REB=2.39920
STR-T-EST C4 1 278.790 / C4 2 282.20 / C4 3 292.030 / &
   C5 1 402.780 / C5 2 414.880 / C5 3 429.50
STR-V-EST C4 1 123.70 / C4 2 122.70 / C4 3 123.40 / &
   C5 1 115.20 / C5 2 125.60 / C5 3 130.40
STR-L-EST C4 1 476.60 / C4 2 477.20 / C4 3 353.90 / &
   C5 1 258.60 / C5 2 263.40 / C5 3 133.0
STR-PSEUDO-S C4 IC1 SOURCE=FEED DRAW=15 / C5 IC2 &
SOURCE=FEED DRAW=18
TRAY-REPORT TRAY-OPTION=ALL-TRAYS
REPORT RESULTS NOCOMPS NOHYDRAULIC NOENTH

FORTRAN DATA

F     LOGICAL THERE
DEFINE F01 STREAM-VAR STREAM=STAB SUBSTREAM=MIXED &
      VARIABLE=STDVOL-FLOW
DEFINE F11 STREAM-PROP STREAM=VAP PROPERTY=V-STDVOL
DEFINE F12 STREAM-VAR STREAM=C1RFLX SUBSTREAM=MIXED &
      VARIABLE=STDVOL-FLOW
DEFINE F13 STREAM-VAR STREAM=DIST-C4 SUBSTREAM=MIXED &
      VARIABLE=STDVOL-FLOW
DEFINE F21 STREAM-VAR STREAM=C1REBL SUBSTREAM=MIXED &
      VARIABLE=STDVOL-FLOW
DEFINE F22 STREAM-VAR STREAM=SPLTFEED SUBSTREAM=MIXED &
      VARIABLE=STDVOL-FLOW
DEFINE F31 STREAM-VAR STREAM=LT-ISO SUBSTREAM=MIXED &
      VARIABLE=STDVOL-FLOW
DEFINE F32 STREAM-VAR STREAM=C2RFLX SUBSTREAM=MIXED &
      VARIABLE=STDVOL-FLOW
DEFINE F41 STREAM-VAR STREAM=IC1 SUBSTREAM=MIXED &
      VARIABLE=STDVOL-FLOW
DEFINE F42 STREAM-VAR STREAM=HV-ISO SUBSTREAM=MIXED &
      VARIABLE=STDVOL-FLOW
DEFINE F51 STREAM-VAR STREAM=IC2 SUBSTREAM=MIXED &
      VARIABLE=STDVOL-FLOW
DEFINE F52 STREAM-VAR STREAM=LT-DIST SUBSTREAM=MIXED &
      VARIABLE=STDVOL-FLOW
DEFINE F61 STREAM-VAR STREAM=C2REBL SUBSTREAM=MIXED &
      VARIABLE=STDVOL-FLOW
DEFINE F62 STREAM-VAR STREAM=SSFEED SUBSTREAM=MIXED &
      VARIABLE=STDVOL-FLOW
DEFINE T01 STREAM-VAR STREAM=STAB SUBSTREAM=MIXED &
      VARIABLE=TEMP
DEFINE T12 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
      SENTENCE=PROFILE ID1=2
DEFINE T13 STREAM-VAR STREAM=DIST-C4 SUBSTREAM=MIXED &
      VARIABLE=TEMP
DEFINE T21 STREAM-VAR STREAM=SPLTFEED SUBSTREAM=MIXED &
      VARIABLE=TEMP
DEFINE T22 STREAM-VAR STREAM=C1REBL SUBSTREAM=MIXED &
      VARIABLE=TEMP
DEFINE T23 STREAM-VAR STREAM=SPLT SUBSTREAM=MIXED &
VARIABLE=TEMP
DEFINE T31 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
   SENTENCE=PROFILE ID1=2
DEFINE T32 STREAM-VAR STREAM=LT-ISO SUBSTREAM=MIXED &
   VARIABLE=TEMP
DEFINE T41 STREAM-VAR STREAM=IC1 SUBSTREAM=MIXED &
   VARIABLE=TEMP
DEFINE T42 STREAM-VAR STREAM=HV-ISO SUBSTREAM=MIXED &
   VARIABLE=TEMP
DEFINE T51 STREAM-VAR STREAM=IC2 SUBSTREAM=MIXED &
   VARIABLE=TEMP
DEFINE T52 STREAM-VAR STREAM=LT-DIST SUBSTREAM=MIXED &
   VARIABLE=TEMP
DEFINE T61 STREAM-VAR STREAM=SSFEED SUBSTREAM=MIXED &
   VARIABLE=TEMP
DEFINE T62 STREAM-VAR STREAM=C2REBL SUBSTREAM=MIXED &
   VARIABLE=TEMP
C WRITE TO FILE MEASURED VARIABLES VALUES AFTER DATA REC
F WRITE(NTERM,*) '+++ PLANT RESULTS FORTRAN STARTED +++'
F INQUIRE (FILE='PLVARS.DAT', EXIST= THERE)
F IF ( THERE ) THEN
F   WRITE(NTERM,*) '*** ERROR: PLVARS.DAT ALREADY EXISTS ***'
F   WRITE(NRPT,*) '*** ERROR: PLVARS.DAT ALREADY EXISTED ***'
F   WRITE(NHSTRY,*) '*** ERROR: PLVARS.DAT ALREADY EXISTS ***'
F GO TO 90
F END IF
F OPEN (UNIT=63, STATUS='NEW', FILE='PLVARS.DAT')
F WRITE(63,100) 'F01', F01
F WRITE(63,100) 'F11', F11
F WRITE(63,100) 'F12', F12
F WRITE(63,100) 'F13', F13
F WRITE(63,100) 'F21', F21
F WRITE(63,100) 'F22', F22
F WRITE(63,100) 'F31', F31
F WRITE(63,100) 'F32', F32
F WRITE(63,100) 'F41', F41
F WRITE(63,100) 'F42', F42
F WRITE(63,100) 'F51', F51
F WRITE(63,100) 'F52', F52
F WRITE(63,100) 'F61', F61
F WRITE(63,100) 'F62', F62
F WRITE(63,100) 'T01', T01
F WRITE(63,100) 'T12', T12
F WRITE(63,100) 'T13', T13
F WRITE(63,100) 'T21', T21
F WRITE(63,100) 'T22', T22
F WRITE(63,100) 'T23', T23
F WRITE(63,100) 'T31', T31
F WRITE(63,100) 'T32', T32
F WRITE(63,100) 'T41', T41
F WRITE(63,100) 'T42', T42
F WRITE(63,100) 'T51', T51
F WRITE(63,100) 'T52', T52
F WRITE(63,100) 'T61', T61
F WRITE(63,100) 'T62', T62
F CLOSE (UNIT=63)
F 90 WRITE( NTERM,* ) '+++ PLANT RESULTS FORTRAN COMPLETED +++'
C FORMAT STATEMENTS
F 100 FORMAT(A13, 2X, E15.8)
    EXECUTE LAST

FORTRAN SPCSET
F     LOGICAL THERE
F     DEFINE STABF STREAM-VAR STREAM=STAB SUBSTREAM=MIXED &
F     VARIABLE=MOLE-FLOW
F     DEFINE STABT STREAM-VAR STREAM=STAB SUBSTREAM=MIXED &
F     VARIABLE=TEMP
F     DEFINE STABP STREAM-VAR STREAM=STAB SUBSTREAM=MIXED &
F     VARIABLE=PRES
F     DEFINE STBZ1 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
F     COMPONENT=H2
F     DEFINE STBZ2 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
F     COMPONENT=METHANE
F     DEFINE STBZ3 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
F     COMPONENT=ETHANE
F     DEFINE STBZ4 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
F     COMPONENT=PROPANE
F     DEFINE STBZ5 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
F     COMPONENT=IBUTANE
F     DEFINE STBZ6 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
F     COMPONENT=IBUTANE
F     DEFINE STBZ7 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
F     COMPONENT=IPENTANE
F     DEFINE STBZ8 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
F     COMPONENT=PENTANE
F     DEFINE STBZ9 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
F     COMPONENT=B4ST85
F     DEFINE STBZ10 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
F     COMPONENT=B6ST85
F     DEFINE STBZ11 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED &
COMPONENT=B85T105
DEFINE STBZ12 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED & COMPONENT=B105T125
DEFINE STBZ13 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED & COMPONENT=B125T145
DEFINE STBZ14 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED & COMPONENT=B145T165
DEFINE STBZ15 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED & COMPONENT=B165T185
DEFINE STBZ16 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED & COMPONENT=B185T205
DEFINE STBZ17 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED & COMPONENT=B205T235
DEFINE STBZ18 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED & COMPONENT=B235T265
DEFINE STBZ19 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED & COMPONENT=B265T295
DEFINE STBZ20 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED & COMPONENT=B295T325
DEFINE STBZ21 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED & COMPONENT=B325T355
DEFINE STBZ22 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED & COMPONENT=B355T395
DEFINE STBZ23 MOLE-FRAC STREAM=STAB SUBSTREAM=MIXED & COMPONENT=B395T510
DEFINE C2RBFD BLOCK-VAR BLOCK=C2SPL1 SENTENCE=MOLE-FLOW & VARIABLE=FLOW ID1=C2RBFD
DEFINE C2RBFD BLOCK-VAR STREAM=C2REBL SUBSTREAM=MIXED & VARIABLE=FLOW
DEFINE C2RBTF BLOCK-VAR BLOCK=F2 PARAM & VARIABLE=TEMP SENTENCE=PARAM
DEFINE C2RBTF BLOCK-VAR STREAM=C2REBL SUBSTREAM=MIXED & VARIABLE=TEMP
DEFINE C2RBP1 BLOCK-VAR BLOCK=F2 PARAM & VARIABLE=PRES SENTENCE=PARAM
DEFINE C2RBP2 BLOCK-VAR STREAM=C2REBL SUBSTREAM=MIXED & VARIABLE=PRES
DEFINE C2RZ1 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=H2
DEFINE C2RZ2 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=METHANE
DEFINE C2RZ3 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=ETHANE
DEFINE C2RZ4 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=PROPANE
DEFINE C2RZ5 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=IBUTANE
DEFINE C2RZ6 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=BUTANE
DEFINE C2RZ7 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=IPENTANE
DEFINE C2RZ8 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=PENTANE
DEFINE C2RZ9 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=B10ST125
DEFINE C2RZ10 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=B125T145
DEFINE C2RZ11 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=B145T165
DEFINE C2RZ12 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=B165T185
DEFINE C2RZ13 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=B185T205
DEFINE C2RZ14 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=B205T235
DEFINE C2RZ15 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=B235T265
DEFINE C2RZ16 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=B255T295
DEFINE C2RZ17 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=B295T325
DEFINE C2RZ18 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=B325T355
DEFINE C2RZ19 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=B355T395
DEFINE C2RZ20 MOLE-FRAC STREAM=C2REBL SUBSTREAM=MIXED & COMPONENT=B395T510
DEFINE EIT BLOCK-VAR BLOCK=E1 VARIABLE=TEMP SENTENCE=PARAM
DEFINE E1P BLOCK-VAR BLOCK=E1 VARIABLE=PRES SENTENCE=PARAM
DEFINE C1RR BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-RR & SENTENCE=COL-SPECS
DEFINE C1RDV BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-R DV & SENTENCE=COL-SPECS
DEFINE C1RBFL BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
SENTENCE=PUMPAROUND ID1=C1REBL
DEFINE C1RBT BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=PUMPAROUND ID1=C1REBL
DEFINE C1P1 BLOCK-VAR BLOCK=C1 VARIABLE=PRES &
   SENTENCE=P-SPEC ID1=1
DEFINE C1P2 BLOCK-VAR BLOCK=C1 VARIABLE=PRES &
   SENTENCE=P-SPEC ID1=2
DEFINE C1D0 BLOCK-VAR BLOCK=C1 VARIABLE=DP-COL &
   SENTENCE=COL-SPECS
DEFINE C2MD BLOCK-VAR BLOCK=C2C4C5 VARIABLE=MOLE-D &
   SENTENCE=COL-SPECS
DEFINE C2SC BLOCK-VAR BLOCK=C2C4C5 VARIABLE=T1 &
   SENTENCE=COL-SPECS
DEFINE C2P1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=PRES &
   SENTENCE=P-SPEC ID1=1
DEFINE C2P2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=PRES &
   SENTENCE=P-SPEC ID1=2
DEFINE C2DP BLOCK-VAR BLOCK=C2C4C5 VARIABLE=DP-COL &
   SENTENCE=COL-SPECS
DEFINE C2IC1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=MOLE-DRAW &
   SENTENCE=STRIPPER ID1=C4
DEFINE C2IC2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=MOLE-DRAW &
   SENTENCE=STRIPPER ID1=C5
DEFINE C4QN BLOCK-VAR BLOCK=C2C4C5 VARIABLE=Q-REB &
   SENTENCE=STRIPPER ID1=C4
DEFINE CSQN BLOCK-VAR BLOCK=C2C4C5 VARIABLE=Q-REB &
   SENTENCE=STRIPPER ID1=C5
DEFINE C1T1 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=T-EST &
   ID1=1
DEFINE C1T2 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=T-EST &
   ID1=2
DEFINE C1T3 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=T-EST &
   ID1=3
DEFINE C1T4 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=T-EST &
   ID1=4
DEFINE C1T5 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=T-EST &
   ID1=5
DEFINE C1T6 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=T-EST &
   ID1=6
DEFINE C1T7 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=T-EST &
   ID1=7
DEFINE C1T8 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=T-EST &
   ID1=8
DEFINE C1T9 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP SENTENCE=T-EST &
   ID1=9
DEFINE C1T10 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=10
DEFINE C1T11 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=11
DEFINE C1T12 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=12
DEFINE C1T13 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=13
DEFINE C1T14 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=14
DEFINE C1T15 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=15
DEFINE C1T16 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=16
DEFINE C1T17 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=17
DEFINE C1T18 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=18
DEFINE C1T19 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=19
DEFINE C1T20 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=20
DEFINE C1T21 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=21
DEFINE C1T22 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=22
DEFINE C1T23 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=23
DEFINE C1T24 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=24
DEFINE C1T25 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=25
DEFINE C1T26 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=26
DEFINE C1T27 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=27
DEFINE C1T28 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=28
DEFINE C1T29 BLOCK-VAR BLOCK=C1 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=29
DEFINE C2T1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=1
DEFINE C2T2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
   SENTENCE=T-EST ID1=2
DEFINE C2T3 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
SENTENCE=T-EST ID1=3
DEFINE C2T4 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=4
DEFINE C2T5 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=5
DEFINE C2T6 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=6
DEFINE C2T7 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=7
DEFINE C2T8 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=8
DEFINE C2T9 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=9
DEFINE C2T10 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=10
DEFINE C2T11 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=11
DEFINE C2T12 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=12
DEFINE C2T13 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=13
DEFINE C2T14 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=14
DEFINE C2T15 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=15
DEFINE C2T16 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=16
DEFINE C2T17 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=17
DEFINE C2T18 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=18
DEFINE C2T19 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=19
DEFINE C2T20 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=20
DEFINE C2T21 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=21
DEFINE C2T22 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=22
DEFINE C2T23 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=23
DEFINE C2T24 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=T-EST ID1=24
DEFINE C4T1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP &
  SENTENCE=STR-T-EST ID1=C4 ID2=1
DEFINE C4T2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP & SENTENCE=STR-T-EST ID1=C4 ID2=2
DEFINE C4T3 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP & SENTENCE=STR-T-EST ID1=C4 ID2=3
DEFINE CST1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP & SENTENCE=STR-T-EST ID1=C5 ID2=1
DEFINE CST2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP & SENTENCE=STR-T-EST ID1=C5 ID2=2
DEFINE CST3 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=TEMP & SENTENCE=STR-T-EST ID1=C5 ID2=3
DEFINE C1L1 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & SENTENCE=L-EST ID1=1
DEFINE C1L2 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & SENTENCE=L-EST ID1=2
DEFINE C1L3 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & SENTENCE=L-EST ID1=3
DEFINE C1L4 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & SENTENCE=L-EST ID1=4
DEFINE C1L5 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & SENTENCE=L-EST ID1=5
DEFINE C1L6 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & SENTENCE=L-EST ID1=6
DEFINE C1L7 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & SENTENCE=L-EST ID1=7
DEFINE C1L8 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & SENTENCE=L-EST ID1=8
DEFINE C1L9 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & SENTENCE=L-EST ID1=9
DEFINE C1L10 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & SENTENCE=L-EST ID1=10
DEFINE C1L11 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & SENTENCE=L-EST ID1=11
DEFINE C1L12 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & SENTENCE=L-EST ID1=12
DEFINE C1L13 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & SENTENCE=L-EST ID1=13
DEFINE C1L14 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & SENTENCE=L-EST ID1=14
DEFINE C1L15 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & SENTENCE=L-EST ID1=15
DEFINE C1L16 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & SENTENCE=L-EST ID1=16
DEFINE C1L17 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW & SENTENCE=L-EST ID1=17
DEFINE C1L18 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
SENTENCE=L-EST ID1=18
DEFINE C1L19 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=19
DEFINE C1L20 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=20
DEFINE C1L21 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=21
DEFINE C1L22 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=22
DEFINE C1L23 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=23
DEFINE C1L24 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=24
DEFINE C1L25 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=25
DEFINE C1L26 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=26
DEFINE C1L27 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=27
DEFINE C1L28 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=28
DEFINE C1L29 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=L-EST ID1=29
DEFINE C1V1 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=1
DEFINE C1V2 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=2
DEFINE C1V3 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=3
DEFINE C1V4 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=4
DEFINE C1V5 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=5
DEFINE C1V6 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=6
DEFINE C1V7 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=7
DEFINE C1V8 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=8
DEFINE C1V9 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=9
DEFINE C1V10 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=10
DEFINE C1V11 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
  SENTENCE=V-EST ID1=11
DEFINE C1V12 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
   SENTENCE=V-EST ID1=12
DEFINE C1V13 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
   SENTENCE=V-EST ID1=13
DEFINE C1V14 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
   SENTENCE=V-EST ID1=14
DEFINE C1V15 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
   SENTENCE=V-EST ID1=15
DEFINE C1V16 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
   SENTENCE=V-EST ID1=16
DEFINE C1V17 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
   SENTENCE=V-EST ID1=17
DEFINE C1V18 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
   SENTENCE=V-EST ID1=18
DEFINE C1V19 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
   SENTENCE=V-EST ID1=19
DEFINE C1V20 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
   SENTENCE=V-EST ID1=20
DEFINE C1V21 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
   SENTENCE=V-EST ID1=21
DEFINE C1V22 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
   SENTENCE=V-EST ID1=22
DEFINE C1V23 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
   SENTENCE=V-EST ID1=23
DEFINE C1V24 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
   SENTENCE=V-EST ID1=24
DEFINE C1V25 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
   SENTENCE=V-EST ID1=25
DEFINE C1V26 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
   SENTENCE=V-EST ID1=26
DEFINE C1V27 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
   SENTENCE=V-EST ID1=27
DEFINE C1V28 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
   SENTENCE=V-EST ID1=28
DEFINE C1V29 BLOCK-VAR BLOCK=C1 VARIABLE=MOLE-FLOW &
   SENTENCE=V-EST ID1=29
DEFINE C2L1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
   SENTENCE=L-EST ID1=1
DEFINE C2L2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
   SENTENCE=L-EST ID1=2
DEFINE C2L3 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
   SENTENCE=L-EST ID1=3
DEFINE C2L4 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
   SENTENCE=L-EST ID1=4
DEFINE C2L5 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=5
DEFINE C2L6 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=6
DEFINE C2L7 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=7
DEFINE C2L8 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=8
DEFINE C2L9 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=9
DEFINE C2L10 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=10
DEFINE C2L11 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=11
DEFINE C2L12 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=12
DEFINE C2L13 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=13
DEFINE C2L14 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=14
DEFINE C2L15 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=15
DEFINE C2L16 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=16
DEFINE C2L17 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=17
DEFINE C2L18 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=18
DEFINE C2L19 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=19
DEFINE C2L20 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=20
DEFINE C2L21 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=21
DEFINE C2L22 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=22
DEFINE C2L23 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=23
DEFINE C2L24 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=L-EST ID1=24
DEFINE C2V1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=V-EST ID1=1
DEFINE C2V2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=V-EST ID1=2
DEFINE C2V3 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SENTENCE=V-EST ID1=3
SEN TENCE=STR-L-EST ID1=C4 ID2=2
DEFINE C4L3 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SEN TENCE=STR-L-EST ID1=C4 ID2=3
DEFINE C5L1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SEN TENCE=STR-L-EST ID1=C5 ID2=1
DEFINE C5L2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SEN TENCE=STR-L-EST ID1=C5 ID2=2
DEFINE C5L3 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SEN TENCE=STR-L-EST ID1=C5 ID2=3
DEFINE C4V1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SEN TENCE=STR-V-EST ID1=C4 ID2=1
DEFINE C4V2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SEN TENCE=STR-V-EST ID1=C4 ID2=2
DEFINE C4V3 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SEN TENCE=STR-V-EST ID1=C4 ID2=3
DEFINE C5V1 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SEN TENCE=STR-V-EST ID1=C5 ID2=1
DEFINE C5V2 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SEN TENCE=STR-V-EST ID1=C5 ID2=2
DEFINE C5V3 BLOCK-VAR BLOCK=C2C4C5 VARIABLE=FLOW &
SEN TENCE=STR-V-EST ID1=C5 ID2=3
C READ PLANT SPECIFICATIONS FROM FILE
F WRITE(NTERM,*) '+++ PLANT SPECIFICATION FORTRAN STARTED +++'
F INQUIRE (FILE='ROSMST.DAT', EXIST=THERE)
F IF (.NOT.THERE) THEN
F WRITE(NTERM,*) '+++ ERROR: ROSMST.DAT DOES NOT EXIST +++'
F WRITE(NRPT,*) '+++ ERROR: ROSMST.DAT WAS NOT FOUND +++'
F WRITE(NHSTRY,*) '+++ ERROR: ROSMST.DAT DID NOT EXIST +++'
F GO TO 92
F END IF
F OPEN (UNIT=63, STATUS='OLD', FILE='ROSMST.DAT')
C STAB STREAM SPECIFICATIONS
F READ(63,100) STABF
F READ(63,100) STABT
F READ(63,100) STABP
F READ(63,100) STBZ1
F READ(63,100) STBZ2
F READ(63,100) STBZ3
F READ(63,100) STBZ4
F READ(63,100) STBZ5
F READ(63,100) STBZ6
F READ(63,100) STBZ7
F READ(63,100) STBZ8
F READ(63,100) STBZ9
F READ(63,100) STBZ10
F READ(63,100) STBZ11
F READ(63,100) STBZ12
F READ(63,100) STBZ13
F READ(63,100) STBZ14
F READ(63,100) STBZ15
F READ(63,100) STBZ16
F READ(63,100) STBZ17
F READ(63,100) STBZ18
F READ(63,100) STBZ19
F READ(63,100) STBZ20
F READ(63,100) STBZ21
F READ(63,100) STBZ22
F READ(63,100) STBZ23
C C2REL STREAM ESTIMATIONS
F READ(63,100) C2RBF1
F C2RBF2 = C2RBF1
F READ(63,100) C2RBT1
F C2RBT2 = C2RBT1
F READ(63,100) C2RBP1
F C2RBP2 = C2RBP1
F READ(63,100) C2RZ1
F READ(63,100) C2RZ2
F READ(63,100) C2RZ3
F READ(63,100) C2RZ4
F READ(63,100) C2RZ5
F READ(63,100) C2RZ6
F READ(63,100) C2RZ7
F READ(63,100) C2RZ8
F READ(63,100) C2RZ9
F READ(63,100) C2RZ10
F READ(63,100) C2RZ11
F READ(63,100) C2RZ12
F READ(63,100) C2RZ13
F READ(63,100) C2RZ14
F READ(63,100) C2RZ15
F READ(63,100) C2RZ16
F READ(63,100) C2RZ17
F READ(63,100) C2RZ18
F READ(63,100) C2RZ19
F READ(63,100) C2RZ20
F READ(63,100) C2RZ21
F READ(63,100) C2RZ22
F READ(63,100) C2RZ23
C E1 HEATER SPECIFICATIONS
F READ(63,100) E1T
READ(63,100) E1P
C1 COLUMN SPECIFICATIONS
READ(63,100) C1RR
READ(63,100) C1RDV
READ(63,100) C1RBFL
READ(63,100) C1RBT
READ(63,100) C1DP
READ(63,100) C1P1
READ(63,100) C1P2
C2 COLUMN SPECIFICATIONS
READ(63,100) C2MD
READ(63,100) C2SC
READ(63,100) C2DP
READ(63,100) C2P1
READ(63,100) C2P2
READ(63,100) C2IC1
READ(63,100) C2IC2
C4 COLUMN SPECIFICATIONS
READ(63,100) C4QN
C5 COLUMN SPECIFICATIONS
READ(63,100) C5QN
C1 TEMPERATURE PROFILE
READ(63,100) C1T1
READ(63,100) C1T2
READ(63,100) C1T3
READ(63,100) C1T4
READ(63,100) C1T5
READ(63,100) C1T6
READ(63,100) C1T7
READ(63,100) C1T8
READ(63,100) C1T9
READ(63,100) C1T10
READ(63,100) C1T11
READ(63,100) C1T12
READ(63,100) C1T13
READ(63,100) C1T14
READ(63,100) C1T15
READ(63,100) C1T16
READ(63,100) C1T17
READ(63,100) C1T18
READ(63,100) C1T19
READ(63,100) C1T20
READ(63,100) C1T21
READ(63,100) C1T22
READ(63,100) C1T23
C2 TEMPERATURE PROFILE
F READ(63,100) C2T1
F READ(63,100) C2T2
F READ(63,100) C2T3
F READ(63,100) C2T4
F READ(63,100) C2T5
F READ(63,100) C2T6
F READ(63,100) C2T7
F READ(63,100) C2T8
F READ(63,100) C2T9
F READ(63,100) C2T10
F READ(63,100) C2T11
F READ(63,100) C2T12
F READ(63,100) C2T13
F READ(63,100) C2T14
F READ(63,100) C2T15
F READ(63,100) C2T16
F READ(63,100) C2T17
F READ(63,100) C2T18
F READ(63,100) C2T19
F READ(63,100) C2T20
F READ(63,100) C2T21
F READ(63,100) C2T22
F READ(63,100) C2T23
F READ(63,100) C2T24
C C4 TEMPERATURE PROFILE
F READ(63,100) C4T1
F READ(63,100) C4T2
F READ(63,100) C4T3
C C5 TEMPERATURE PROFILE
F READ(63,100) C5T1
F READ(63,100) C5T2
F READ(63,100) C5T3
C C1 LIQUID AND VAPOUR FLOW PROFILES
F READ(63,100) C1L1
F READ(63,100) C1L2
F READ(63,100) C1L3
F READ(63,100) C1L4
F READ(63,100) C1L5
F READ(63, 100) C1L6
F READ(63, 100) C1L7
F READ(63, 100) C1L8
F READ(63, 100) C1L9
F READ(63, 100) C1L10
F READ(63, 100) C1L11
F READ(63, 100) C1L12
F READ(63, 100) C1L13
F READ(63, 100) C1L14
F READ(63, 100) C1L15
F READ(63, 100) C1L16
F READ(63, 100) C1L17
F READ(63, 100) C1L18
F READ(63, 100) C1L19
F READ(63, 100) C1L20
F READ(63, 100) C1L21
F READ(63, 100) C1L22
F READ(63, 100) C1L23
F READ(63, 100) C1L24
F READ(63, 100) C1L25
F READ(63, 100) C1L26
F READ(63, 100) C1L27
F READ(63, 100) C1L28
F READ(63, 100) C1L29
F READ(63, 100) C1V1
F READ(63, 100) C1V2
F READ(63, 100) C1V3
F READ(63, 100) C1V4
F READ(63, 100) C1V5
F READ(63, 100) C1V6
F READ(63, 100) C1V7
F READ(63, 100) C1V8
F READ(63, 100) C1V9
F READ(63, 100) C1V10
F READ(63, 100) C1V11
F READ(63, 100) C1V12
F READ(63, 100) C1V13
F READ(63, 100) C1V14
F READ(63, 100) C1V15
F READ(63, 100) C1V16
F READ(63, 100) C1V17
F READ(63, 100) C1V18
F READ(63, 100) C1V19
F READ(63, 100) C1V20
F READ(63, 100) C1V21
F READ(63,100) C1V22
F READ(63,100) C1V23
F READ(63,100) C1V24
F READ(63,100) C1V25
F READ(63,100) C1V26
F READ(63,100) C1V27
F READ(63,100) C1V28
F READ(63,100) C1V29
C  C2 LIQUID AND VAPOUR FLOW PROFILES
F READ(63,100) C2L1
F READ(63,100) C2L2
F READ(63,100) C2L3
F READ(63,100) C2L4
F READ(63,100) C2L5
F READ(63,100) C2L6
F READ(63,100) C2L7
F READ(63,100) C2L8
F READ(63,100) C2L9
F READ(63,100) C2L10
F READ(63,100) C2L11
F READ(63,100) C2L12
F READ(63,100) C2L13
F READ(63,100) C2L14
F READ(63,100) C2L15
F READ(63,100) C2L16
F READ(63,100) C2L17
F READ(63,100) C2L18
F READ(63,100) C2L19
F READ(63,100) C2L20
F READ(63,100) C2L21
F READ(63,100) C2L22
F READ(63,100) C2L23
F READ(63,100) C2L24
F READ(63,100) C2V1
F READ(63,100) C2V2
F READ(63,100) C2V3
F READ(63,100) C2V4
F READ(63,100) C2V5
F READ(63,100) C2V6
F READ(63,100) C2V7
F READ(63,100) C2V8
F READ(63,100) C2V9
F READ(63,100) C2V10
F READ(63,100) C2V11
F READ(63,100) C2V12
F  READ(63,100) C2V13
F  READ(63,100) C2V14
F  READ(63,100) C2V15
F  READ(63,100) C2V16
F  READ(63,100) C2V17
F  READ(63,100) C2V18
F  READ(63,100) C2V19
F  READ(63,100) C2V20
F  READ(63,100) C2V21
F  READ(63,100) C2V22
F  READ(63,100) C2V23
F  READ(63,100) C2V24
C  C4 LIQUID AND VAPOUR FLOW PROFILES
F  READ(63,100) C4L1
F  READ(63,100) C4L2
F  READ(63,100) C4L3
F  READ(63,100) C4V1
F  READ(63,100) C4V2
F  READ(63,100) C4V3
F  READ(63,100) C5L1
F  READ(63,100) C5L2
F  READ(63,100) C5L3
F  READ(63,100) C5V1
F  READ(63,100) C5V2
F  READ(63,100) C5V3
F  CLOSE (UNIT=63)
F  WRITE(NTERM,*), 'ROSMST.DAT READ SUCCESSFULLY'
F  92 WRITE(NTERM,*), '+++ PLANT SPECIFICATION FORTRAN COMPLETED +++'
C FORMAT STATEMENTS
F  100 FORMAT(15X, E15.8)
EXECUTE FIRST

CONV-OPTIONS
  PARAM TRACEOPT=GRADUAL CHECKSEQ=YES

CONVERGENCE C2REBL WEGSTEIN
  DESCRIPTION "C2 REBOILER TEAR STREAM"
  BLOCK-OPTION RESTART=YES
  TEAR C2REBL

REPORT NOINSERT NOADA NOSENSITIVIT NOPROPERTYS NOCOSTBLOCK &
  NOUNITS NOUNILITIES NOECONOMIC

BLOCK-REPORT NOSORT NOTOTAL NOINPUT
F.2 randdata.f

The following FORTRAN77 randdata.f. adds normally distributed random noise to the measured plant data. This program requires the NAG Library FORTRAN Routines.

C $\text{RANDDATA.F - ROUTINE FOR ADDING NORMALLY DISTRIBUTED NOISE TO DATA}$
C $\text{C}$
C $\text{NOTE: This routine uses NAG Library Routines, Compile on Cape with the}$
C $\text{command line: f77 randdata.f -lnag}$
C $\text{C}$
C $\text{DECLARATIONS:}$
C $\text{INTEGER M, NPTS}$
C $\text{DOUBLE PRECISION V(28), RV(28), SV(28)}$
C $\text{CHARACTER *13 VLAB(28)}$
C $\text{LOGICAL THERE}$
C $\text{C}$
C $\text{External Functions:}$
C $\text{DOUBLE PRECISION G05DDF}$
C $\text{EXTERNAL G05DDF}$
C $\text{C}$
C $\text{External Subroutines:}$
C $\text{EXTERNAL G05CBF}$
C $\text{C}$
C $\text{Set Up Variables:}$
C $\text{NPTS=28}$
C $\text{WRITE (*,*)) >>>RANDDATA CALLED'}$
C $\text{C}$
C $\text{READ IN DATA:}$
C $\text{C}$
C $\text{Read in PLVARS.DAT}$
C $\text{INQUIRE (FILE='PLVARS.DAT', EXIST= THERE)}$
C $\text{IF (.NOT. THERE) THEN}$
C $\text{GO TO 915}$
C $\text{ENDIF}$
C $\text{OPEN (UNIT=50, STATUS='OLD', ERR=910, FILE='PLVARS.DAT')}$
C $\text{REWIND (UNIT=50)}$
C $\text{DO 20 M=1,NPTS}$
C $\text{READ (50,100,ERR=900,END=905) VLAB(M), V(M)}$
20 CONTINUE
   CLOSE (UNIT=50)
C Read in RVARNC.DAT
   INQUIRE (FILE='RVARNC.DAT', EXIST= THERE)
   IF (.NOT. THERE) THEN
      GO TO 916
   ENDIF
   OPEN (UNIT=50, STATUS='OLD', ERR=910, FILE='RVARNC.DAT')
   REWIND (UNIT=50)
   DO 25 M=1,NPTS
      READ (50,110,ERR=902,END=906) SV(M)
   25 CONTINUE
   CLOSE (UNIT=50)
C Main Program:
   CALL G05CBF(O)
   DO 30 M=1,NPTS
      RV(M) = V(M) + G05DDF(O, SV(M))
   30 CONTINUE
C Write Out Data:
   INQUIRE (FILE='IMEAS.DAT', EXIST= THERE)
   IF ( THER E) THEN
      GO TO 920
   ENDIF
   OPEN (UNIT=51, STATUS='NEW', ERR=910, FILE='IMEAS.DAT')
   WRITE(*,107) 'VARIABLE', 'OLD VALUE', 'VALUE WITH NOISE'
   DO 40 M=1,NPTS
      WRITE(51,100,ERR=901) VLAB(M), RV(M)
   40 CONTINUE
   CLOSE (UNIT=51)
   WRITE ('*,*') '>>RANDDATA - NOISY VARIABLES WRITTEN SUCCESSFULLY'
   GO TO 1000
C Format Statements:
   100 FORMAT(A13, 2X, E15.8)
   105 FORMAT(A13, 2X, E15.8, 2X, E15.8)
   107 FORMAT(A13, 2X, A15, 2X, A17)
   110 FORMAT(15X, E15.8)
C Error Statements:
   900 WRITE(*,*) 'RANDDATA: Error reading PLVARS.DAT line:', M
   GO TO 1000
   901 WRITE(*,*) 'RANDDATA: Error writing IMEAS.DAT line:', M
   GO TO 1000
   902 WRITE(*,*) 'RANDDATA: Error reading RVARNC.DAT line:', M
   GO TO 1000
   905 WRITE(*,*) 'RANDDATA: EOF in PLVARS.DAT reading line: ', M
GO TO 1000
906 WRITE(*,*) 'RANDATA: EOF in RVARNC.DAT reading line: ', M
   GO TO 1000
910 WRITE(*,*) 'RANDATA: Error opening file'
   GO TO 1000
915 WRITE(*,*) 'RANDATA: PLVARS.DAT does not exist'
   GO TO 1000
916 WRITE(*,*) 'RANDATA: RVARNC.DAT does not exist'
   GO TO 1000
920 WRITE(*,*) 'RANDATA: IMEAS.DAT already exists'
   GO TO 1000
1000 WRITE(*,*)
      END