An Optimization Approach for Integrating Planning and CO$_2$ Mitigation in the Power and Refinery Sectors

by

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I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

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ABSTRACT

Climate change is one of the greatest and probably most challenging environmental, social and economical threats facing the world this century. Human activities have altered the chemical composition of the atmosphere through the buildup of significant quantities of greenhouse gases (GHGs), which remain in the atmosphere for long periods of time and intensify the natural greenhouse effect. Increasing concentrations of greenhouse gases, mainly CO_2, are likely to accelerate the rate of climate change. Concerns are growing about how increases in CO_2 caused by human activities are contributing to the natural greenhouse effect and raising the Earth's average temperature.

Electricity generation, especially from fossil fuel, and petroleum industries contribute the most to greenhouse gases emissions in Canada. As of 2004, they contributed to about 37% of total (GHGs). Risks of climate change and subsequent future environmental regulations are pressing electricity and petroleum refining industries to minimize their greenhouse gas emissions, mainly CO_2. Fossil fuel power plants and refineries are now being challenged to comply with the Kyoto protocol by the United Nations Framework Convention and Climate Change (UNFCC). Canada's target is a reduction in CO_2 emissions of 6% from 1990 level.

In this thesis, an optimization approach for integrating planning and CO_2 reduction is developed for electricity and refinery sectors. Three different CO_2 mitigation options are considered in each case. For the electricity sector, these mitigation options were 1) fuel balancing (optimal adjustment of the operation of existing generating stations to reduce CO_2 emissions without making structural changes to the fleet), 2) fuel switching (switching from carbon intensive fuel to less carbon intensive fuel, essentially switching from coal to natural gas) and 3) implementing different technologies for efficiency improvement. The optimization model takes into account meeting electricity demand and achieving a certain CO_2 reduction target at a minimum overall cost. The model was formulated as a Mixed Integer Non Linear Program (MINLP) and was implemented in GAMS (General Algebraic Modeling System). Exact linearization techniques were employed to facilitate solution development. The computer program was capable of determining the best strategy or mix of

strategies to meet a certain CO_2 reduction target at minimum cost. The model was illustrated on a case study for Ontario Power Generation (OPG) fleet. The results showed that for 1% CO_2 reduction target, only fuel balancing need to be applied and even a decrease of about 1.3% in overall cost was obtained. The optimizer chose to increase production from all non fossil fuel power plants and to decrease production from natural gas power plant. This is because natural gas is the most expensive fuel that OPG uses. For higher reduction targets, it was necessary to implement fuel switching. For 30% reduction, for example, 11 boilers out of 27 (4 are already natural gas) are switched from coal to natural gas and the cost increases by about 13%. Applying efficiency improvement technologies such as installing new turbine blades was a good option only at small reduction targets. As the reduction target increases, the optimizer chose not to implement efficiency improvement technologies and only fuel switching was the best option to select in addition to fuel balancing.

For the refinery sector, a similar strategy was applied. An optimization model was developed to maximize profit from selling final products and to meet a given CO_2 reduction target with products demand and specifications. Three CO_2 mitigation options were considered and these were: 1) balancing that implies the increase in production from units that emit less CO_2 emissions provided that demand is met, 2) fuel switching that involves switching from current carbon intensive fuel to less carbon intensive fuel such as natural gas, 3) implementation of CO_2 capture technologies. Chemical absorption (MEA) process was used as the capture process.

Prior to the development of the refinery planning model, a sub-model was developed for each unit in a refinery layout. Then, the sub-models were integrated into a master planning model to meet final products demand and specifications with the objective of maximizing profit without CO_2 mitigation options. The model was solved first as a Non Linear Program (NLP). Then, binary variables representing the existence or no existence of fuel switching option and CO_2 capture processes were introduced into the model. The model was formulated as a Mixed Integer Non Linear Program (MINLP), coded in GAMS, and applied to different case studies. The results showed that the refinery planning model tends to produce more from the most profitable product, which is gasoline, and chose to blend products into the most

profitable pool unless the demand needs to be satisfied for certain other products. The model, for example, chose to send kerosene from the diesel hydrotreater to the kerosene pool and not to the diesel pool since kerosene has higher selling value than diesel. When CO_2 mitigation options were introduced into the model, only 0.4% CO_2 reduction was achieved by simply decreasing production from the hydrocracker (HC) unit and increasing production from the fluidized catalytic cracking (FCC) unit. This was done because the FCC unit tends to emit less CO_2 compared to the HC unit. At higher reduction target such as 1%, fuel switching was implemented by choosing the FCC to run with natural gas. The profit decreased slightly because of the retrofit cost of switching. It was noticed also that fuel switching can achieve a maximum of 30% reduction in CO_2 emissions. This was achieved by switching all units to run with natural gas that emits less CO_2 emissions. For a reduction target higher than 30%, CO_2 capture technologies need to be applied. For 60% reduction, the optimization chose to switch three units (out of 8) and to capture CO_2 emissions coming from four units. Only the FCC remained unchanged. A decrease in the profit was noticed as the reduction target increases since more units need to be switched and more CO_2 need to be captured. The results showed that adding sequestration cost further decreased the profit. However, it was noticed that the selling price of final products had the most effect on the profit. An increase of 20%, for example, in final products' prices, leads to a 10% increase in profit even when the CO_2 reduction target was as high as 80%. When the retrofit cost for switching and capture was decreased by 30%, the effect on the profit was noticed only at higher reduction targets since more units were switched and more CO_2 capture units were implemented

ACKNOWLEDGEMENTS

**Dedicated to my parents, my wife,
my loving daughter… Lama
and my loving son… Saleh**

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NOMENCLATURE

1. POWER PLANTS

NOTATION

I	Power plant
J	Type of fuel
K	Technology for efficiency improvement
X_{ij}	Binary variable representing fuel selection
y_{ik}	Binary variable representing existence/non existence of efficiency improvement technology k
F	Set of fossil fuel power plants
NF	Set of non fossil fuel power plants
N	Set of nuclear energy power plants
H	Set of hydroelectric energy power plants
A	Set of alternative energy power plants
Z	Annualized capital and operating cost of the fleet of power stations
C_{ij}	Cost of electricity generation if fuel j is used on fossil power plant i ($/MWh)
C_i	Cost of electricity generation from non fossil power plant i ($/MWh)
C_{ik}	Cost of applying improvement technology k in plant i ($/yr)
E_{ij}	Electricity generated from i^{th} fossil fuel boilers operating with j fuel, MWh/yr
E_i^{max}	Maximum electricity generated from i^{th} non fossil, MWh/yr
E_{ij}^{max}	Maximum electricity generated from i^{th} fossil fuel boilers running with j fuel, MWh/yr
E_{ij}^{min}	Minimum electricity production for i^{th} fossil fuel boilers running with j fuel
E_i^{min}	Minimum electricity production for i^{th} non fossil fuel boilers
R_{ij}	Retrofit cost ($/yr)
$\%CO_2$	CO_2 reduction target
ε_{ik}	Gain in efficiency associated with applying technology k on boiler i

ABBREVIATIONS

CCS	Carbon Capture and Storage
GAMS	General Algebraic Modeling System
MEA	Monoethanolamine
MILP	Mixed Integer Linear Programming
MINLP	Mixed Integer Nonlinear Programming
OPG	Ontario Power Generation

2. Oil refinery

I	Set of units (*i*) in the refinery
J	Set of units (*j*) that can send products to unit (*i*)
N	Set of streams (*s*) of unit (*j*) can be sent to unit (*i*)
M	Set of units (*m*) can received stream (*s*) from unit (*i*)
B	Set of final blending units (*b*)
E	Set of unit (*e*) received external feed
S	Set of product streams (*s*) of unit (*i*)
P	Set of properties (*p*) of stream (*s*)
PF	Set of properties (*p*) of feed to unit (*i*)
OV	Set of operating parameter of unit (*i*)
IF	Set of unit (i) furnaces
Indices	
i, j, m, b	For refinery unit
s, n	For stream
p	For property
ov	For operation parameter
w	Fuel type
k	Capture process

Parameters

$Umax_i$	Maximum capacity of unit (i)
TE_s^U , TE_s^L	Upper and lower bounds of the end point (EP) of product s from (CDU) unit, °F
Cp_i	Price of product from unit (i)
Cf_i	Cost of feed to unit (i)
Cp_i	Cost of operating unit (i)
Cs_{iw}	Cost of switching for unit (i) to fuel w
$a_{k,p}$	Coefficient for calculating the property (p) of stream (s)
$TE_{CDU,s}$	End point (EP) cut temperature for product (s) of (CDU) unit
Cut_s	Volume percent vaporized of product (s) at the TE_s
ε_{ik}	Percent of CO_2 capture

Variables

F_i	Volume flowrate of feed to unit (i), BPD
$V_{i,s}$	Volume flowrate of product (s) from unit (i), BPD
$VS_{i,s,m}$	Volume flowrate of stream (s) splited from product $V_{i,s}$ of unit (i) received by unit (m), BPD
$PV_{i,s,p}$	Property (p) of stream (s) from unit (i)
$FP_{i,p}$	Property (p) of feed to unit (i)
X_{iw}	A binary variable represents switching for unit (i) or not
Y_{ik}	A binary variable represents existing or not of capture process k on unit (i)
CO_{2iw}	CO_2 emissions from unit (i) using fuel w (tonne/yr)
$\alpha_i^{released}$	CO_2 emissions to be release to the atmosphere (tonneyr)
α_i^{cap}	CO_2 emissions to be captured (tonne/yr)
Cc_{ik}	Cost of capture by technology k

ABBREVIATIONS

CDU	Crude distillation unit
RDHT	Residual hydrotreater
GOHT	Gas oil hydrotreater
DHT	Diesel hydrotreater

NHT	Naphtha hydrotreater
HC	Hydrocracker
FCC	Fluidized catalytic cracking
Ref	Reformer
LSRN	Light straight run naphtha
TLN	Treated light naphtha
REFORMATE	Reformate
LNHC	Light naphtha from hydrocracker
LNFCC	Light naphtha from FCC
HNFCC	Heavy naphtha from FCC
Kero (CDU)	Kerosene from CDU
KHC	Kerosene from HC
KDHT	Kerosene from diesel hydrotreater
TDiesel	Treated diesel
DHC	Diesel from HC
DGOHT	Diesel from gas oil hydrotreater
LCOFCC	Light cycle oil from FCC
DRDHT	Diesel from residual hydrotreater
HCOFCC	Heavy cycle oil from FCC
LSFO	Low sulfur fuel oil

CHAPTER 1

INTRODUCTION

1.1 Background

The risks associated with global warming or climate change have been the subject of much debate in recent years. Climate change is one of the most significant environmental issues facing the world today (Environment Canada, 2004). While other environmental risks can be highly relevant to specific sectors, climate risk distinguishes itself through its widespread potential for impact on individual companies, across sectors and whole economies. The impact of climate change will be felt directly (in terms of damage to agriculture, forestry and water), and will also have serious consequences for the sectors impacted by policy-driven strategies to mitigate climate change (such as energy, and automobile sectors).

Concern is growing because average global temperatures are rising. This seems to be occurring because of an increase in greenhouse gases, which trap heat in the atmosphere which is called the greenhouse effect (Figure 1.1). The natural greenhouse effect has made life on earth possible. It is the excess of greenhouse gases that causes concern. Modernisation and human activities have led to the risk of global warming, climate change and bad impacts on our quality of life (Environment Canada, 2004).

The international policy response to climate change began with the negotiation of the United Nations Framework Convention on Climate Change (UNFCCC), opened for signature at the 1992 Earth Summit in Rio de Janeiro, Brazil. The UNFCCC's ultimate objective is to achieve stabilization of greenhouse gas concentrations in the atmosphere at a level that would prevent dangerous anthropogenic (human-caused) interference with the climate system. The UNFCCC provides a legal framework for global action to cut
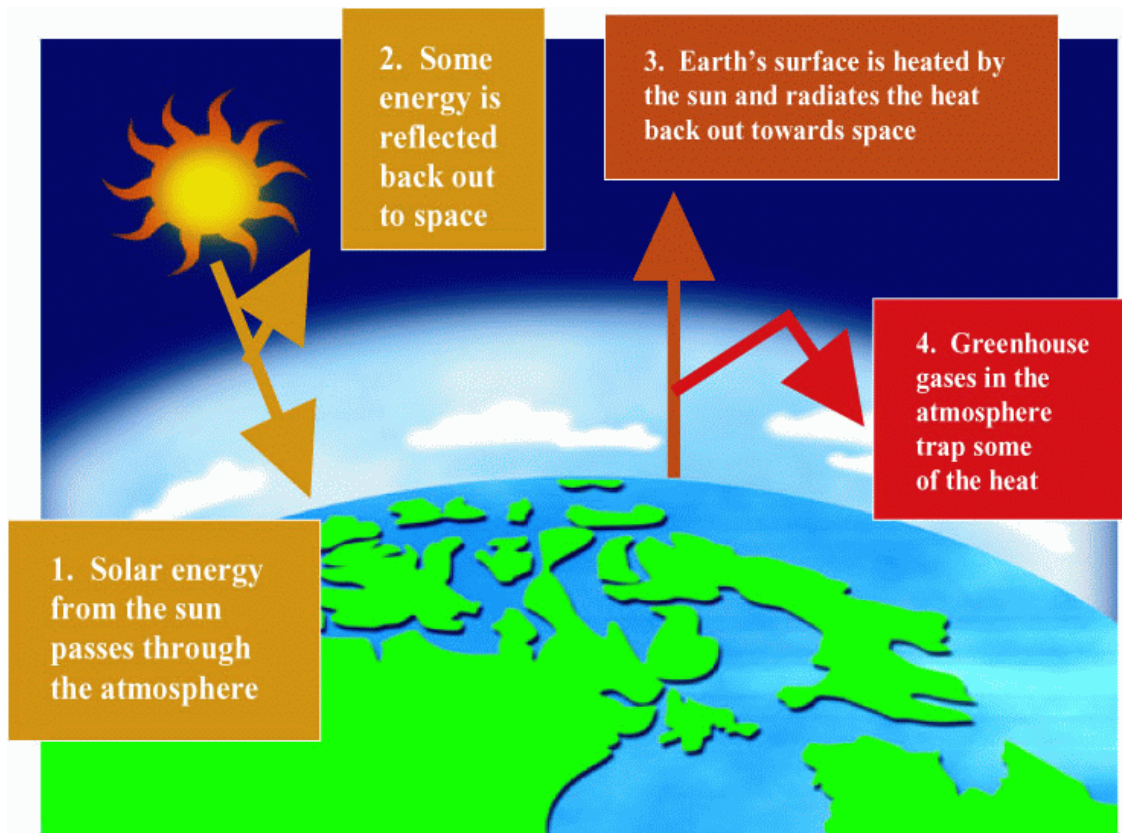
Figure 1.1. Greenhouse gas effect (Environment Canada, 2004)

greenhouse gas (GHG) emissions. In 1995 the Parties to the UNFCCC therefore agreed on the need for an additional treaty to set legally binding targets and timelines for the GHG emissions of industrialized countries. The result was the negotiation, in December 1997, of the Kyoto Protocol to the UNFCCC. The protocol sets legally binding GHG emission targets for each of 38 industrialized countries, including Canada, for the period 2008-2012. The protocol had been ratified by enough countries to enter into force as international law on February 16, 2005. Canada ratified the Kyoto Protocol in December 2002, thereby agreeing to be legally bound to meet a target of reducing its GHG emissions to 6% below the 1990 level during 2008-12.

As a matter of fact, across Canada, greenhouse gas emissions from all sources increased by 26% from 1990 to 2004 (Environment Canada, 2004). Figure 1.2 shows this data. If no action is taken to address climate change ('business as usual' scenario), it is

estimated that Canada's GHG emissions will rise to approximately 809 Mt by 2010, about 35% greater than what they were in 1990. The actual extent of the challenge to meet Kyoto's target should be understood when comparing the predicted value of GHG emissions in 2010 if no action is taken (809 Mt) with the target value of 563 Mt. The actual reduction target is therefore 30% and not 6%.
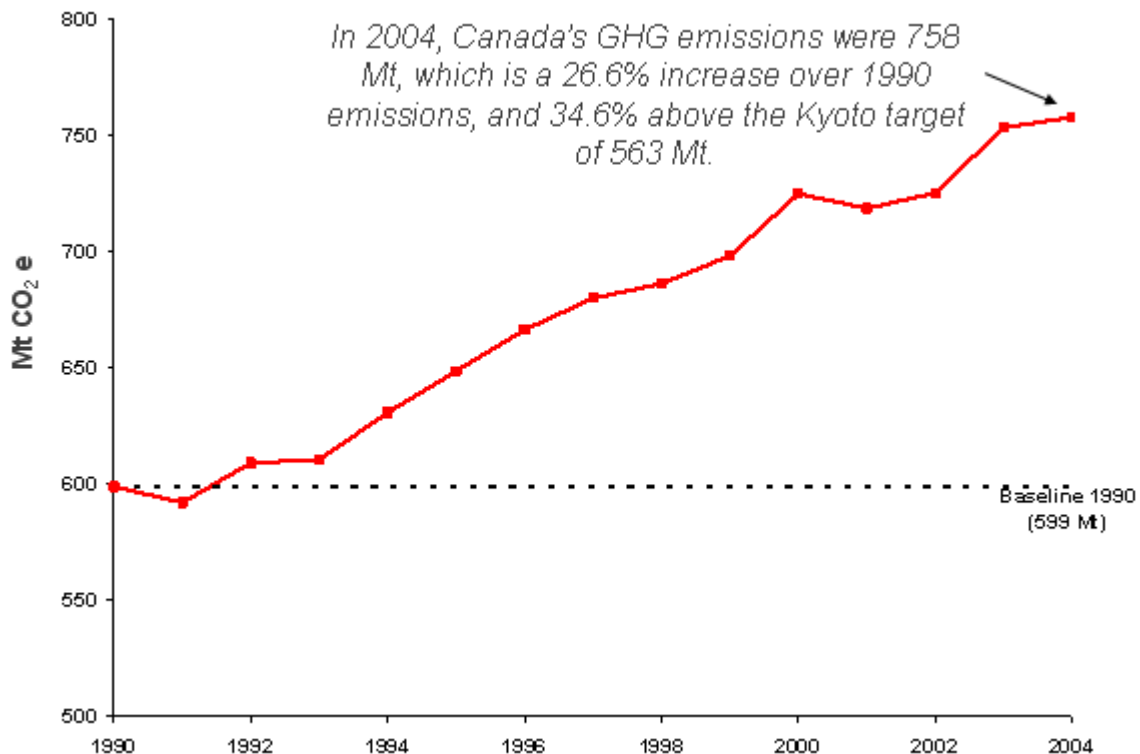
Figure 1.2. Canadian emission trend 1990-2004 (Environment Canada, 2004)

There are six greenhouse gases covered under the Kyoto Protocol - carbon dioxide (CO_2), methane (CH_4), nitrous oxide (N_2O), hydrofluorocarbons (HFCs), perfluorocarbons (PFCs) and sulphur hexafluoride (SF_6). Carbon dioxide makes up the largest share of greenhouse gas emissions (79% of Canada's 2004 total GHG) and has become the most important anthropogenic greenhouse gas. Methane contributed 13% and nitrous oxide 7% (with other gases totalling 1%) to the total 2004 greenhouse gas releases (Environment Canada, 2004).

The greatest contributions to GHG emissions in 2004 were from the electricity and petroleum industries, which accounted for 37% of total national emissions followed by other industries that contributed about 29% and the transportation sector, which contributed 20% (Figure 1.3). These sectors are also responsible for nearly all of the growth in Canadian emissions since 1990. Since the electricity and petroleum industries contribute the most to overall GHG emissions (essentially CO_2), they are the focus of the research presented in this thesis.

Mining
2%

Waste and others
5%

Agriculture
7%

Electricity & Petroleum industries
37%

Other industries
29%

Transportation
20%
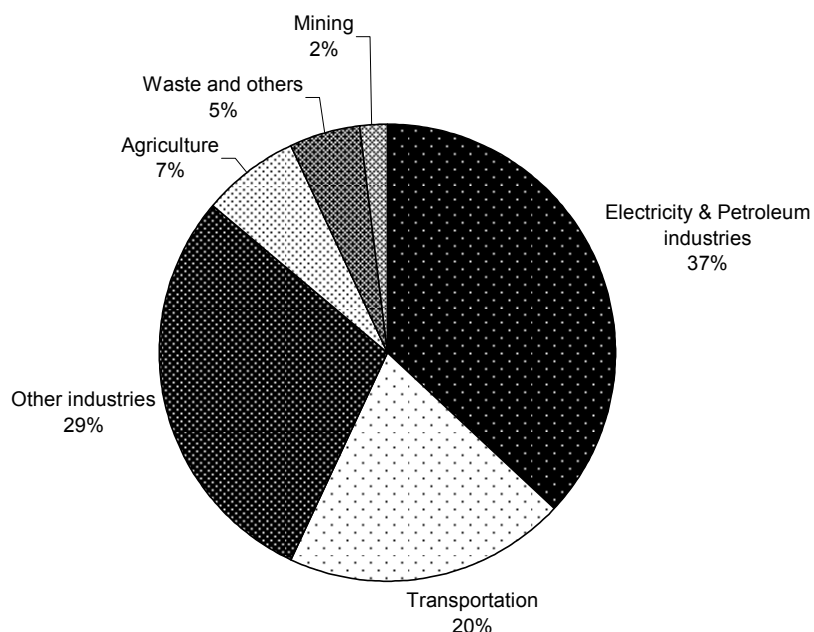
Figure 1.3. Canadian emission contribution by sector (Environment Canada, 2004)

In 2004, the electricity generation sector contributed (17%) to Canada's GHG emissions. Since 1990, electricity generation has increased by about 21% and emissions have grown by 40%. This is due to an increase in the percentage of electricity generated by coal and natural gas and a decrease in the amount generated by hydro and nuclear sources in the overall makeup of electricity generation in Canada. In 2004, the petroleum industry, including refinery, contributed (about 20%) of Canada's GHG

emissions. The petroleum industry has experienced (43%) increase in GHG emissions since 1990 (Environment Canada, 2004).

Electricity in Canada is generated by hydroelectric, fossil fuel (coal and natural gas) and nuclear power, while solar energy and wind generators are used to a very limited extent (less than 1% in 2003). Figure 1.4 gives a breakdown of the power plant type used for generating electricity in Canada (Canadian Electricity Association, 2003).
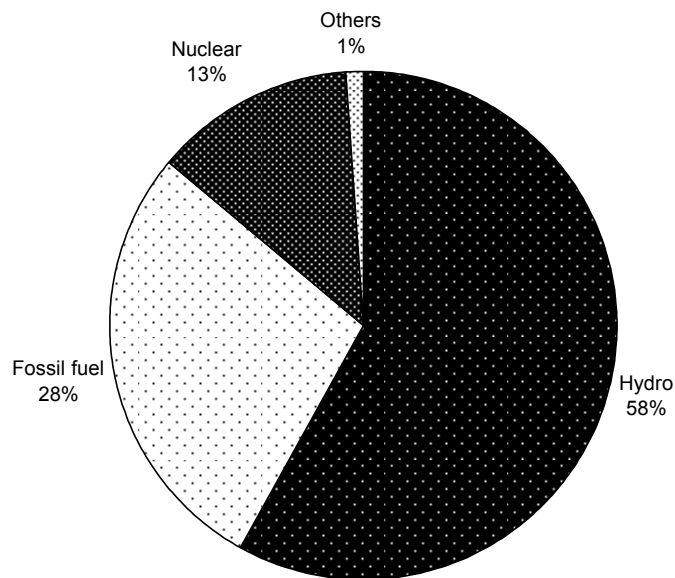
Figure 1.4. Breakdown of electricity generation in Canada (Canadian Electricity Association, 2003).

Burning of fossil fuels for electricity generation is the major sources of CO_2 emissions since others like hydro or nuclear do not emit CO_2. Combustion of fossil fuel for electricity generation accounted for about 17% of total CO_2 emissions in 2004 (Environment Canada, 2004).

Oil refineries are considered as another important source of CO_2 emission mainly from fuel combustion. Petroleum refinery operations range from the receipt and storage of

crude oil at the refinery to petroleum handling and refining operations and, finally, to storage and shipping of the finished products. A refinery's processing scheme is determined largely by the composition of the crude oil input and the chosen mix of petroleum products. The mix and arrangement of refining processes will vary among refineries; few, if any, use all of the same processes.

Canada, for example, has twenty refineries. In 2002, the Canadian Council of Ministers of the Environment (CCME), Environmental Planning and Protection Committee, directed the National Air Issues Coordinating Committee (NAICC) to consider undertaking and funding the development of CO_2 emissions reduction strategy for the petroleum refining sector (Environment Canada, 2002).

1.2 Options to Reduce CO_2 Emissions from Electricity and Refinery Sectors

Carbon dioxide, produced from fuel combustion, either to generate electricity or provide heat to units within an oil refinery, needs to be reduced. If no action is taken, the CO_2 emissions will continue to increase. It is vital for Canada, to meet its target of 6% below the 1990 level and to find an economic strategy to reduce CO_2 emissions from major contributing sectors. The electricity and refinery sectors, which are the main contributors to CO_2 emissions in Canada, are the main focus of this research.

Thus, any technology that can significantly reduce CO_2 emissions need to be considered. In general, there are several possible ways that electricity or refinery sectors can implement to reduce CO_2 emissions from fuel combustion. These include:

1. Balancing which means increasing production from the sources that emit less or no CO_2 emissions and decreasing production from those that emit more CO_2. For example, in power plants, one option to reduce CO_2 emissions is by increasing

the production from non fossil fuel, such as hydro and nuclear power plants, and decreasing the production from fossil fuel power plants. For a refinery, it means to decrease production from a unit that emits more CO_2 emissions and increase production from units that emit less CO_2 providing that final products demand is met.

2. Increasing plant efficiency (especially for power plants) by applying different technologies such as installing new turbine blades. CO_2 emission is decreased as a result of increasing plant efficiency.

3. Switching from carbon intensive fuel to low carbon intensive fuel (e.g. from coal to natural gas as in the case of power plants). This will change the plant structure to run with fuel that emits less CO_2.

4. Capturing CO_2 from flue gas, "end of pipe solution", using one of the available technologies and these include:
   - Chemical capture process such as MEA.
   - Physical adsorption in solid and liquid.
   - Membrane separation.

Among these options, the method with potentially the greatest impact on CO_2 reduction in the medium term is carbon capture and storage (CCS). However, storage sites must be at a reasonable distance from the sources and must be such that no CO_2 will leak back to the surface.

1.3 Research Objectives

The overall objective of this research is to determine the best strategy or mix of strategies for the electricity and refinery sectors to meet a given CO_2 reduction target at

a minimum cost while maintaining a desired production level. A mathematical model will be formulated for each sector to meet the overall objective. Each model is formulated as a MINLP (Mixed Integer Non-linear Program) and implemented in GAMS (General Algebraic Modeling System).

A flowchart of optimal CO_2 reduction strategies is presented in Figure 1.5. For a given sector, either electricity or refinery, the aim is to satisfy demand requirement and determine the best CO_2 mitigation techniques to achieve a certain CO_2 emission reduction target at minimum cost.

For electricity generation, a mathematical model to find the best strategy to reduce CO_2 emissions at minimum cost while maintaining electricity demand is presented. Three potential CO_2 mitigation strategies have been integrated in the model and these include: fuel balancing (optimal adjustment of the operation of existing generating stations to reduce CO_2 emissions without making structural changes to the fleet), fuel switching (switching from carbon intensive fuel to less carbon intensive fuel, e.g. coal to natural gas) and increasing power plant efficiency through available technologies on coal power plants. CO_2 capture technologies are not included in the power plant model because a similar study by a member in our group has recently investigated this issue in details. The objective of the optimization is to determine the best strategies to reduce emissions to a certain target and satisfy electricity demand in the most economical way. The results of the study show the implication of CO_2 emission mitigation in term of generation mix, capacity mix and optimal configuration on power generation fleet at minimum cost. The developed mathematical model for energy sector will be illustrated on a case study from Ontario Power Generation (OPG).

For an oil refinery, a mathematical model, that aims at maximizing the profit of selling final products with quality specifications and reduce CO_2 emissions from fuel combustion to a certain target with least cost, is also presented. To achieve this objective, a non-linear refinery planning model is integrated with a CO_2 management model. Prior to mathematical model development, sub-models were developed for each

```
                    ┌─────────────────────┐
                    │    Existing Plant   │
                    └─────────────────────┘
                              │
                              ▼
Demand requirement ▶  ┌─────────────────────┐  ◀ CO₂ emissions
                      │    Information      │
                      │     Gathering      │
Emission rates from each ▶ │              │  ◀ Identify control
unit                  └─────────────────────┘    technologies and cost
                              │
                              ▼
                    ┌─────────────────────┐
                    │   Data Management   │
                    │    and Analysis     │
                    └─────────────────────┘
                              │
                              ▼
Appropriate Solvers ▶ ┌─────────────────────┐ ◀ Solution Algorithm
                      │    Mathematical     │
                      │ Programming Model   │
                      └─────────────────────┘
                              │
                              ▼
                    ╭─────────────────────╮
                    │ Output = Best CO₂ control │
                    │ strategy and operational  │
                    │      planning       │
                    ╰─────────────────────╯
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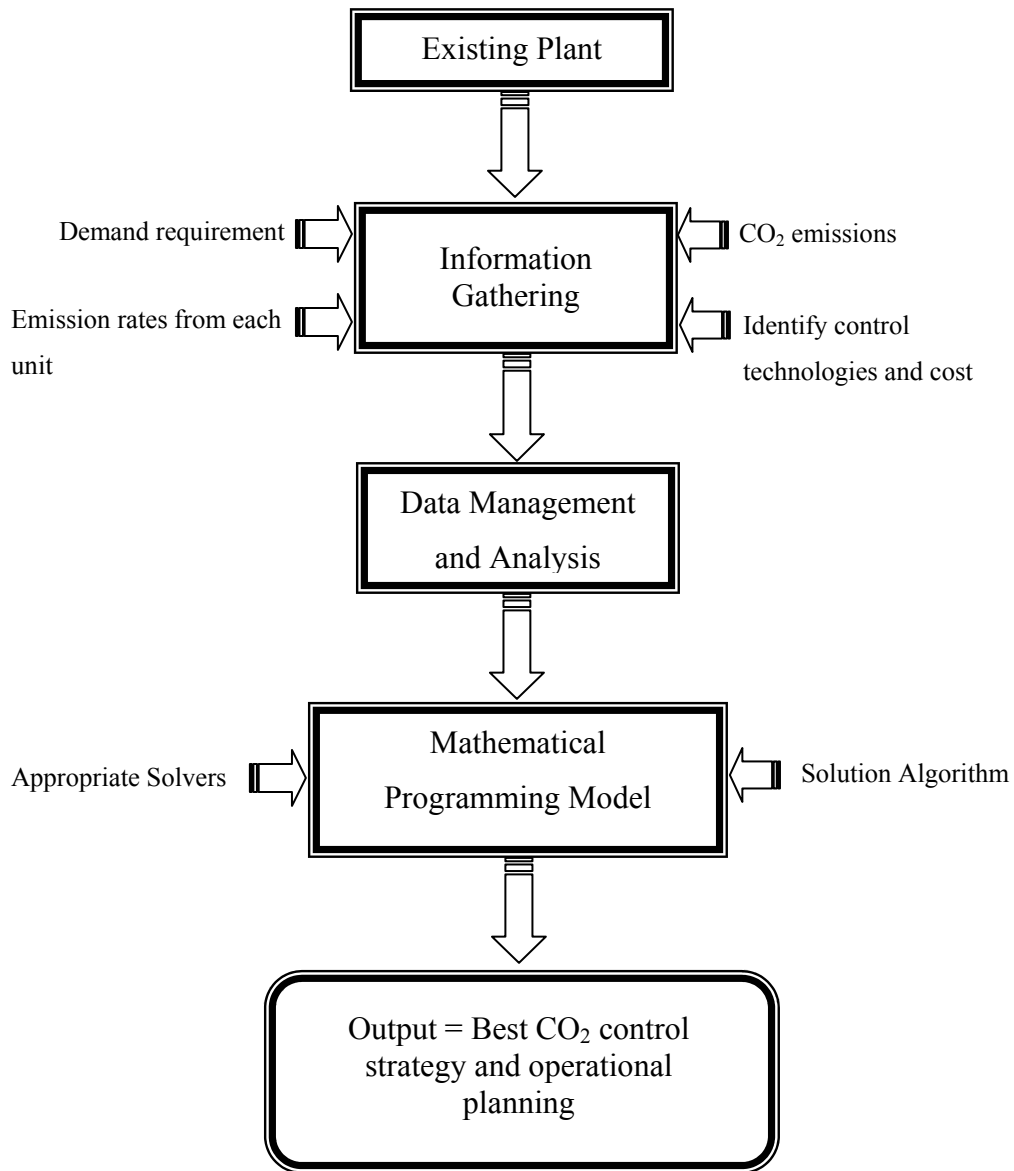
Figure 1.5. Flowsheet of the optimal CO_2 emission reduction strategy

unit within an oil refinery and these were integrated within a master overall refinery planning model. Three potential CO_2 mitigation options are considered, for this sector, and these are: balancing which means increase production from units that emit less CO_2

emissions providing that demand is met for each product; fuel switching which involves a structural change since the current fuel will be replaced with another fuel that emits less CO_2 emission; and the installation of carbon capture technologies to reduce CO_2 emissions. The developed model is illustrated for different case studies.

1.4 Contributions of the Research

The contributions of this research are:

- The development of MINLP mathematical models that take into account both the planning problem and the CO_2 abatement strategies.
- The exact linearization procedures of the MINLP model for the case of CO_2 management in a fleet of power generating units.
- The coding of optimization models for each sector (energy or refinery), in a general, self documenting style, will allow them to be adapted to other industries.
- The optimization programs can be used as tools for evaluating various strategies that might be suggested by industries or governments.
- The work on refinery is the first attempt on CO_2 management in this sector trying to maximize profit while achieving a given CO_2 reduction target. It is unique in that no information has been found in the literature on optimization studies of this nature.
- Highlighting areas where further R & D is required e.g. better CO_2 capture processes.

1.5 Organization of the Thesis

The organization of this thesis is as follows:

Chapter 1: *INTRODUCTION*

Provides an introduction and background about Kyoto accord, addresses the issues of greenhouse gas in the electricity and refinery sectors, primarily CO_2 emission in Canada. Different CO_2 mitigation options are also discussed in this chapter.

Chapter 2: *LITERATURE REVIEW*

Provides a background on electricity generation and describes the processes involved in electricity power generation including fossil-fuel power stations, nuclear, hydroelectric and renewable energy. Gives an overview of an oil refinery and how it works. Presents previous studies carried out on CO_2 capture process, sequestration and the prospects of carbon mitigation to decrease CO_2 emission. Reviews a number of energy planning models that have been developed for the electricity sector. This chapter also provides a survey of refinery planning models.

Chapter 3: *MODEL DEVELOPMENT FOR POWER PLANT*

This chapter presents the problem statement for a power plant. It then describe the development of the superstructure representation that comprises several configurations for CO_2 mitigation options. This chapter also provides the mathematical model formulation for power plants and discusses model application and model coding.

Chapter 4:   *CASE STUDY: A MINLP MODEL FOR CO_2 EMISSION REDUCTION IN THE POWER GENERATION SECTOR*

Presents the results of applying the mathematical model, developed in Chapter 3, on a case study. The model is applied to Ontario Power Generation (OPG). Three CO_2 mitigation strategies are considered: fuel balancing, fuel switching from coal to natural gas, and efficiency improvement through available technologies in order to achieve certain CO_2 reductions while maintaining or enhancing electricity to the grid.

Chapter 5:   *MODEL DEVELOPMENT FOR OIL REFINERIES*

Presents the statement of the problem followed by the superstructure representation. Three CO_2 mitigation options are shown and these are: balancing which includes increasing production from the unit that emits less CO_2 provided that demand is met, fuel switching from current fuel to another fuel with less CO_2 emission, and implementation of CO_2 capture technologies such as chemical absorption process (MEA) to reduce CO_2. The mathematical model for refinery planning is developed in this chapter. Different sub-models are developed for each unit within a refinery. The crude distillation unit (CDU) sub-model is illustrated as an example. The chapter also gives a general methodology to calculate CO_2 emissions from fuel combustion and gives different correlations that may be used for blending products' properties. The model is illustrated through different case studies as will be shown in chapter 6.

Chapter 6:   *CASE STUDIES: AN OPTIMIZATION APPROACH FOR INTEGRATING PLANNING AND CO_2 EMISSIONS REDUCTION IN THE PETROLEUM REFINING INDUSTRY*

Presents the results of the mathematical model developed in Chapter 5. Realistic case studies are shown in this chapter. The first case study considers one CO_2 mitigation option only (balancing) and is incorporated into the model with and without quality constraints to investigate the effect of this option. In a second case study, fuel switching is added to the model of case 1 with products' specifications. CO_2 capture technologies are considered in a third case study. A typical capture process (MEA) is applied to the refinery units. CO_2 sequestration cost is then incorporated in the model and illustrated in a fourth case study. Sensitivity analysis is carried out in this chapter to investigate the effect of increasing or decreasing product prices and the cost of mitigation options.

Chapter 7:   *CONCLUSIONS AND RECOMMENDATIONS*

This chapter presents the conclusions from this study and gives recommendations for future investigations.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

The main greenhouse gas, carbon dioxide, is produced from different sources and different industrial sectors. Stationary sources represent a major contributor to carbon dioxide emissions in Canada. These stationary sources include combustion of any carbon rich fuel, either to generate electricity or to supply energy for different units within a plant, such as an oil refinery. The electricity generation and oil refinery industries account for about 37% of total CO_2 emissions in Canada as of 2004 (Environment Canada, 2004).

In this chapter, a general overview of the electricity and refinery sectors is presented. The following section describes different types of power plants followed by a section on a general overview of an oil refinery. Since one promising way to mitigate CO_2 emissions is to capture and sequester CO_2, different CO_2 capture processes and sequestration technologies will also be discussed in this chapter. This chapter also presents a literature review on the current research in optimization relevant to the energy and refinery sectors. It also discusses a number of studies related to energy models that has been developed for the electricity sector. Finally this chapter highlights the research which has been done related to refinery planning models.

2.2 Overview of Power Generation

The power generation industry became one of the most important global industries generating electricity for all other industries as well as for domestic use. The power generation industry has the mission to generate electric power for all users under all kinds of weather conditions at any level of demand. Electric power has to be generated in the most economical way. The power generation industry depends on the available fuel sources and has to apply the best technologies for converting fuel into electric power with the lowest adverse effect on the environment. This section gives an overview of different types of electricity generation. These include:

1. Fossil fuel power plants.
2. Hydroelectric power plants.
3. Nuclear power plants.
4. Renewable sources power plants.

1. Fossil fuel power plants

Fossil fuel-fired power plants are responsible for producing a large percentage of the electricity that is currently being generated around the world. Demand for that electricity is increasing rapidly, in both the developed and developing countries. In many parts of the world, steadily growing demand for electricity is heightening the need for additional capacity. Fossil fuels will continue to play a crucial role in the development of many national economies well into the future. The fossil fuels currently supplying the major part of the world's energy needs will remain in abundant supply well into coming years. Consequently, if concerted action is not taken, atmospheric levels of CO_2 will continue to increase. Fossil fuel power plants are considered one of the two major contributors to greenhouse gas emissions in Canada. They are being challenged to comply with the Kyoto protocol by United Nations Framework Convention and Climate Change (UNFCC). Canada's target is 6% from 1990 level. (Environment Canada, 2004)

In coal power plants, coal is usually pulverized into a fine powder before being sent to the furnace. The coal powder is then burned, yielding hot gases that boil water to create steam. The steam spins a turbine, which in turn, drives a generator to produce electricity. Steam from power generation is condensed by cooling water and then reused in the boiler. Like any fossil fuel fired thermal power plant, only about 35% of the potential energy in the coal is converted into electricity (OPG, 2003). The remaining energy is released into the environment in the form of heat. Figure 2.1 shows a sketch for a coal power plant with the main processes involved for electricity generation.
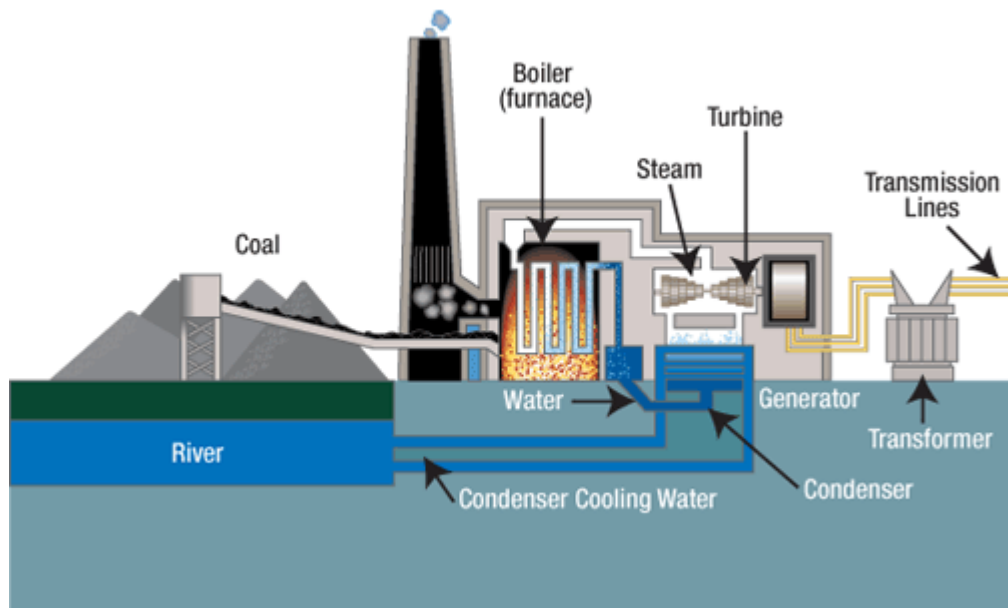
Figure 2.1. A sketch of coal power plant (www.tva.gov)

The major processes are given briefly as (Canadian Clean Power Coalition):

1. **Coal Supply**

- Coal from the mine is delivered to the coal hopper, where it is crushed to five centimetres in size.
- The coal is processed and delivered by a conveyor belt to the generating plant.

2. **Pulverizer**

- The coal is then pulverized, or crushed, to a fine powder, mixed with air and blown into the boiler, or furnace for combustion.

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3. Boiler

- The coal / air mixture ignites instantly in the boiler.

- Millions of litres of purified water are pumped through tubes inside the boiler.

- Intense heat from the burning coal turns the purified water in the boiler tubes into steam, which spins the turbine to create electricity.

4. Precipitator, stack

- Burning coal produces carbon dioxide (CO_2), sulphur dioxide (SO_2) and nitrogen oxides (NO_x). These gases are vented from the boiler.

- Fly ash, which is very light, exits the boiler along with the hot gases.

- An electrostatic precipitator (a huge air filter) removes 99% of fly ash before the flue gases are dispersed into the atmosphere.

5. Turbine, generator

- Water in the boiler tubes picks up heat from the boiler and turns into steam.

- The high-pressure steam from the boiler passes into the turbine (a massive drum with thousands of propeller blades).

- Once the steam hits the turbine blades, it causes the turbine to spin rapidly.

- The spinning turbine causes a shaft to turn inside the generator, creating an electric current.

6. Condensers and the cooling water system

- Cooling water is drawn into the plant and circulated through condensers, which cools steam discharged from the turbine.

- Steam from the turbine also passes through the condensers in separate pipes from cooling water.

- The cold water is warmed by the steam, which condenses back into pure water and circulates back to the boiler to begin the process of generating electricity again.

7. Water treatment plant: water purification

- To reduce corrosion, water must be purified for use in the boiler tubes.

8. Precipitator, Ash systems

- Ash that builds up on the precipitator's plates is vibrated off and collected in large hoppers or bins.

9. Substation, transformer, transmission lines

- Once the electricity is generated, transformers increase the voltage so it can be carried across the transmission lines.
- Once electricity is delivered to substations in cities and towns, the voltage flowing into the distribution lines is reduced, and then reduced again to distribute electricity to customers.

2. Hydroelectric power plant

Most hydroelectric stations use either the natural "drop" of the river or build a dam across the river to raise the water level and provide the drop needed to create a driving force. Water at the higher level goes through the intake into a pipe, called a penstock, which carries it down to the turbine. The turbine is a type of water wheel. The turbine is connected to a generator. When the turbine is set in motion, it causes the generator to rotate, and electricity is produced. The falling water, having served its purpose, exits the generating station through the draft tube and the tailrace where it rejoins the main stream of the river (Brown, 1961; OPG, 2005). Figure 2.3 illustrates how hydroelectric power plants work.
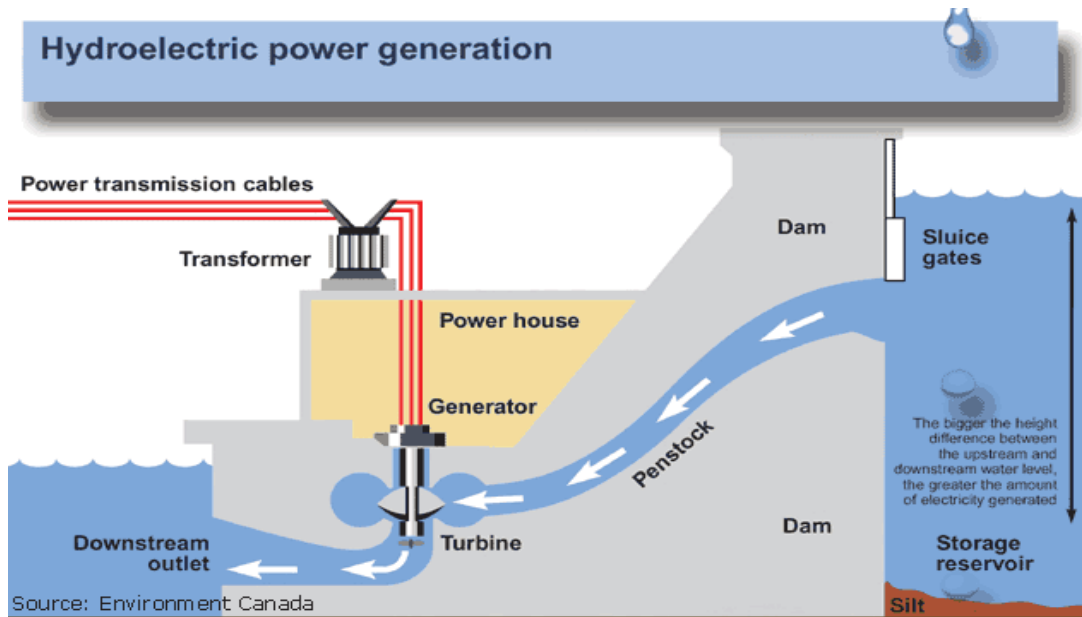
Figure 2.2. Hydroelectric power plant (Environment Canada, 2004)

3. Nuclear power plants

A nuclear power plant is not all that different from coal, oil, or gas fired plants. The main difference is that at a nuclear power plant, the heat used to make steam is produced by fission. Fission is the splitting of atoms into smaller parts. Some atoms, themselves tiny, split when they are struck by even smaller particles, called neutrons. Each time this happens more neutrons come out of the split atom and strike other atoms. This process of energy release is called a chain reaction. The plant controls the chain reaction to keep it from releasing too much energy too fast. In this way, the chain reaction can go on for a long time. As atoms split and collide, they heat up. The plant uses this heat to create steam. The pressure of the expanding steam turns a turbine which is connected to a generator in which electricity is produced. (Termuehlen, 2001; Arbor, 1979)

4. Renewable sources power plants

Renewable energy offers a potential to decrease emissions of greenhouse gases (GHGs). Renewable energy sources include wind and solar energy. Presently, technologies of power generation from these sources attract a great interest because they are non-polluting. However, the fraction of electricity produced from renewable sources remains very limited (Termuehlen, 2001).

Wind turbines convert the kinetic energy of wind into mechanical energy, which is used to generate electricity or to pump water for irrigation. Turbines can be used both as a source of power in remote areas and in "wind farms" to generate power for utilities. The cost of generation has decreased dramatically (Termuehlen, 2001).

Solar thermal power plants use the sun's rays to heat a fluid, from which heat transfer systems may be used to produce steam. The steam, in turn, is converted into mechanical energy in a turbine and into electricity from a conventional generator coupled to the turbine. Solar thermal power generation is essentially the same as conventional technologies except that in conventional technologies the energy source is from the stored energy in fossil fuels released by combustion. Solar thermal technologies use concentrator systems due to the high temperatures needed for the working fluid (Termuehlen, 2001).

2.3 Overview of an Oil Refinery

The modern petroleum refinery is a very sophisticated and capital-intensive industrial complex. To the casual observer, the typical petroleum refinery appears to be a maze of piping with scattered process units containing very tall equipment and massive storage tanks. This section gives a general overview of an oil refinery.

Petroleum refining has evolved continuously in response to changing consumer demand for better and different products. No two major petroleum refineries are identical. This uniqueness stems predominantly from the geographical location of the refinery, which in conjunction with the refinery process configuration, determines how efficiently crude oils can be delivered to the refinery and products to the markets served by the refinery. An overview of the various processes typically incorporated into a modern petroleum refinery is provided in this section. A simplified flow diagram of a typical fuels refinery is shown in Figure 2.3. (Kevin, 2004; Gary, 1994; Watkins, 1979; Jones, 1995)

The key function of most refinery processes is to effect chemical reactions on the hydrocarbons being processed. Generally, the reactions are carried out at high temperatures in the 600-1,000°F (300-550°C) range depending on the process, and in most cases at high pressures, from 200 (1.4 MPa) to as high as 3,000 psi (20 MPa). Those processes involving reactions will typically incorporate a fractionator to distill the reactor effluent into different product streams. The primary function of some refinery processes, such as crude distillation for example, is fractionation only (Kevin, 2004). A general description of a refinery processing unit is that the unit feedstocks are pumped and/or compressed up to the required pressures, preheated via heat exchangers with reactor effluent and/or product streams, and finally heated via heat exchangers in a direct-fired furnace before entering the reactor(s) or distillation tower (if no reaction is intended). The reactor effluent is then cooled via heat exchange with unit feedstocks, fractionated into the desired product streams via distillation, which are then further cooled via heat exchange with unit feedstocks. (Gary, 1994; Watkins, 1979; Kevin, 2004)
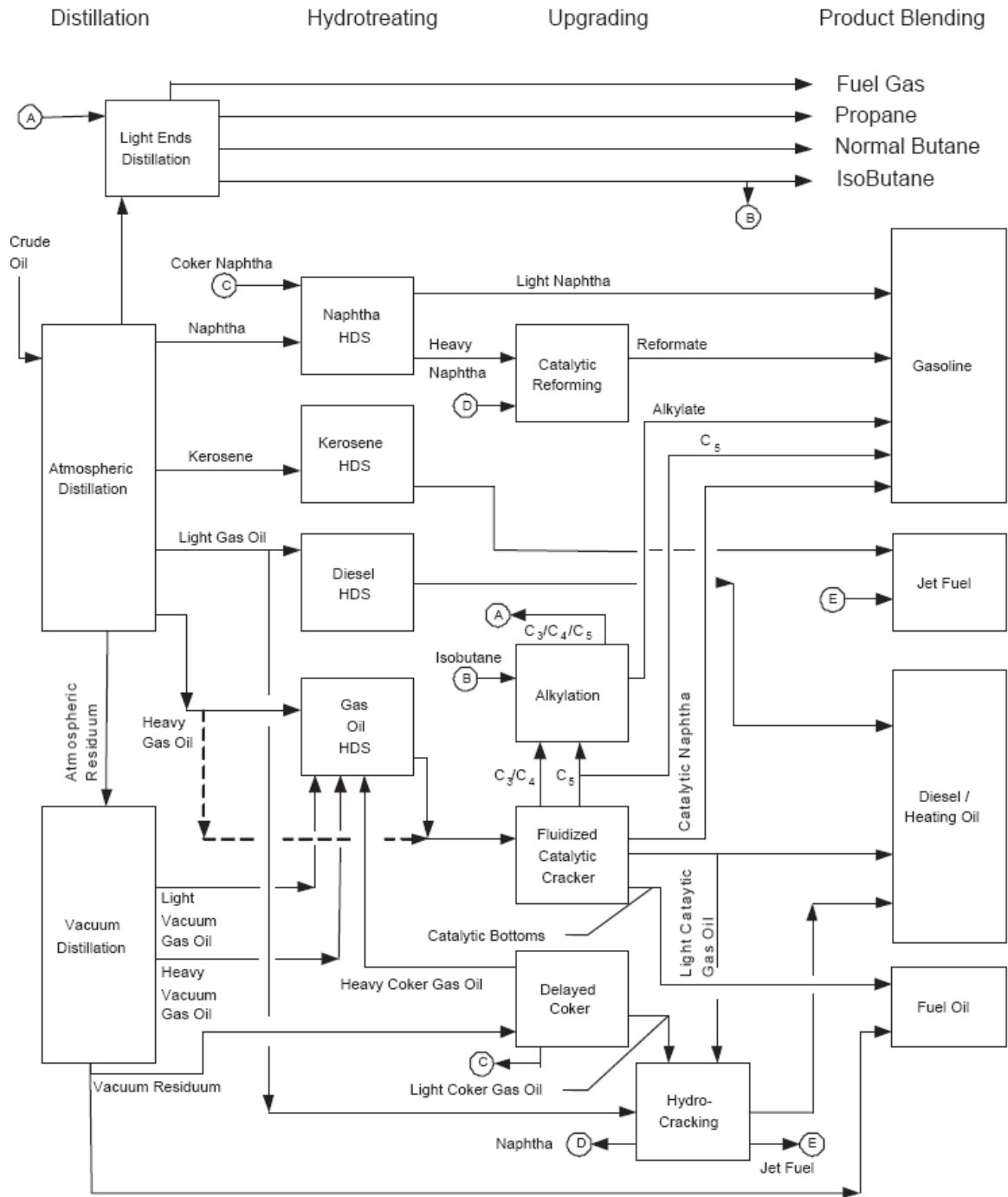
Figure 2.3. Simplified refinery process flow diagram (Kevin, 2004)

A brief description of crude oil will be given before discussing the refinery processes. Crude oil is a mixture of hydrocarbon organic molecules ranging from 1 to 60 carbon chains. The refining process uses chemicals, catalysts, heat, and pressure to separate and combine the basic types of hydrocarbon molecules naturally found in crude oil into groups of similar molecules. The refining process also rearranges their structures and bonding patterns into different hydrocarbon molecules and compounds. Therefore it is the type of hydrocarbon (paraffinic, naphthenic, or aromatic) rather than its specific chemical compounds that is significant in the refining process. Paraffinic hydrocarbon compounds are saturated organic compounds with no double bonds. They exist as long chains and isomers. Aromatic hydrocarbon compounds are organic compounds with ring type structure. All aromatic compounds have at least one benzene ring. Naphthenes are saturated hydrocarbon groupings arranged in the form of closed rings (cyclic) and found in all fractions of crude oil except the very lightest. These are the three principal groups that occur naturally in crude oil. Other undesirable hydrocarbon molecules are formed during the refining process (cracking) such as alkenes (Ethylene or ethene) and alkynes. All these compounds are unsaturated organic compounds. Other non-hydrocarbon compounds or molecules that may be present in the crude oil include sulphur compounds (e.g hydrogen sulphide), oxygen compounds (e.g phenols), nitrogen compounds (e,g ammonia), trace metals, salts (e.g NaCl), and carbon dioxide. (Gary, 1994; Kevin, 2004)

Most of the non-hydrogen, non-carbon elements found in crude oils are undesirable and are removed from the hydrocarbons in total or in part during refinery processing. One of the key attributes for characterizing the hydrocarbons composing crude oils is by boiling point (Watkins, 1979). This attribute is determined through laboratory test methods by measuring the temperature at which the components of the crude oil will evaporate at a given pressure (typically atmospheric pressure unless stated to be a different pressure basis). A True Boiling Point (TBP) curve is developed as a part of the crude assay to plot or tabulate the liquid volume percent of the crude oil that evaporates relative to temperature at atmospheric pressure. The numerous hydrocarbon components constituting crude oil will generally have individual boiling points ranging from less

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than 60^{o}F (15^{o}C) to greater than 1200^{o}F (650^{o}C). Crude oils are named and grouped into broad categories typically based on the geographic location of origin, along with the level of sulphur contained in the crude and/or density of the crude oil. For example, West Texas Intermediate (WTI) and West Texas Sour (WTS) are two families of crude oils produced in the oilfields of West Texas. WTI is a light, sweet (i.e., low levels of sulphur relative to high sulphur sour crude oils) crude oil when compared to the heavier, higher sulphur content WTS (Kevin, 2004). Higher sulphur crude oils are more corrosive than lower sulphur crude oils. To ensure a reasonable life expectancy for equipment processing the higher sulphur crude oils, refiners specify that such equipment be built from more expensive alloys with a higher corrosion resistance (Kevin, 2004). The American Petroleum Institute (API) has developed the term Degrees API Gravity (API) which is widely used as another general characterization of the density of crude oils. The relationship is as follows (Gary, 1994):

$$API = \frac{141.5}{S.Gr(60^o F)} - 131.5$$

where S.Gr (60)^o F is specific gravity at 60^o F (15^{o}C) which is the density of the crude oil measured at 60^{o}F divided by the density of water at 60^{o}F.

Therefore, when comparing two crude oils, the higher density crude (i.e., the one with the highest specific gravity) will have a correspondingly lower API. For example, the 35 API crude oil is heavier than the 40 API crude oil. Crude oil assays are the results of numerous laboratory analyses conducted on the whole crude oil or fractions of the crude oil (Watkins, 1979). These tests characterize a crude oil and enable refiners to evaluate the feasibility and economics of processing a given crude in their refinery. Crude oil assays vary widely in the degree of details. However, qualities of interest with respect to the whole crude, as well as various fractions of the crude are presented in the assay (Watkins, 1979).

All units within an oil refinery can fall into one of the following four categories (Kevin, 2004):

1. Fractionation or Distillation.
2. Hydrotreating.
3. Upgrading.
4. Product Blending.

1. Fractionation or Distillation

Fractionation utilizes a mass separation technique called distillation in which the feedstock is distilled into various cuts of target boiling ranges or even separated into individual hydrocarbon compounds. Distillation is accomplished by imposing a temperature profile across the tower enabling differences in the equilibrium compositions of the vapour and liquid phases to change the compositions throughout the distillation tower (Watkins, 1979).

Distillation concentrates the lower boiling point material towards the top of the tower. The lowest boiling point product is the tower overhead vapour which is condensed as distillate. Higher boiling point materials are present further down the tower. The liquid phase flows down the tower because of gravity force. Additional intermediate boiling range streams may be withdrawn at various levels from the tower as side-stream products. The highest boiling range material is the liquid product withdrawn from the bottom of the tower (Watkins, 1997; Kevin, 2004).

The first refinery process unit that a crude oil or mixture of crude oils is charged to is a crude distillation unit which consists of an atmospheric distillation tower and typically also includes a vacuum distillation tower. The crude oil or mixture of crude oils that represents the feed to a crude distillation unit is pumped from crude oil storage tanks into banks of heat exchangers which pre-heat the crude oil to approximately 250^oF (120^oC) by cross exchanging heat with various product streams. Most crude oils contain appreciable levels of inorganic salts which would cause downstream corrosion and equipment fouling. The crude oil is then desalted by emulsifying the crude oil with water. The salts are dissolved in the water and the brine phase is then separated from the

oil phase and withdrawn. The crude oil is further preheated to the maximum possible temperature (typically about 500-550^{o}F or 260-290^{o}C) through heat exchange with distillation product streams. Finally, the crude oil is heated to approximately 750^{o}F (400^{o}C) in a direct-fired furnace and fed to the atmospheric distillation tower. The most common fractions withdrawn from an atmospheric distillation unit (progressing from lightest to heaviest) are naphthas, kerosene, diesel, gas oils, and residual (the liquid bottoms stream). Figure 2.4 gives a sketch of a crude distillation unit with the main products. An atmospheric distillation unit operates normally at atmospheric pressure. The maximum process temperature in the atmospheric distillation unit is approximately 750^{o}F (400^{o}C). At temperatures above 750^{o}F (400^{o}C), thermal cracking of the petroleum into light gases and coke occurs (Kevin, 2004). Coke is essentially pure carbon in a solid form. The presence of coke is undesirable in refinery process units because solid coke formation fouls refinery process equipment and severely reduces equipment performance. The residual stream is usually further fractionated in a vacuum distillation tower. Hydrocarbons existing as a liquid at a given temperature at atmospheric pressure will boil at a lower temperature when the pressure is sufficiently reduced. Table 2.1 shows boiling range of typical crude oil fractions. (Gary, 1994; Watkins, 1979; Kevin, 2004)

Table 2.1. Boiling range of typical crude oil fractions (Gary, 1994)

Fraction	TBP - Boiling range (^{o}F)
Light straight run naphtha (LSRN)	90 – 220
Heavy straight run naphtha (HSRN)	180 – 380
Kerosene	380 – 520
Diesel	520 – 610
Light vacuum gas oil (LVGO)	610 – 800
Heavy vacuum gas oil (HVGO)	800 – 1050
Residue	1050 +
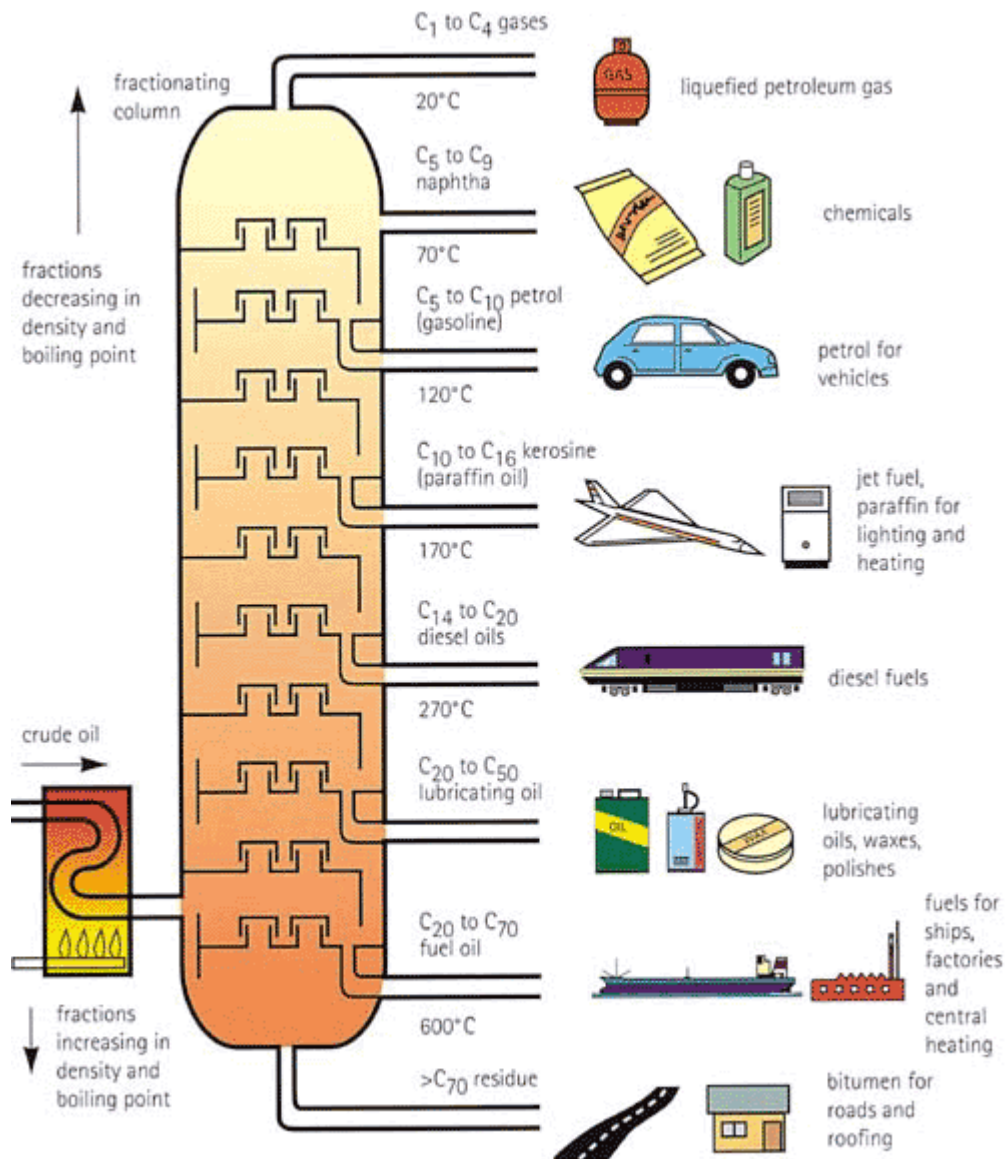
Figure 2.4. Crude distillation unit with products (www.energyinst.org.uk)

Distillation/fractionation does not produce desirable refined products because impurities have not yet been removed. Hence, the products from distillation are converted into more useable products by changing the size and structure of the hydrocarbon molecules through cracking, reforming, and other conversion processes. This is done after treatment methods such as hydrotreating to remove impurities and improve product quality. Finally, a blending operation is carried out to add additives to produce finished

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products with specific performance properties. Many more operations can be carried out on the products to obtain compounds that meet specific requirements. Therefore, there are no end limitations in the refining process (Watkin, 1979; Kevin, 2004).

2. Hydrotreating

Hydrotreating is a hydrogenation process used to remove about 90% of contaminants such as nitrogen, sulphur, oxygen, and metals from liquid petroleum fractions. These contaminants, if not removed from the petroleum fractions as they travel through the refinery processing units, can have detrimental effects on the equipment, the catalysts, and the quality of the finished product (Gary, 1994).

With rare exceptions, the intermediate hydrocarbon product streams from the crude distillation unit contain levels of sulphur that exceed the specifications for the finished product stream and/or the catalyst specifications for downstream processing units. Hydrotreating is the most common process configuration utilized to remove the sulphur from the intermediate stream (Kevin, 2004). Hydrotreating may also reduce the levels of nitrogen contained in the stream. In addition, some of the metals (such as nickel and vanadium) may be removed from the hydrocarbon stream during hydrotreating. Hydrotreaters may be designated to continuously process one particular hydrocarbon feedstock, or may alternate processing of different feed streams. Hydrotreating is a refinery process in which hydrogen gas is mixed with the hydrocarbon stream and contacted with a fixed-bed of catalyst in a reactor vessel at a sufficiently high enough temperature and pressure to effect the hydrodesulfurization (HDS) reactions (Gary, 1994; Kevin, 2004).

3. Upgrading

Upgrading is a broad term applied to refinery processing which significantly increases the market value of the hydrocarbons processed. This is accomplished through chemical reactions to yield more desirable hydrocarbon compounds. The upgrading reactions

result in either improving product specification qualities or rearranging the molecular structure (i.e., converting) so that the hydrocarbons boil in a more desirable boiling range. These upgrading units include:

a) Catalytic Reforming.
b) Fluidized Catalytic Cracking.
c) Hydrocracker.
d) Alkylation.
e) Isomerization.
f) Polymerization.

a) Catalytic Reforming

Catalytic reforming is the refinery process that reforms the molecular structure of the heavy naphtha to increase the percentage of high-octane components while reducing the percentage of low-octane components. This is mainly to increase the octane number of the final gasoline (Kevin, 2004). More details on octane number will be given in the section on product blending (section 5.5 in this thesis).

The hydrocarbon compounds that constitute heavy naphtha are classified into four different categories: paraffins, olefins (a very low percentage of olefins occur in the heavy naphthas from crude), naphthenes and aromatics. Simplistically, the paraffins and olefins are compounds with straight or branched carbon chains, whereas the naphthenes and aromatics are carbon rings (Kevin, 2004). The paraffins and naphthenes are saturated hydrocarbons. Saturated means that they have the maximum number of hydrogen atoms attached to the carbon atoms. The olefins and aromatics, however, are unsaturated hydrocarbons because the compounds contain carbon atoms that are double bonded to other carbon atoms. The straight chain, saturated compounds exhibit very low octane numbers, the branched, saturated compounds exhibit progressively higher octane numbers, while the unsaturated compounds exhibit very high octane numbers (Gary, 1994; Kevin, 2004).

b) Fluidized Catalytic Cracking

The Fluidized Catalytic Cracking (FCC) process unit is considered by many refiners to be the heart of the petroleum refinery. This derives from the fact that the FCC is a key tool to correct the imbalance reflected by the markets demand for predominantly lighter, lower boiling petroleum products, whereas fractionated crude oils typically provide an excess of heavy, high boiling range oils. The FCC process converts heavy gas oils into lighter products which are then used as blendstocks for gasoline and diesel fuels. The olefinic FCC catalytic naphtha product exhibits a very high-octane value for gasoline blending. The FCC process cracks the heavy gas oils by breaking carbon-to-carbon bonds in the large molecules comprising the gas oils and splitting them into multiple smaller molecules which boil at a much lower temperatures. The FCC may achieve conversions of 70-80% of the feed hydrocarbons boiling above the gasoline range (i.e., $430^{o}F$ or $220^{o}C$) to products boiling below $430^{o}F$ (Kevin, 2004). The lower density of the FCC products relative to the gas oil feedstocks has the added benefit of producing a volume gain in which the combined volume of the liquid product streams is greater than the volume of the unit feed stream. Since most petroleum products are bought and sold on a volume basis, the volume gain aspect of the FCC process is a key aspect in how it enhances refinery profitability (Kevin, 2004; Gary, 1994; www.osha.gov). The resulting FCC product hydrocarbons are highly olefinic (i.e., unsaturated).

The FCC cracking reactions are catalytically promoted at very high temperatures of $950-1,020^{o}F$ ($510-550^{o}C$). At these temperatures, coke (i.e., essentially pure carbon) formation deactivates the catalyst by blocking catalyst surface area which prevents intimate contact between the catalyst and the hydrocarbons (Kevin, 2004). To retain catalyst activity, the FCC utilizes a very fine powdery, zeolite catalyst that behaves like a fluid (i.e., is able to flow). The fluidized catalyst is continuously circulated in the FCC from the reactor to a regenerator vessel and then returned to the reactor. Coke is removed from the catalyst in the regenerator vessel through controlled incomplete combustion of the carbon with oxygen to form carbon monoxide and carbon dioxide.

The gas oil feed to the FCC is preheated via heat exchange with reactor products and then a direct-fired furnace before being mixed with the hot (1,200-1,350°F or 650-730°C) regenerated catalyst. The hot catalyst vaporizes the gas oil and heats the oil to the reactor temperature (Kevin, 2004). Figure 2.5 shows a schematic of a FCC unit.
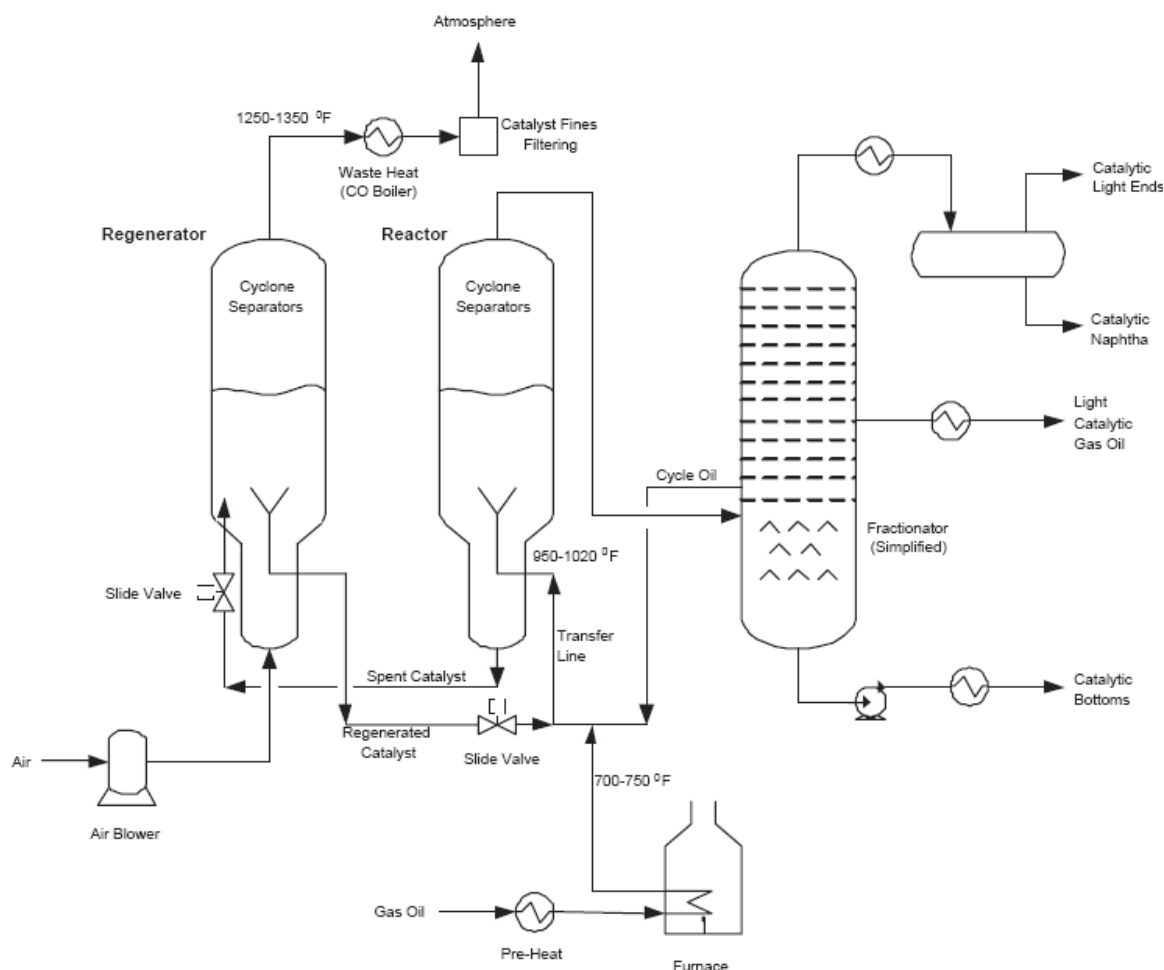
Figure 2.5. Simplified sketch of FCC (Kevin, 2004)

c) **Hydrocracker**

Hydrocracking is a similar process to FCC to the extent that this process catalytically cracks the heavy molecules that comprise gas oils by splitting them into smaller molecules which boil in the gasoline, jet fuel, and diesel fuel boiling ranges (Gary, 1994). The fundamental difference is that hydrocracking reactions are carried out in an

extremely hydrogen-rich environment. In hydrocracking, two different reactions are occurring in the reactor(s). These are cracking and hydrogenation reactions. First, a carbon-to-carbon bond is broken (endothermic cracking reaction), followed by the attachment of hydrogen to the carbon atom (exothermic hydrogenation reaction). The resulting product from the hydrocracking process are saturated. The net effect of the endothermic (consumes heat) and exothermic (creates heat) reactions is a temperature increase across each hydrocracking reactor bed because more heat is generated in the hydrogenation reactions than is consumed in the cracking reactions. Typical hydrocracking feedstocks are gas oils (Gary, 1994; Kevin, 2004).

The heavy naphtha produced from hydrocracking makes an excellent catalytic reformer feedstock due to the significant presence of naphthenes created by saturating aromatics in the gas oil feedstock with hydrogen. Hydrocracking also produces an excellent blendstock for jet fuels. The yields across a hydrocracking unit may exhibit liquid volume gains of as much as 20-25 percent (Gary, 1994).

d) Alkylation

Alkylation combines low-molecular-weight olefins (primarily a mixture of propylene and butylene) with isobutene in the presence of a catalyst, either sulphuric acid or hydrofluoric acid. The product is called alkylate and is composed of a mixture of high-octane, branched-chain paraffinic hydrocarbons. Alkylate is a premium blending stock because it has exceptional antiknock properties and burns cleanly (Gary, 1994; Kevin, 2004).

e) Isomerization

Isomerization converts n-butane, n-pentane and n-hexane into their respective isoparaffins of substantially higher octane number. The straight-chain paraffins are converted to their branched-chain counterparts whose component atoms are the same but are arranged in a different geometric structure. Isomerization is important for the

conversion of n-butane into isobutane, to provide additional feedstock for alkylation units, and the conversion of normal pentanes and hexanes into higher branched isomers for gasoline blending. Isomerization is similar to catalytic reforming in that the hydrocarbon molecules are rearranged, but unlike catalytic reforming, isomerization just converts normal paraffins to isoparaffins (Gary, 1994; Kevin, 2004).

f) Polymerization

Polymerization in the petroleum industry is the process of converting light olefin gases including ethylene, propylene, and butylene into hydrocarbons of higher molecular weight (Gary, 1994).

4. Product blending

Refinery products are typically the result of blending several component streams or blendstocks. In most cases, product blending is accomplished by controlling the volumes of blendstocks from individual component storage tanks that are mixed in the finished product storage tank. Samples of the finished blend are then analyzed by laboratory testing for all product specifications prior to shipping. The applicable specifications vary by product but typically include density, and sulphur content specifications (Kevin, 2004; Riazi, 2005).

Taking gasoline as an example since it is the major product from an oil refinery, motor gasoline has numerous specifications that must be satisfied to provide the performance demanded by our high-performance motor vehicles. The most widely recognized gasoline specification is the octane number. Gasoline is typically retailed in grades of regular, mid-grade and premium, which are differentiated by the posted octane number. The Octane Number of a test fuel refers to the percentage by volume of isooctane in a mixture of isooctane and heptane in a reference fuel that when tested in a laboratory engine, matches the antiknock quality, as measured by a knockmeter, of the fuel being

tested under the same conditions (Kevin, 2004). The octane number posted at the gasoline pump is actually the average of the Research Octane Number (RON) and Motor Octane Number (MON), commonly referred to as (R+M)/2. RON and MON are two different test methods that quantify the antiknock qualities of a fuel. Since the MON is a test under more severe conditions than the RON test, for any given fuel, the RON is always higher than the MON. Unfortunately, the desulphurized light and heavy naphtha fractions of crude oils have very low octane numbers. The heavy naphtha fraction is roughly 50 (R+M)/2 (Kevin, 2004; Riazi, 2005).

Examples of other product specifications include Cetane number, Reid Vapour Pressure, Smoke Point, etc. Many of these product specifications do not blend linearly by component volumes. In these circumstances, the finished blend properties are predicted using experience-based algorithms for the applicable blendstock components. These algorithms are very sophisticated and their precision is absolutely critical for in line blending (Kevin, 2004).

2.4 CO$_2$ Capture and Sequestration

Because power plants and oil refineries contribute to about 37% of Canada CO$_2$ emissions, CO$_2$ capture and storage processes have been viewed as a potential solution to achieve deep reduction of CO$_2$ from these sectors. The goal of CO$_2$ capture technologies is to separate the CO$_2$ from its sources in appropriate forms for transportation and sequestration. Once CO$_2$ is captured, it needs to be pipelined and stored securely and permanently. Therefore, the applicability of CO$_2$ capture technologies to power plants must be evaluated in a context of the total system including capture, transportation and storage. This section gives a brief description of available CO$_2$ capture technologies and sequestrations. Most of the research found in the literature has focused on CO$_2$ capture from power plants but the technology would not change if it is applied to flue gas from an oil refinery.

2.4.1 CO_2 capture

Carbon capture can be defined as the reduction of carbon that would otherwise be emitted to, or remain, in the atmosphere. Various approaches could potentially be applied to flue gas from fossil fuel-fired power plants or oil refineries. CO_2 capture systems that are possible candidates are described below and summarized in Figure 2.4 (Rubin, 2004).
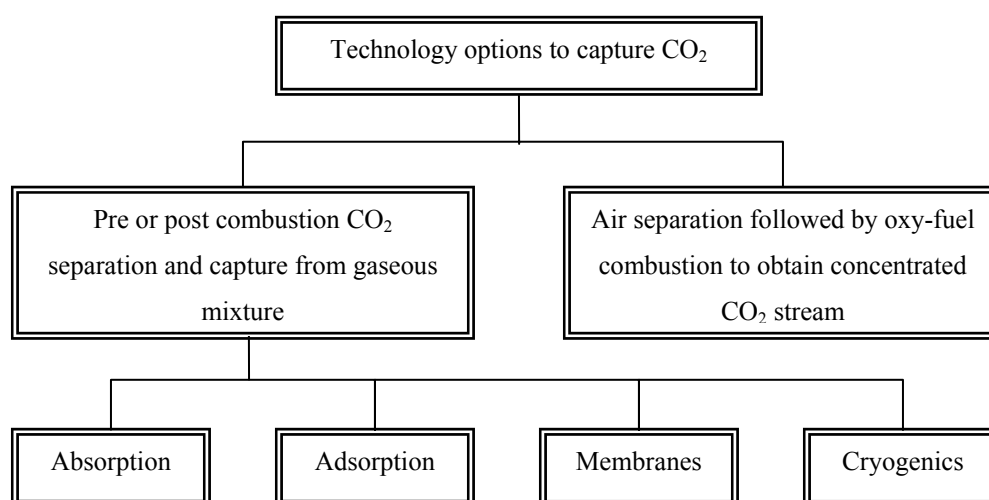
Figure 2.6. Options for CO_2 capture (Rubin, 2004)

A brief description of each process shown in the figure will be given as follows:

1. Chemical solvent absorbtion

These are well established and are usually based on use of amines (often monoethanolamine-MEA) for removing CO_2 from exhaust gases. Typically, prior to the CO_2 removal stage, the flue gas is cooled, treated to reduce the levels of particulates and other impurities present, then passed into an absorption tower where it is brought into contact with the absorption solution. The amine solvent selectively absorbs the CO_2 by chemically reacting with it to form a loosely bound compound. The CO_2-rich absorbent

is then pumped into a stripper tower where the pressure is reduced and/or the temperature increased to roughly $120^{o}C$ in order to release the CO_2. As the released CO_2 is compressed, the regenerated absorbent is recycled to the stripper in a fully continuous process. Most systems of this sort were developed originally for the chemical and oil industries and can achieve a CO_2 recovery rate of up to 98%, with a purity of 99+%. At present, a handful of coal- and gas-fired power plants in operation use amine scrubbers for CO_2 capture (Rubin, 2004). As other capture processes, the amine scrubbing process often requires large amount of energy.

2. Adsorption

Some solids can be used to separate CO_2 from gas mixtures. The most important adsorbents are activated carbon, zeolite, silica gel, and aluminium oxide. The separation is based on the difference in gas molecule sizes or different binding forces between gas species and the adsorbent. Because of the large volume of CO_2 in the flue gas, physical adsorption might not be an effective and economical solution for separating CO_2 from flue gas. The other limit for this technology is the low gas selectivity of the available adsorbents (Meisen et al., 1997).

3. Membranes

These can be used to separate gases by exploiting differences in physical or chemical interactions between gases and the membrane material. The differences allow one component to pass more speedily through the membrane. A range of separation membranes are available or being developed. The degree of separation, however, is generally only modest, while systems tend to be relatively complex and energy consumption may be high (Meisen, 1997).

4. Cryogenics

CO_2 can be separated from other gaseous compounds through cooling and condensation. This method's main application is for purifying gas streams that contain a high percentage of CO_2 (some with more than 90%), and the technology is not at present applied to more dilute CO_2 streams such as those encountered with typical power

generation plant. A disadvantage is that the process requires a significant amount of energy, as well as the removal of water from the gas stream (Plasynki, 2000).

5. Oxy-fuel (O$_2$/CO$_2$) combustion processes

The use of oxygen (or oxygen enriched air) significantly improves the combustion of fossil fuels, therefore achieving higher combustion rate, higher thermal efficiency, reduction in the volume of flue gas and heat loss and elimination of NO$_x$ control that can partially offset the costs (Plasynski et al., 2000). Through this burning process, the system increases the CO$_2$ concentration in the flue gas to more than 90% and recovers the CO$_2$ gas directly. The O$_2$/CO$_2$ pulverized coal-fired power plants consist of four main processes: 1) oxygen generation, 2) O$_2$/CO$_2$ combustion, 3) flue gas treatment and 4) CO$_2$ recovery/disposal. An important disadvantage of the O$_2$/CO$_2$ combustion process is the need for oxygen which is expensive to produce from air.

Although there are several methods that have been proposed for the capture and separation of CO$_2$, one of the few methods that has been proven to work on an industrial scale for capturing CO$_2$ from flue gas is chemical absorption using monoethanolamine (MEA). Other processes like membrane separation, cryogenic fractionation, and adsorption technologies are also possible to separate the carbon from the flue gases, but they have not been yet demonstrated on large scale.

2.4.2 Sequestration

Following the capture process, CO$_2$ needs to be stored, so that it will not be emitted into the atmosphere. Several key criteria must be applied to the storage method (Herzog and Dan, 2004):

    a. The storage period should be prolonged, preferably hundreds to thousands of years.

    b. The cost of storage, including the cost of transportation from the source to the storage site, should be minimized.

c. The risk of accidents should be eliminated.

d. The environmental impact should be minimal.

e. The storage method should not violate any national or international laws and regulations.

Storage media include geologic sinks and the deep ocean. Geologic storage includes deep saline formations, depleted oil and gas reservoirs and enhanced oil recovery (Herzog and Dan, 2004; Shafeen et al., 2004). Deep ocean storage includes direct injection of liquid carbon dioxide into the water column at intermediate depths (1000-3000 m), or at depths greater than 3000 m, where liquid CO_2 becomes heavier than sea water, so it would drop to the ocean bottom and form a so-called "CO_2 lake" (Herzog and Dan, 2004).

1. Geologic storage

Geological sinks for CO_2 include depleted oil and gas reservoirs and enhanced oil recovery. Together, these can hold hundreds to thousands of gigatonnes of carbon (GtC), and the technology to inject CO_2 into the ground is well established (Bachu, 2000; Herzog and Dan, 2004; Shafeen et al., 2004).

Depleted oil and gas reservoirs

Injecting CO_2 into depleted oil and gas fields has been practiced for many years. The major purpose of these injections was to disposing of "acid gas," a mixture of CO_2, H_2S and other byproducts of oil and gas exploitation and refining. In 2001, nearly 200 million cubic meters of acid gas were injected into formations across Alberta and British Columbia at more than 30 different locations (Herzog and Dan, 2004).

Enhanced oil recovery

Carbon dioxide injection into geological formations for enhanced oil recovery (EOR) is a mature technology. In CO_2-EOR projects, much of the CO_2 injected into the oil reservoir is only temporarily stored. This is because the decommissioning of an EOR

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project usually involves the "blowing down" of the reservoir pressure to maximize oil recovery. This blowing down results in CO_2 being released, with a small but significant amount of the injected CO_2 remaining dissolved in the immobile oil (Herzog and Dan, 2004).

Deep saline formations

Deep saline formations may have the greatest CO_2 storage potential. These reservoirs are the most widespread and have the largest volumes. These reservoirs are very distinct from the more familiar reservoirs used for fresh water supplies. Research is currently underway in trying to understand what percentage of these deep saline formations could be suitable CO_2 storage sites (Herzog and Dan, 2004; Shafeen, 2004).

The density of CO_2 depends on the depth of injection, which determines the ambient temperature and pressure. The CO_2 must be injected below 800 m, so that it is in a dense phase. When injected at these depths, the specific gravity of CO_2 ranges from 0.5 to 0.9, which is lower than that of the ambient aquifer brine. Therefore, CO_2 will naturally rise to the top of the reservoir (Herzog and Dan, 2004).

2. Ocean Storage

The ocean represents the largest potential sink for anthropogenic CO_2. It already contains an estimated 40,000 GtC (billion metric tonnes of carbon) compared with only 750 GtC in the atmosphere. Apart from the surface layer, deep ocean water is unsaturated with respect to CO_2. It is estimated that if all the anthropogenic CO_2 that would double the atmospheric concentration were injected into the deep ocean, it would change the ocean carbon concentration by less than 2%, and lower its pH by less than 0.15 units. Furthermore, the deep waters of the ocean are not hermetically separated from the atmosphere. Discharging CO_2 directly to the ocean would accelerate this ongoing but slow natural process and would reduce both peak atmospheric CO_2 concentrations and their rate of increase (Herzog and Dan, 2004).

In order to understand ocean storage of CO_2, some properties of CO_2 and seawater need to be elucidated. For efficiency and economics of transport, CO_2 would be discharged in its liquid phase. If discharged above about 500 m depth, that is at a hydrostatic pressure less than 50 atm, liquid CO_2 would immediately flash into a vapor, and bubble up back into the atmosphere. Between 500 and about 3000 m, liquid CO_2 is less dense than seawater, therefore it would ascend by buoyancy (Herzog and Dan, 2004).

2.5 Optimization and Planning Models

The wide range of solution techniques and the advantage of mathematical programming and optimization have been combined to enable the chemical process systems engineer (PSE) to solve various problems in different areas in chemical engineering. Chemical process design, planning, and operations problems received a huge attention in the last two decays due to the change in the picture of process integration and to an increased understanding of the physical principles underlying problems and developing the practical methodologies to solve them. This section gives a brief description of optimization strategies in process system engineering. It also presents energy models with CO_2 and refinery planning models reported in the literature.

Optimization strategy in Process System Engineering is to quantify the best solution to a problem within constraints. Floudas (1995) stated that optimization models consist of:

- Variables: the variables can be continuous, integer or a mixed set of continuous and integer
- Parameters: the parameters are fixed to one or more specific values, and each fixation defines a different model
- Constraints: the limitation on the variables value
- Mathematical relationships or equations: the mathematical models can be classified as equalities, inequalities and logical conditions. The model equalities are usually composed of mass balances, energy balances, equilibrium relations and engineering

relations which describe the physical phenomena of the system. The model inequalities often consists of allowable operating limits, specification on qualities, performance requirement and bounds on availability's and demand. The logical conditions provide the connection between the continuous and integer variables.

Mathematical models for optimization fall into four categories:
- Linear programming (LP) problems
- Mixed Integer Linear Programming (MILP) problems
- Nonlinear Programming (NLP) problems
- Mixed Integer Nonlinear Programming (MINLP) problems

The aim of this study is to present the structural and operating optimization of large scale problems of power plants or oil refineries to meet a given CO_2 reduction target while meeting the demand at a minimum overall cost. The structural optimization approach can be performed effectively with MINLP techniques. The integer variables in the MINLP problem can be used to model, for example sequences of events, alternative candidates, existence or non-existence of units (in their 0–1 representation); while the continuous variables are used to model the input-output and interaction among individual units/operations.

Currently several commercial optimizer-simulator packages, such as ASPEN PLUS, SPEEDUP, GAMS etc. are available and have been applied to many practical problems (Kocis and Grossmann 1989; Diaz and Bandoni, 1996; Turkay and Grossmann, 1996).

In this research, the optimization problem for power plants and oil refinery will be solved using GAMS. GAMS is an algebraic modeling system which has a library of solvers for modeling linear, nonlinear and mixed integer optimization problems. In the past, the user had to spend more time on computer coding to solve mathematical programming problem. Substantial progress was made recently with the development of algorithms and computer codes, reducing the time required to form a solution procedure. Therefore, more time can be allocated to the development of models rather

than on coding and solver development. GAMS has implemented a MINLP algorithms (Viswanathan and Grossmann, 1990). GAMS allows the user to concentrate on the modeling problem by defining variables, equations and data and selecting appropriate solvers in a simple way. The user can change the formulation quickly and easily, and can change from one solver to another with little trouble. All algorithms, which are available in GAMS, can be used without requiring changes in existing models, resulting in significant reduction in development time. The basic GAMS system is file oriented with no special editor or graphic input/output routines.

2.5.1 Energy Model and CO_2 in Electricity Sector

Several papers have been published which addressed the cost effectiveness of CO_2 control strategies in power plants. Yamaji et al. (1993) presented a study on the effectiveness of CO_2 emission control strategies in Japan. They considered applying a CO_2 tax as one control option.

Wu et al. (1994) analyzed the characteristics of China's CO_2 emissions from the energy sector and proposed several options for mitigating CO_2 emissions on a large scale, such as strengthening energy conservation, introducing energy-efficient technologies into the energy system, speeding up non-fossil fuels development and importing oil and natural gas as substitute for coal. They evaluated the effectiveness of the different CO_2 mitigation options but they did not employ any optimization techniques.

Rovere et al. (1994) summarized a cost benefit analysis based on applying alternative energy strategies, such as increasing hydroelectric power for abatement of carbon emissions in Brazil.

Elmahgary et al. (1994) considered a case study in Egypt to mitigate CO_2 emissions from the energy sector. They considered several technologies including energy conservation, fuel switching and use of renewable energy to decrease CO_2 emissions.

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The impact of energy conservation measures on the economy of the country was found to be positive.

Climaco et al. (1995) developed new techniques that incorporate multiple objective linear programming and demand-side management (DSM). The techniques were able to determine the minimum expansion cost by changing the levels and forms of the electricity use by the consumers and generating alternatives from the supply side. The model also considered the emissions caused by the electricity production.

Bai and Wei (1996) developed a linear programming model to evaluate the effectiveness of possible CO_2 mitigation options for the electric sector. The options considered were fuel alternatives, energy conservation, reduced peak production and improved electric efficiency. The results indicated that energy conservation can significantly reduce CO_2 emissions only when combined with reduced peak production and improved electric efficiency.

Noonan et al. (1997) studied and developed an optimization program for planning investments in electricity generating systems. The optimization program determined the mix of plant types, sizes of the individual plants to be installed and the allocation of installed capacity to minimize total discounted cost while meeting the system's forecasted demand for electricity. This problem is referred to as the Generation Planning Problem (GPP). In order to comply with the variation in electricity demand, the electricity demand to be met was described by the Load Duration Curve (LDC). The mathematical model was solved using Benders' Decomposition Method (BDM) and it was applied to New England Generation Planning Task Force**.**

Spyros (1997) developed a methodology to investigate strategies to reduce CO_2 emissions from the electricity sector. The model enabled the investigation of optimal strategies for satisfying a limit on CO_2 emissions from the electricity sector. The model also can estimate the cost of CO_2 emission limit and the optimal tax required to achieve the optimal strategy for reducing emissions to a desired level. In selecting the optimal

strategy, the methodology considered commercial technologies and other new types of technology such as new coal or lignite, natural gas technologies with CO_2 capture.

Mavrotas et al. (1999) developed a mixed integer multiple objective linear programming (MOLP) model applied to the Greek electricity generation sector for identifying the number and output of each type of power units needed to satisfy the expected electricity demand in the future. Their model is a branch and bound algorithm, which has been modified for the multi-objective case and is capable of generating the complete set of efficient solutions.

Linares and Romero (2000) proposed a methodology that combines several multi-criteria methods to address electricity planning problems within a realistic context. The method was applied to an electricity planning scenario in Spain with a planning horizon set for the year 2030. The model included the following objectives: (1) total cost; (2) CO_2; (3) SO_2; and (4) NO_x emissions as well as the amount of radioactive waste produced.

Yokoyama et al. (2002) formulated a mixed integer linear programming model for the structural design problem to determine an optimal structure of energy supply system to match energy demand requirement, by expressing the selection and on/off status of operation of equipment by binary variables and capacities and load allocation of equipment by continuous variables. The effect of equipment performance characteristics on their capacities as well as capital cost, were incorporated into the optimization model. The objective was to minimize annual capital cost, and was evaluated as the sum of the annualized capital and operational costs of energy purchased.

Rao and Rubin (2002), conducted more advanced plant-level analyses of CCS by incorporating uncertatinty and variablility for about 30 independent model parameters using the Integrated Environmental Control Model (IECM). This analysis considered the following effects: energy efficiency improvement, changing fuel prices, response of

electricity demand on price changes, effect of electricity demand by incorporating advanced power generation and CCS technologies, fuel switching and plant retirement.

Genchi et al. (2002) developed a prototype model for designing regional energy supply systems. Their model calculates a regional energy demand and then recommends a most effective combination of eleven different power supply systems to meet required CO_2 emission targets with minimum cost. The new energy system, to be installed, included co-generation systems, garbage incineration and solar energy.

Zhou et al. (2004) developed an expert system to assist power plant decision makers in selecting an economical and efficient pollution control system that meets new stringent emission standards. A fuzzy relation model and a Gaussian dispersion model were integrated into the expert system.

Antunes et al. (2004) presented a multiple objective mixed integer linear programming model for power generation expansion planning that allows the consideration of modular expansion capacity values of supply side options.

Rubin et al. (2004) developed the Integrated Environmental Control Model (IECM) to provide an analytical tool to compare various environmental control options for fossil-fuel power plants. The model is built in a modular fashion that allows new technologies to be easily incorporated into an overall framework. A user can then configure and evaluate a particular environmental control system design. Current environmental control options include a variety of conventional and advanced systems for controlling SO_2, NOx, CO_2, particulates and mercury emissions for both new and retrofit applications. The IECM framework now is being expanded to incorporate a broader array of power generating systems and carbon management options.

Johnson and Keith (2004) proposed a linear programming (LP) model to illustrate the importance of considering competition between new plant with and without capture, and the economic plant dispatch in analyzing mitigation costs. Model results illustrate how

both, carbon capture and sequestration technologies and the dispatch of generating units vary with the price of carbon emissions, and thereby determine the relationship between mitigation cost and emissions reduction.

Wise et al. (2004) developed the Carbon Management Electricity Model (CMEM), a new electricity generation and dispatch optimization model to explore the effect of carbon taxes and constraints on investment and operating decisions for new generating capacity as well as on the operation and market value of existing plants in a specific region of the United States and across three carbon dioxide scenarios. In computing the least cost decision to meet the constraints, the model considered the economic trade offs among several factors, including capital costs for new plants, capacities of existing plants, efficiencies, operation and maintenance cost, availabilities for new and existing plants, CCS technologies for new plants and CCS retrofit for existing units, natural gas and coal prices, carbon prices resulting from the imposed CO_2-emissions constraints and the hourly load profile of electricity demand.

Gielen (2004) analyzed the potential role of CO_2 capture and storage for 15 regions in the world, using the IEA Secretariat's Energy Technology Perspectives (ETP) model. This linear programming model determined the least cost energy system for the period 2000-2050. Emission reduction strategies accounted in this model include renewable energy, nuclear energy, energy efficiency, as well as CCS on existing and new plants. Model results indicate that electricity production from coal fired power plants without CCS will be ceased by 2030 and no new coal fired power plants without CCS are being built.

Davison et al. (2004) reviewed the technologies that could be used to capture CO_2 from use of fossil fuels. They described three main overall methods of capturing CO_2 in power plants: post combustion capture, oxyfuel combustion and pre-combustion capture. They also discussed the impacts of different CO_2 capture technologies on the thermal efficiencies and costs of power plants based on recent studies carried out by process technology developers and plant engineering contractors.

More recently, Hashim et al. (2005) considered the problem of reducing CO_2 emissions from a fleet of generating stations consisting of coal, natural gas, nuclear, hydroelectric, and renewable energy. The problem was formulated as a mixed integer linear program (MILP) and implemented in GAMS. Two carbon dioxide mitigation options were considered in their study: fuel balancing and fuel switching. The optimization results showed that fuel balancing can contribute to the reduction of the amount of CO_2 emissions by up to about 3%. Beyond 3% reductions, more stringent measures that include fuel switching and plant retrofitting have to be employed. Improving power plant efficiency was not considered in their study.

In another study, Hashim et al. (2006) considered three potential CO_2 mitigation strategies which include: fuel balancing (optimal adjustment of the operation of existing generating stations to reduce CO_2 emissions without making structural changes to the fleet), fuel switching (switching from carbon intensive fuel to less carbon intensive fuel, e.g. coal to natural gas) and retrofitting of carbon capture and storage (CCS) on existing coal-fired power plants. The model is illustrated on a case study to Ontario Power Generation (OPG).

Several studies have been conducted in order to increase power plant efficiency and, as a consequence, decrease CO_2 emissions. The thermal efficiency of a plant can be defined as a percentage determined by the ratio of electrical energy output to the fuel energy input. Increased plant efficiency means that less coal is burned (producing less CO_2) for the same power output (Audus, 1993). Improved efficiency in any power plant can produce noticeable reductions in CO_2 emissions- typically, a 1% point gain in efficiency reduces CO_2 output by 2% (Torrens and Stenzel, 2001).

Boiler efficiency in any power plant is a function of size, capacity factor, the fuel fired, operating and ambient conditions and unit design. Existing coal boilers use mostly subcritical or in some cases supercritical steam cycles. A supercritical steam cycle operates above the water critical temperature ($374^{\circ}C$) and critical pressure (221 bar) where water can exist only in the gaseous phase. Subcritical systems historically have

achieved thermal efficiencies (HHV) of 34 to 36%. Supercritical systems can achieve thermal efficiencies 3 to 5% higher than subcritical systems (US Department of Energy, 2001).

There are various measures that can be used to increase power plant efficiency relative to current design. Increasing the steam pressure and temperature can increase the efficiency by nearly 2%. Controlling the excess air is an important function in boiler operation and reducing the excess air ratio from 25% to 15% can increase the efficiency by about 1%. Controlling the excess air is an important issue since too much air will cool the furnace and carry away useful heat and too little air will lead to incomplete combustion. Using a second reheat stage can add another 1% and decreasing the condenser pressure can further increase efficiency. Table 2.2 shows some actions that can be employed to improve the efficiency of coal power plants (Audus, 1993).

Table 2.2. Some actions for efficiency improvement (Andus, 1993)

Action	Efficiency Improvement (%)
Restore Plant to Design Conditions	
Boiler chemical cleaning	0.84
Reinstate any feedheaters out of service	0.46
Refurbish feedheaters	0.84
Reduce steam leaks	1.0
Reduce turbine gland leakage	0.84
Change to Operational Settings	
Low excess air operation	1.22
Improved combustion control	0.84
Retrofit Improvements	
Extra air heater surface in the boiler	2.1
Install new high efficiency turbine blades	0.98
Install variable speed drives	1.97
Install on-line condenser cleaning system	0.84

For a number of the initiatives listed in Table 2.2, the gain in efficiency stated would appear to be optimistic. For example, low excess air operation might bring slightly more than 1% gain in efficiency. In order to advance practical options for efficiency improvement, a soundly based techno-economic engineering study would need to be undertaken for each station (US Department of Energy, 2001).

Wisconsin Electric Power Company (WEPCO) in the USA has implemented a number of actions to improve the efficiency at five of their coal power plants (US Department of Energy, 2001). These plants are namely Oak Creek, Pleasant Prairie, Port Washington, Presque Isle and Valley. At Oak Creek for example, the efficiency improved by 3.9%. Projects that contributed to efficiency improvements include variable speed drives on the forced and induced draft fans, reduced air in-leakage and feed water heater replacements. At the Pleasant Prairie power plant, the efficiency improved by 3.2%. This improvement came from variable pressure operation, unit and equipment performance monitoring, reduced air in-leakage and installation of variable speed drives. Additional projects may include operation at lower cooling water tower temperatures to improve condenser vacuum and variable speed drives on boiler fans and other large motors. At the Port Washington power plant, the efficiency improved by 11%. This improvement was the result of a major plant renovation project, which included the refurbishment or replacement of most major plant equipment. The result of the project was a restoration of the units to their original capacity and improved efficiency. At the Presque Isle power plant, the efficiency improved by 4%. Some actions that contributed to improvements include reduced air in-leakage, reduced excess boiler O_2, boiler chemical cleaning, CO_2 monitors on the boiler, improved turbine pressure and updated or additional instrumentation. At the Valley power plant, the efficiency improved by 2.3% due to last row turbine blade replacement, variable speed drives for the forced and induced draft fans and reduced air in-leakage.

Several power plants in different countries have implemented improvement technologies for increasing power plant efficiency. For example, Ontario Power Generation (OPG) was involved in a project to help Jordan to improve the efficiency of its oil fuelled electricity generating units (Jordan Central Electricity, 2000). In 2000, the project was completed and the total emissions savings resulting from the project estimated over a three year period was about 6% of carbon dioxide (Jordan Central Electricity, 2000).

Although increasing plant efficiency is one way to reduce CO_2 emissions but it can not achieve a high percent reduction. The most promising option to mitigate CO_2, while still using fossil fuel based power plant, is CCS.

2.5.2 Planning Model and CO_2 in the Petroleum Refining Sector

Production planning is the discipline related to the macro-level problem of allocation of production capacity and production time (with less emphasis on the latter); raw materials, intermediate products, and final products inventories; as well as labour and energy resources. Its primary objective is to determine a feasible operating plan consisting of production goals that optimizes a suitable economic criterion, typically maximizing total profit over a specific extended period of time into the future, typically in the order of a few months to a few years; given marketing forecasts for prices, market demands for products, and considerations of equipment availability and inventories (Birewar and Grossmann, 1995). In essence, its fundamental function is to develop a good set of operating goals for the future period. In the present settings of the oil and gas or hydrocarbon industry, planning requirements have become increasingly difficult and demanding because of the need to produce more varied, higher-quality products while simultaneously meeting increasingly tighter environmental legislations and policies as reported by Fisher and Zellhart (Bodington, 1995).

On the other hand, production scheduling, which is outside the scope of this research, in the context of the chemical processing industry, deals with micro-level problems embedded in the production planning problem that involves deciding on the methodology that determines the feasible order or sequence and timing in which various products are to be produced in each piece of equipment so as to meet the production goals that are laid out by the planning model. Its major objective is to efficiently utilize the available equipment among the multiple types of products to be manufactured, to an extent necessary to satisfy the production goals by optimizing a suitable economic or systems performance criterion; typically over a short-term time horizon ranging from

several shifts to several weeks. Scheduling functions specify the task(s) of each stage of production and this includes defining and projecting the inputs to and outputs from each production operation. It is particularly required whenever a processing system is used to produce multiple products by allocating the available production time between products (Sahinidis et al., 1989; Birewar et al., 1995; Bodington, 1995).

Hartmann (1998) stresses the differences between a planning model and a scheduling model. In general, process manufacturing planning models consider economics of the operations by handling the issues of what to do and how to do it whereas process manufacturing scheduling models consider feasibility of the operations by addressing the question of when to do it. In particular, planning models ignore changeovers and treat products grouped into aggregated families. Conversely, scheduling models explicitly consider changeovers and consider products in greater details, including the shipment of specific orders for specific products to specific customers.

Fisher and Zellhart (Bodington, 1995) also emphasize that a planning model differs from a daily scheduling model or an operational process controller. For example, they point out that the product or process yields predicted or estimated in the planning model should not be expected to be used exactly in executing operating conditions. This is because planning models are almost always an average over time. As opposed to planning models, operations are not averaged over the scheduling period as time and operations move continuously from the beginning of the particular period to the end. The schedule is revised as needed so that it always starts from what is actually happening with revisions typically occur on each day or on each shift.

As was mentioned in the previous section, oil refinery is one of the most complex chemical industries involving different processes with various possible connections. The aim in refinery operation is to generate as much profit as possible by converting crude oils into valuable products. Mathematical programming or optimization has become indispensable tools to realize this goal. Linear programming (LP) is the most widely used technique in refinery operation optimization, which is called planning and

scheduling in industry. The goal in planning is to determine high-level decisions such as production levels and product inventories for given marketing demands.

Linear programming (LP) is an approach to the solution of a particular class of optimization problems. It is concerned with finding values for a set of variables that maximize or minimize a linear objective function of the variables, subject to a set of linear equality or inequality constraints. Linear programming was first proposed by Dantzig in 1947 (Edgar, 2001) to refer to the optimization problems in which both the objective function and the constraints are linear. LP problems exhibit the special characteristic that the optimal solution of the problem must lay on some constraints or at the intersection of several constraints. Dantzig first proposed the most popular algorithm in LP called the simplex algorithm.

Despite the many contributions that have been reported on planning models, very few can be found that specifically address the petroleum refining industry. Symonds (1956) developed an LP model for solving a simplified gasoline refining and blending problem. The advantage of LP is its quick convergence and ease of implementation. Allen (1971) presented in his paper an LP model for a simple refinery that consists mainly of three units; distillation, cracking and blending.

One of the first contributions to consider nonlinearity in production planning is that of Moro et al. (1998). A nonlinear planning model for refinery production was developed. The model represented a general refinery topology. Also, a real world application was developed for the planning of diesel production in one of the refineries in Brazil. The model was solved and the results were compared to the current situation where no computer algorithm was being used. The developed model gives a better result compared to the current situation.

Pinto and Moro (2000) also developed a nonlinear planning model for refinery production. The model described represents a general petroleum refinery and its framework allows for the implementation of nonlinear process models for few units as

well as blending relations. This model assumes the existence of several processing units, producing a variety of intermediate streams, with different properties, that can be blended to constitute the desired products. Two real world applications are developed and in both cases, different market scenarios were analysed using the planning model and the results were compared with the current situation. However, the model was based on the assumption that many of the refinery processes are linear which affect the overall predictability of the model.

Pinto et al. (2000) discussed planning and scheduling applications for oil refinery operations. They presented a nonlinear planning model in the first part similar to the one developed earlier by Moro et al. (1998). In the second part, they addressed scheduling problems in oil refineries that were formulated as mixed integer optimization models and relied on both continuous and discrete time representations. The paper considered the development and solution of optimization models for short term scheduling of a set of operations including products received from processing units, storage and inventory management in intermediate tanks, blending in order to attend oil specifications and demands, and transport sequencing in oil pipelines. Important real-world examples on refinery production and distribution were reported. The diesel distribution problem at one refinery in Brazil and the production problems related to fuel oil, asphalt and LPG were considered.

Zhang and Zhu (2000) showed in their paper a novel modelling and decomposition strategy for overall refinery optimization to tackle large scale optimization problems. The approach was derived from an analysis of the mathematical structure of a general overall plant model. This understanding forms the basis for decomposing the model into two levels. These levels were a site level (master model) and a process model (sub-models). The master model determined common issues among the processes. Then, sub-models optimized the individual processes. The results from these sub-models were fed back to the master model for further optimization. This procedure terminates when convergence criteria are met. Linear yield correlations were used in their study.

Zhang et al. (2001) studied a simultaneous optimization strategy for overall integration in refinery planning. They presented a method for overall refinery optimization through integration of the hydrogen network and the utility system with the material processing system. To make the problem of overall optimization solvable, they adopted a decomposition approach, in which material processing was first optimized using linear programming (LP) techniques to maximize the overall profit. Then, the supporting systems, including the hydrogen network and the utility system, were optimized to reduce operating costs for the fixed process conditions determined from the LP optimization.

Recently, Li et al. (2005) presented a refinery planning model that utilizes simplified empirical non-linear process models with considerations for crude characteristics, products' yields and qualities. The study integrated crude distillation, FCC and product blending modules into refinery planning models.

Neiro and Pinto (2005) studied multi-period optimization for production planning of petroleum refineries. The developed model was based on a nonlinear programming formulation that was developed to plan production over a single period of time. First, the model incorporates multiple planning periods and the selection of different crude oil types. Uncertainties related to petroleum and product prices as well as demand were then included as a set of discrete probabilities. The model was successfully applied to a real world case study.

No refinery planning models taking into consideration CO_2 mitigation options were found in the literature.

CHAPTER 3

MODEL DEVELOPMENT FOR POWER PLANT

3.1 Introduction

This chapter presents the mathematical model for power plants. This section has been divided into 4 phases. Phase 1 shows the word and mathematical statements of the problem to be solved. Phase 2 presents a superstructure framework that includes many alternatives to reduce CO_2 emissions from power plants. The mathematical model that is used to solve the problem is developed in Phase 3. The mathematical models developed in phase 3 is then applied to a case study in the next chapter and coded into GAMS in Phase 4 to find the best strategies for the energy sector in order to reduce CO_2 to a given level with a minimum overall cost.

For power plants, structural and operating optimization are modified to meet a given CO_2 reduction target while maintaining or enhancing the electricity output to the grid at minimum overall cost. The structural optimization approach for the energy sector can be performed effectively with MINLP techniques. The integer variables in MINLP problem can be used to model, for example sequences of events, alternative candidates, existence or non-existence of units (in their 0–1 representation), while continuous variables are used to model the input-output and interaction among individual units/operations. A summary of these phases is given in Figure 3.1.

Phase 1: Statement of the problem
"given a CO_2 reduction target, what is the best combination of power plants, fuels, efficiency improvement technologies for a set of power plants to pursue ?"

Phase 2: Superstructure representation			
Base case	*Fuel balancing*	*Fuel switching*	*Efficiency improvement*

Phase 3: Mathematical model development	
Objective Minimize annual total cost	*Constraints* Demand satisfaction, capacity constraints on existing plants, fuel selection and plant shut down, selection of efficiency improvement technologies, upper & lower boundaries on operational changes, CO_2 emission constraints

Phase 4: Model application and coding
Case study   Consider 3 mitigation strategies: fuel balancing, fuel switching from coal to natural gas and efficiency improvement to meet electricity demand requirement and satisfy certain CO_2 reduction target
Code the mathematical model into GAMS

Figure 3.1. Steps in model development for power plant

3.2 Phase 1: Statement of Problem

For power plants, the basic problem can be addressed as follows: "having a number of power plants that are emitting CO_2 to the environment, the target is to find the best technologies and alternatives, such as fuel balancing, fuel switching or improving power plants efficiency, to meet electricity demand at minimum cost, while reducing CO_2 emissions to a specific target".

The mathematical statement of the above problem statement consists of minimizing an objective function while observing equality and inequality constraints. It can be written in a general form as the following MINLP (Mixed Integer Non-Linear Programming):

$$\min_{x,y} f(x,y,p)$$

such that,

$$h(x,y,p) = 0$$
$$g(x,y,p) \leq 0$$

$$x \in X \leq R^n \qquad \text{(x is a vector of continuous variables)}$$
$$y \in Y = \{0,1\} \qquad \text{(y is a vector of binary variables)}$$
$$p \qquad\qquad \text{(p is a vector of parameters)}$$

Variables

The continuous variables, x, are real numbers that may represent flow rates of fuels, electricity generated from each power plant, capacity factor, CO_2 emissions etc. The binary variables, y, are assigned (0-1) to represent the existence or non-existence of technology for power plants efficiency improvement.

Objective Function

In this thesis the objective for the power plant model is to minimize the total cost of reducing CO_2 emission by a specified amount. f(x,y,p) is a single objective function which represents the total cost including operating costs for generating electricity and

retrofit costs for fuel switching and other retrofit costs for implementing the technology for power plants efficiency improvement.

Constraints

$h(x,y,p) = 0$, are the equality constraints; these equations would include operating cost models for each type of power plant and cost models for power plants efficiency improvement.

$g(x,y) \leq 0$ are the inequality constraints which correspond to design specifications, restrictions and feasibility constraints. The constraints considered in this work are as follows:

- Quality constraints: The total CO_2 emissions must be less than or equal to a given CO_2 reduction target.
- Demand constraints: The total electricity generated must be equal or greater than the nominal electricity demand.
- Limitations of process/size: Capacity factor for each power plant must be between 0 and 1.
- Binary constraints: Existence or non existence of technology for power plant efficiency improvement.

3.3 Phase 2: Superstructure Representation

In order to solve the problem stated earlier in this chapter, a superstructure will be developed for power plants. The three CO_2 mitigation options considered in this section are:

1. Fuel balancing, which basically consists of increasing the production from non fossil fuel power plants and in decreasing the production from fossil fuel power plants.
2. Fuel switching, which involves a structural change since the plant is run using less carbon intensive fuels such as replacing coal by natural gas.
3. Increasing power plant efficiency by different available technologies.

<u>Superstructure of Alternatives for Power Plants</u>

Four different options are presented in this section to illustrate the impact of a CO_2 reduction strategy on the structure of energy supply. The options considered here are fuel balancing, fuel switching and improving power plant efficiency. A superstructure representing all possible alternatives is very complex. Figures 3.2 to 3.5 show the four scenarios starting from the base case without any mitigation option. Here, C, NG, O, N, H and A represent coal, natural gas, oil, nuclear, hydroelectric and alternative energy power plants, respectively. Figure 3.3 gives one simple possible way to decrease CO_2 emissions by increasing electricity production from existing non fossil power plants and decreasing production from existing fossil power plants. Figure 3.4 shows a second option to decrease CO_2 emissions by fuel switching from coal to the less intensive carbon fuel, natural gas. Figure 3.5 shows another set of options for decreasing CO_2 emissions through increasing boilers efficiencies. Only boilers operating with coal are represented in the figure.
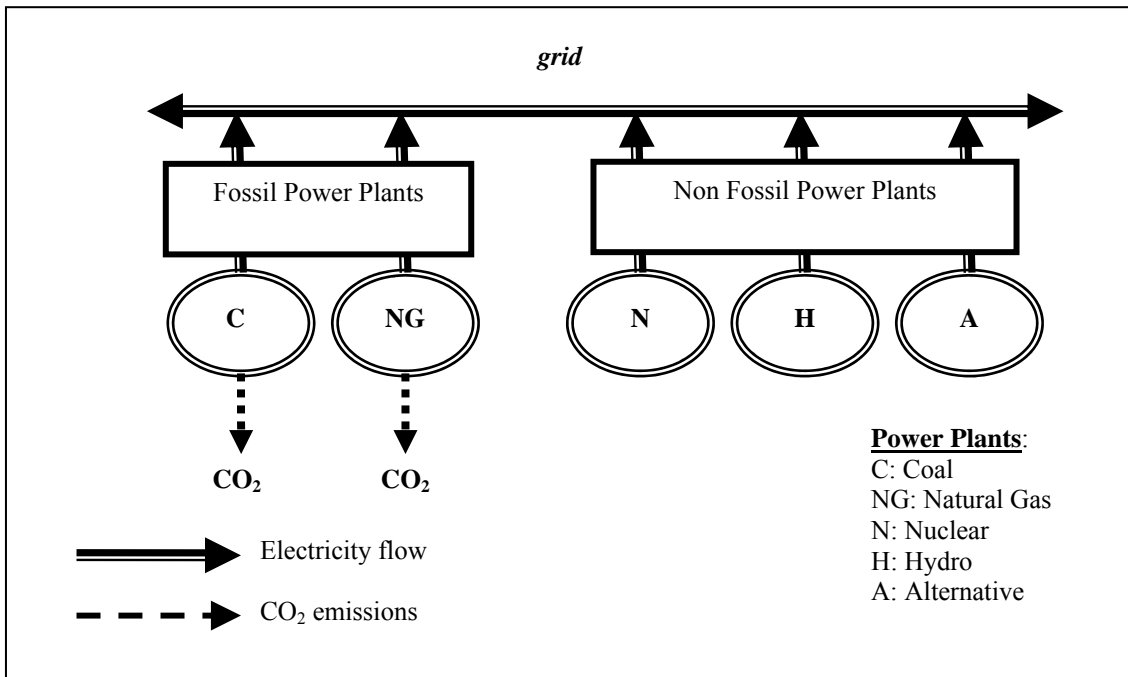
Figure 3.2. Superstructure of base case scenario
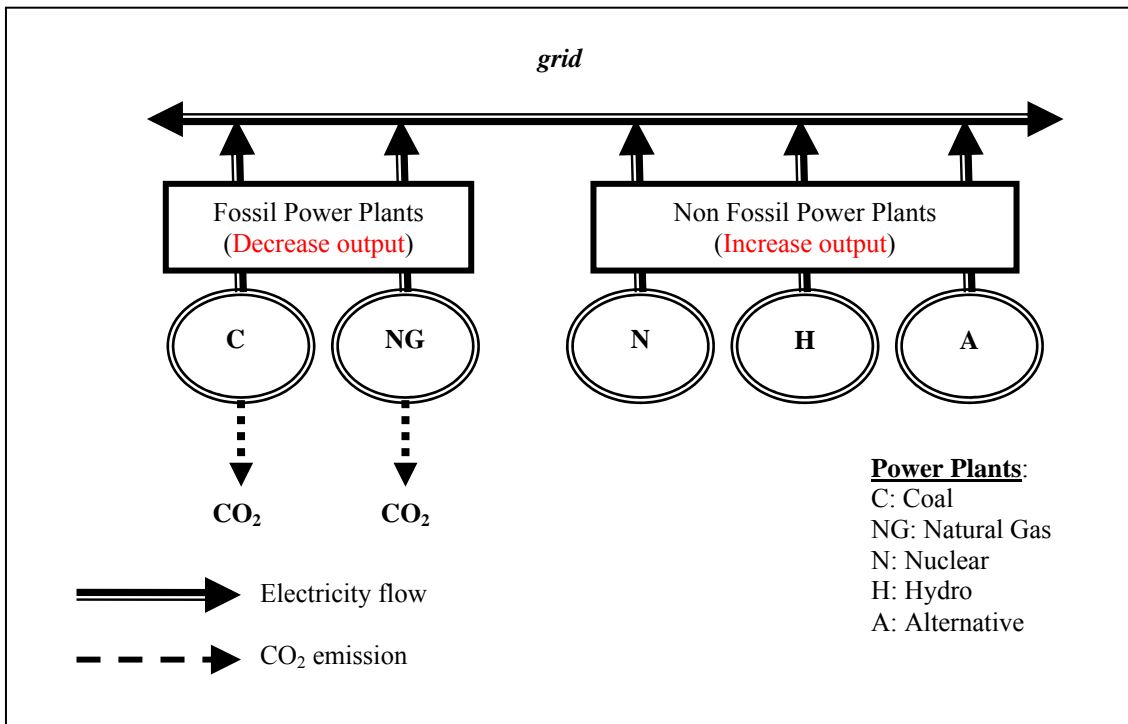
Figure 3.3. Superstructure of fuel balancing

Figure 3.4. Superstructure for fuel switching

Figure 3.5. Superstructure for efficiency improvement

3.4 Phase 3: Mathematical Model Development

A mathematical model to represent the unit operations of the postulated superstructure for the electricity sector was developed. The model corresponds to a system of equalities and inequalities that describe the performance of process units in the superstructure and the objective function.

Large scale optimization model for the energy sector is formulated according to the superstructure presented in the previous section. The model was initially formulated as a Mixed Integer Non-Linear Programming (MINLP) model. The model was then linearized to avoid the difficulties encountered with non linear models. Hence, the MINLP model was reformulated as a Mixed Integer Linear programming (MILP) but still keeping the consistency of the solution. This can be accomplished by using exact linearization method. This model was implemented in GAMS (General Algebraic Modeling System). A case study is presented in Chapters 4 to illustrate the application of the model.

This section describes the strategy for developing the model and then presents the actual development of the model. First, fossil and non fossil power plants are defined as different sets. Then, the set of boilers is defined for each power plant. The interest here is on the fossil fuel power plants since non fossil fuel power plants do not emit much CO_2. The model is then formulated as MINLP. The binary variables represent the selection of fuel and technology for power plant efficiency improvement. Since solving linear model is easier and ensures finding a global optimum, the model is linearized and solved as MILP. The output of the model finds the best mix of electricity generation, fuel switching and selection of technologies for power plant efficiency improvement with minimum overall cost of electricity generation.

In order to efficiently compute this large scale optimization problem, model reduction has been applied for the sake of simplification. We first develop an optimization model that represents the electricity generation fleet. This optimization problem is decomposed

into two main groups representing fossil-fuel and non fossil fuel power plants. Non fossil power plants generate electricity without emitting CO_2 and their operating cost is cheaper than the operational cost of existing fossil fuel power plants with and without CO_2 mitigation. Therefore, the existing non fossil power stations will be operated at maximum capacity in order to maximize their contribution to the electricity demand requirement while minimizing the total cost.

Two main groups of continuous variables are defined as:

(1) E_{ij} representing the electricity generated/load distribution from the i^{th} fossil fuel boilers using j^{th} fuel type

(2) E_i representing electricity generated/load distribution from the existing non fossil power plants (nuclear, hydroelectric, alternative energy power plants).

There are two sets of binary variables in this MINLP model:

(1) Fuel switching on i^{th} coal fired boilers (e.g. coal to natural gas) can be represented by a binary variable, $X_{i,j}$

$$X_{i,j} = \begin{cases} 1 & \text{if } j^{th} \text{ fuel is used in } i^{th} \text{ boiler} \\ 0 & \text{otherwise} \end{cases}$$

(2) Selection of technology k for efficiency improvement can be represented by a binary variable, $Y_{i,k}$

$$Y_{i,k} = \begin{cases} 1 & \text{if technology k is applied in the } i^{th} \text{ boiler} \\ 0 & \text{otherwise} \end{cases}$$

The mathematical model consists of an objective function to be minimized and equality and inequality constraints. The objective of the model is to find the best strategy or mix of strategies to reduce CO_2 up to a certain target with minimum overall cost for electricity generation while meeting the demand.

The objective function can be written as:

Minimize objective ($/yr) = Sum of operating cost for electricity generation from fossil fuel power plants + Sum of operating cost for electricity generation from non fossil fuel power plants + Retrofit cost for switching from coal to natural gas + Retrofit cost for applying technology for efficiency improvement.

The objective function can be written as:

$$Z = \underbrace{\sum_{i \in F}\sum_{j} C_{ij} E_{ij}}_{\substack{\text{Cost of electricity generation} \\ \text{from fossil fuel power plant}}} + \underbrace{\sum_{i \in NF} C_{i} E_{i}}_{\substack{\text{Cost of electricity generation} \\ \text{from non-fossil fuel power plant}}} + \underbrace{\sum_{i \in F}\sum_{j} R_{ij} X_{ij}}_{\substack{\text{Retrofit cost for switching} \\ \text{from coal to natural gas}}} + \underbrace{\sum_{i}\sum_{k} C_{ik} Y_{ik}}_{\substack{\text{Cost of applying technology} \\ \text{for effeciency improvement}}} \quad (3.1)$$

Where Z ($/yr) is annualized capital and operating cost of the fleet of power stations; F represents the set of fossil power stations that includes coal and natural gas; NF represents the set of non-fossil power stations that includes nuclear, hydroelectric and wind turbine; i is the index for the power plant; j is the index for the type of fuel (coal or natural gas); k is the index for the technology applied to increase power plant efficiency; C_{ij} ($/MWh) is cost of electricity generation if fuel j is used in fossil power plant i; C_i ($/MWh) is the cost of electricity generation for non fossil fuel power plants i; C_{ik} ($/yr) is the cost of applying improvement technology k in plant i given; E_{ij} (MWh/yr) is the amount of electricity generated from i^{th} power plant if fuel j is used; E_i (MWh/yr) is the amount of electricity generated from i^{th} non fossil power plants; R_{ij} ($/yr) is the retrofit cost to switch from coal to natural gas; X_{ij} is a binary variable either to switch plant i to natural gas or not; Y_{ik} represents a binary variable either to implement improvement technology k for efficiency improvement in plant i or not.

The objective is to minimize, (Z), the total annualized cost of operating a fleet of generating stations while satisfying the electricity demand and specified CO_2 reduction targets. The first term in equation (3.1) above represents the cost associated with electricity generated from fossil power plants whereas the second term shows the cost for electricity generated from non-fossil power plants. The third term represents the

retrofit cost if the fuel is to be switched from coal to natural gas. The last term is the cost associated with applying technologies on fossil fuel power plants for efficiency improvement.

Constraints:

The constraints for power demand satisfaction, fuel selection and emission reduction are given in details as follows:

a) Power demand satisfaction:
The electricity generated from all power plants must be equal to or greater than the demand (D).

$$\sum_{i \in F} \sum_{j} E_{ij} + \sum_{i \in NF} E_i \geq D \tag{3.2}$$

b) Fuel selection or plant shut down:
For each fossil fuel power plant i, the plant either operates with a given fuel or is shut down. For this reason, a binary variable is introduced to represent the type of fuel used in a given fossil fuel plant. $X_{ij}=1$ if fuel j is used in plant i otherwise it is 0.

$$\sum_{j} X_{ij} \leq 1 \qquad \forall i \in F \tag{3.3}$$

c) Upper bound on operational changes:
The adjusted electricity generated from each power plant should be less than or equal to a certain percentage higher than current production.

$$E_{ij} \leq (1 + r_i) E_i^{current} X_{ij} \qquad \forall i \in F \tag{3.4}$$

$$E_i \leq (1 + r_i) E_i^{current} \qquad \forall i \in NF \tag{3.5}$$

This constraint set requires that the electricity produced from any plant i should not exceed the current electricity produced from the same plant by r_i which is the maximum increase in the base load due to operational constraints.

d) Lower bound on operational changes:

These constraints introduce a lower bound for each power plant and the plant production must be at least equal to this lower limit or otherwise the plant should be shut down. The electricity generated from each power plant must be greater than some minimum (E_i^{min}), otherwise the plant will be shut down.

$$E_{ij} \geq E_i^{min} X_{ij} \qquad \forall i \in F \tag{3.6}$$

$$E_i \geq E_i^{min} \qquad \forall i \in NF \tag{3.7}$$

e) Emission constraints:

The CO_2 emitted from electricity generation must satisfy a CO_2 reduction target. Different technologies, k, to increase the power plant efficiency are implemented in the mathematical model. It is assumed that the effects of these technologies is additive. If this is not the case, then different sets or combinations of technologies can be defined as a single composite technology with a proper corresponding overall efficiency.

$$\sum_{i \in F} \sum_j CO_{2ij} \left(1 - \sum_k \varepsilon_{ik} Y_{ik}\right) E_{ij} \leq (1 - \%CO_2) CO_2 \tag{3.8}$$

CO_{2ij} is the CO_2 emissions from fossil fuel power plant i in (million tonnes per MWh); $\%CO_2$ is reduction target; CO_2 is total fleet CO_2 emissions in (million tonnes per year); ε_{ik} is the gain in efficiency associated with applying technology k in coal power plant i. Y_{ik} is a binary variable defined earlier.

f) Technology selection:

A binary variable (Y_{ik}) is introduced in the model to represent whether technology k for efficiency improvement should be implemented in power plant i or not.

$$\sum_k Y_{ik} + Card(K) * X_{ij\text{æ}ng} \leq Card(K) \qquad \forall i \in F \tag{3.9}$$

Where Card(K) is the cardinality of the set of technologies k. $X_{ij \in NG}$ is a binary variable representing running plant i with natural gas fuel. This constraint imposes the fact that no improvement technology should be implemented in a plant that is to be switched from coal to natural gas.

g) Non-negativity constraints:
The electricity produced from all power plants must be greater than zero.

$$E_{ij} \geq 0 \quad and \quad E_i \geq 0 \tag{3.10}$$

The resulting model is formulated as a mixed integer non linear program (MINLP) because of a constraint set where there is a multiplication of a decision variable (E_{ij}) and a binary variable (Y_{ik}) in the CO_2 emissions term (equation 3.8). The model has been linearized and proved to have the same optimum as the original one; the linearization and proof are given in the next section:

3.4.1 Model Linearization

The emission constraint (3.8) is the one that causes non-linearity to the model. The nonlinear equation is:

$$\sum_{i \in F} \sum_j CO_{2ij} \left(1 - \sum_k \varepsilon_{ik} Y_{ik} \right) E_{ij}$$

The non-linearity is due to the product ($Y_{ik} E_{ij}$). Linearization can be performed by first defining a new variable for this product as follows:

Let $\gamma_{ijk} = Y_{ik} E_{ij}$ (non-linear term) $\tag{3.11}$

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The term can be linearized by adding these constraints to the model:

$$0 \le \gamma_{ijk} \le E_{ij} \tag{3.12}$$

$$E_{ij} - E_{ij}^{\max}(1 - Y_{ik}) \le \gamma_{ijk} \le E_{ij}^{\max} Y_{ik} \tag{3.13}$$

Where $E_{ij}^{\max}$ is a maximum upper bound on E_{ij}.

Proof:

From equation (3.11), we want to show that $\gamma_{ijk} = 0$ if $Y_{ik} = 0$

and $\gamma_{ijk} = E_{ij}$ if $Y_{ik} = 1$

Case 1: (*No technology is selected*)

$Y_{ik} = 0$

Since $\gamma_{ijk} = Y_{ik} E_{ij}$ (from equation 3.11),   then we want to show that indeed $\gamma_{ijk} = 0$

Equation (3.12) becomes:

$$0 \le \gamma_{ijk} \le E_{ij} \tag{3.14}$$

And equation (3.13) becomes:

$$E_{ij} - E_{ij}^{\max} \le \gamma_{ijk} \le 0 \tag{3.15}$$

From equations (3.14) and (3.15), γ_{ijk} will be chosen to be zero.

Case 2: (*technology is selected*)

$Y_{ik} = 1$

Since $\gamma_{ijk} = Y_{ik} E_{ij}$ (from equation 3.11), then we want to show that indeed $\gamma_{ijk} = E_{ij}$

Equation (3.12) becomes:

$$0 \le \gamma_{ijk} \le E_{ij} \tag{3.16}$$

And equation (3.13) becomes:

$$E_{ij} \le \gamma_{ijk} \le E_{ij}^{\max} \tag{3.17}$$

From equations (3.16) and (3.17), γ_{ijk} is set equal to E_{ij}.

3.5 Phase 4: Model Application and Coding

The mathematical model for the energy sector developed in the previous section is illustrated in a case study in chapter 4 and was coded into GAMS. GAMS is a high-level modelling system that provides a flexible framework for formulating and solving linear, nonlinear, mixed integer linear and nonlinear optimization problems. Among other attributes, its syntax allows for declaring associations among equations (objective function, equality constraints, inequality constraints), variables, parameters and scalar. GAMS provides a wide array of solvers to optimize a variety of problem formulation, including linear programs (LPs), nonlinear programs (NLPs), mixed integer linear programs (MILPs), and mixed integer nonlinear programs (MINLPs). The GAMS system is file-oriented with no special editor or graphical input/output routines. The user can change the formulation quickly and easily and can change from one solver to another with little trouble. An overview of GAMS system is illustrated in Figure 3.6.

Figure 3.6 shows that the user must specify all the equations representing the objective function and constraints. In addition the user must specify all the scalars, parameters and variables. The GAMS input file which contained sets, scalar, parameters and variables for the power plants is presented in Appendix B. Finally, the user must choose either to minimize or maximize the objective function and the solver required to solve the optimization problem. The optimization algorithm will determine the solution and yield the optimum objective function by adjusting decision variables. GAMS consists of a language compiler and solvers which operate on an input file in two stages:

Stage 1: *Compilation*. This stage ensures that the input file is understood by GAMS. The compiler checks for errors in the input file, ensuring that the file follows a specific layout, does not contain syntax errors, and uses an appropriate solver. The compiler does not solve the problem or indicate that a solution exists. When the compiler locates errors in the input file, the errors are flagged and written in the output file before GAMS
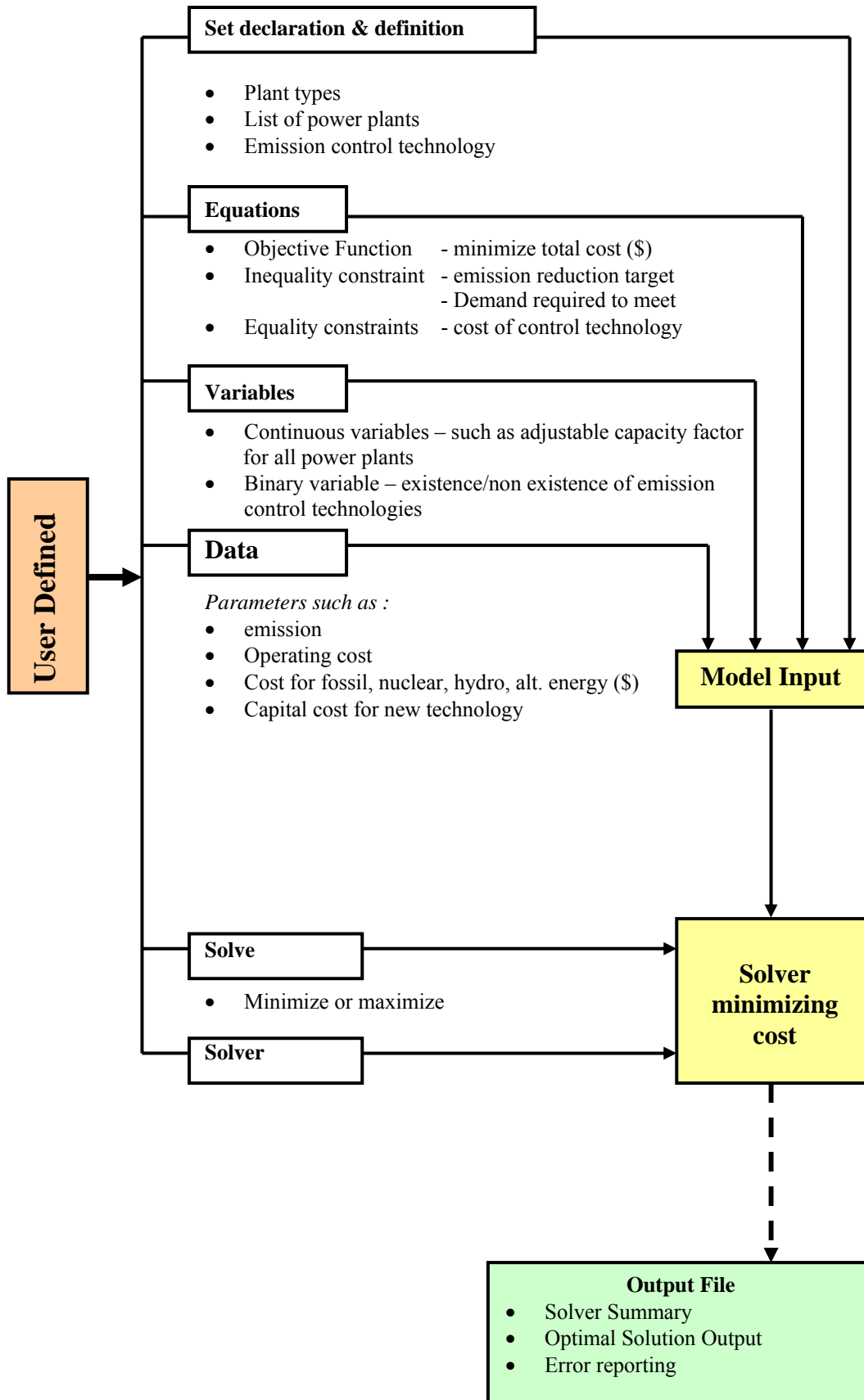
Figure 3.6. The basic GAMS simulator and optimizer system

terminates. The user must modify the input file accordingly. When the compilation is successful, GAMS proceeds to Stage 2.

Stage 2**: *Execution.* Once the input file syntax is correct, GAMS proceeds to carry out the optimisation using an appropriate solver for the problem formulation (e.g., LP, NLP, MIP or MINLP). Note that the solver declared by the user must be applicable to the formulation. For instance, an LP solver cannot be used to solve an NLP. GAMS writes in the output file providing information on whether the solution was obtained, and if so, the solution values. The output can be controlled using the display options in the input file.

CHAPTER 4

CASE STUDY: A MINLP MODEL FOR CO_2 EMISSION REDUCTION IN THE POWER GENERATION SECTOR

4.1 Introduction

The mathematical model developed in Chapter 3 for the power plants is illustrated in this chapter on a case study for Ontario. This section considers the problem of reducing CO_2 emissions from Ontario Power Generation (OPG) by three different options. The first option is fuel balancing in which the production from non fossil fuel power plants is increased while decreasing the production from fossil fuel power plants. The second option for reducing CO_2 emissions is by switching from high carbon content fuel to less carbon content fuel. Typically, this is done here by switching from coal to natural gas. The third option being considered in this section is to apply different technologies for efficiency improvement which might leads to CO_2 emissions reduction. The objective of the model is to find the minimum cost solution for CO_2 mitigation while reducing CO_2 emission by a fixed target.

Ontario Power Generation (OPG), the main electricity producer in Ontario, is one of the largest electricity generators in North America. OPG currently operates approximately 74% of the available generating capacity in Ontario. About 35% of OPG electricity is produced through combustion of fossil fuels, same percentage from nuclear, 29% from hydroelectricity and the remaining 1% comes from renewable energy sources, such as wind turbines.

4.2 Superstructure Development

The superstructure representing the OPG energy supply systems and fuel alternatives is presented here. The following notation is adopted throughout the chapter: C_i, NG_i, O_i, N_i, H_i and A_i represent a set of coal, natural gas, oil, nuclear, hydroelectric and alternative energy power plants, respectively. Figure 4.1 represents OPG current configuration of power stations. The mix of all electricity generated by OPG sources is injected into the grid.
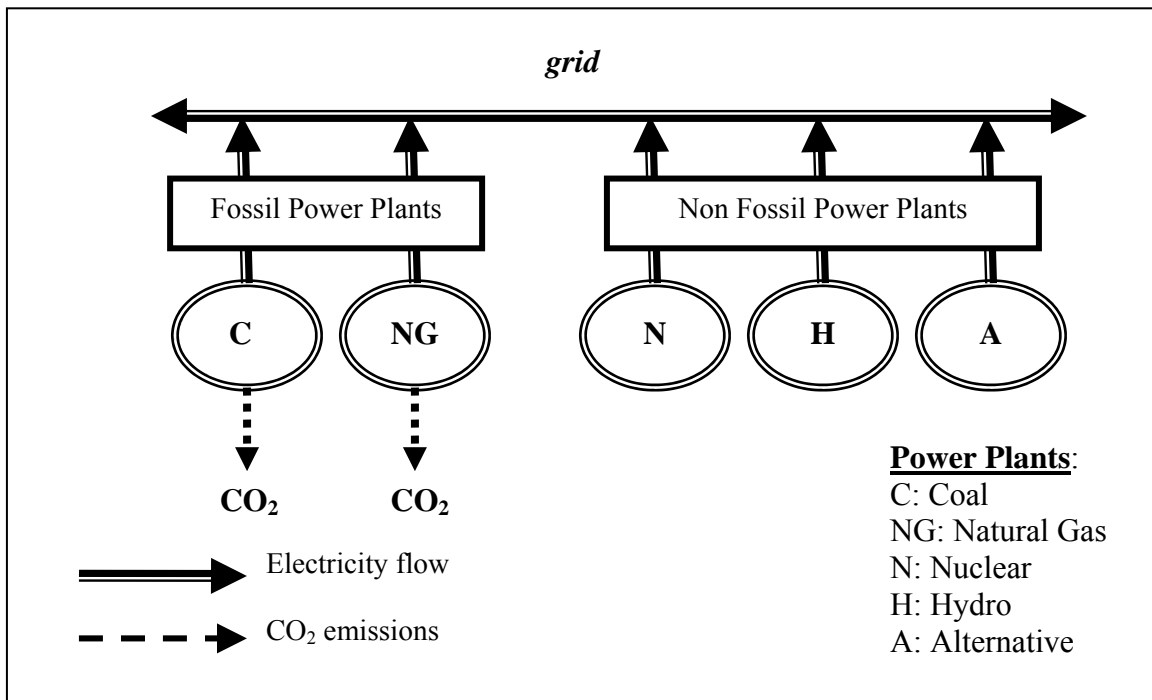
Figure 4.1. Superstructure for OPG's existing fleet

Figure 4.2 illustrates the fuel balancing technique to reduce CO_2 emissions by increasing the load on existing non fossil fuel power plants and decreasing the load on existing fossil fuel power plants.
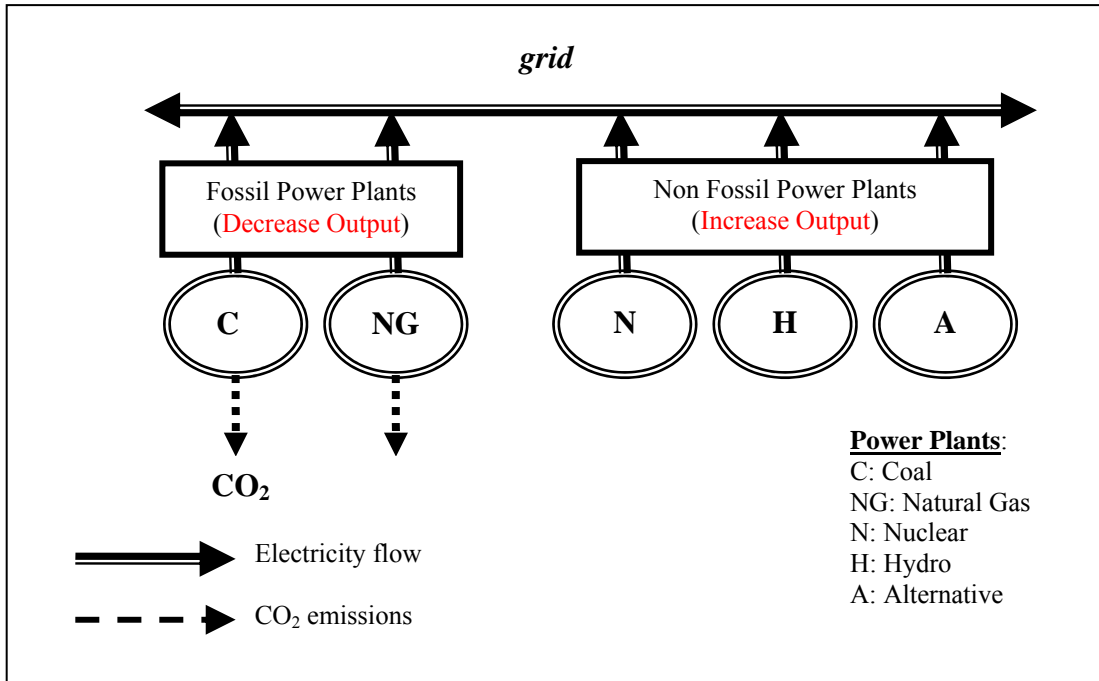
Figure 4.2. Superstructure for fuel balancing

Figure 4.3 illustrates another technique, the so-called fuel switching technique, i.e. switching from carbon intensive fuels to lower carbon intensive fuels, e.g. switching from coal to natural gas.
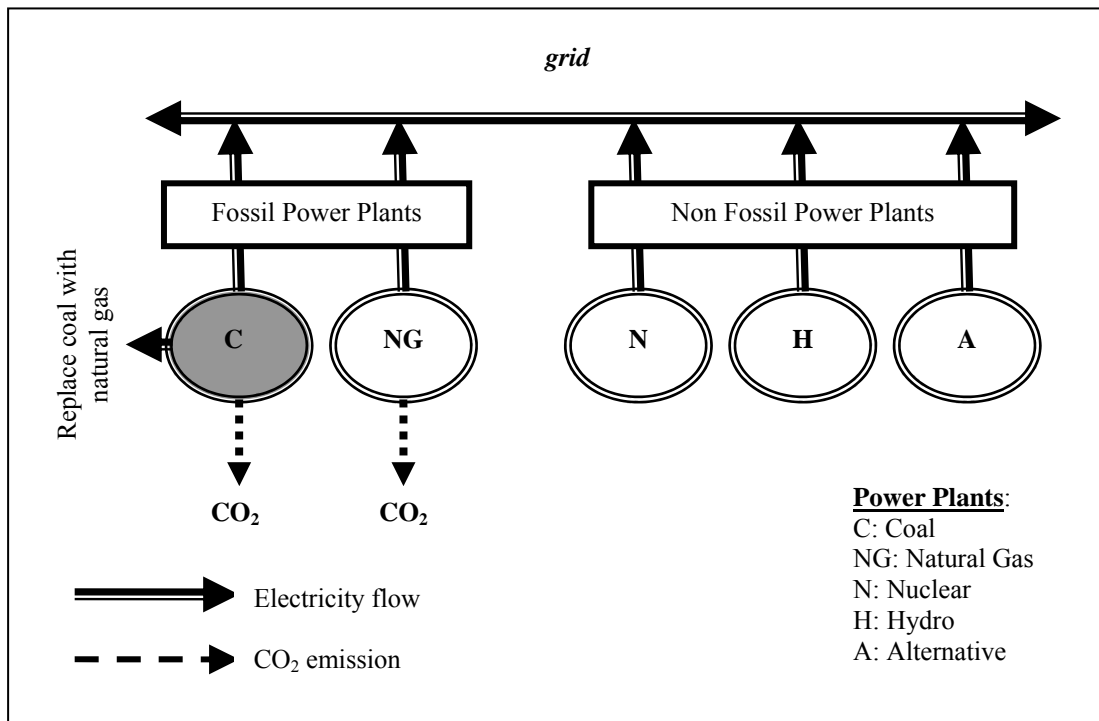
Figure 4.3. Superstructure for fuel switching

Figure 4.4 represents the option of applying technology for efficiency improvement on existing power plants.
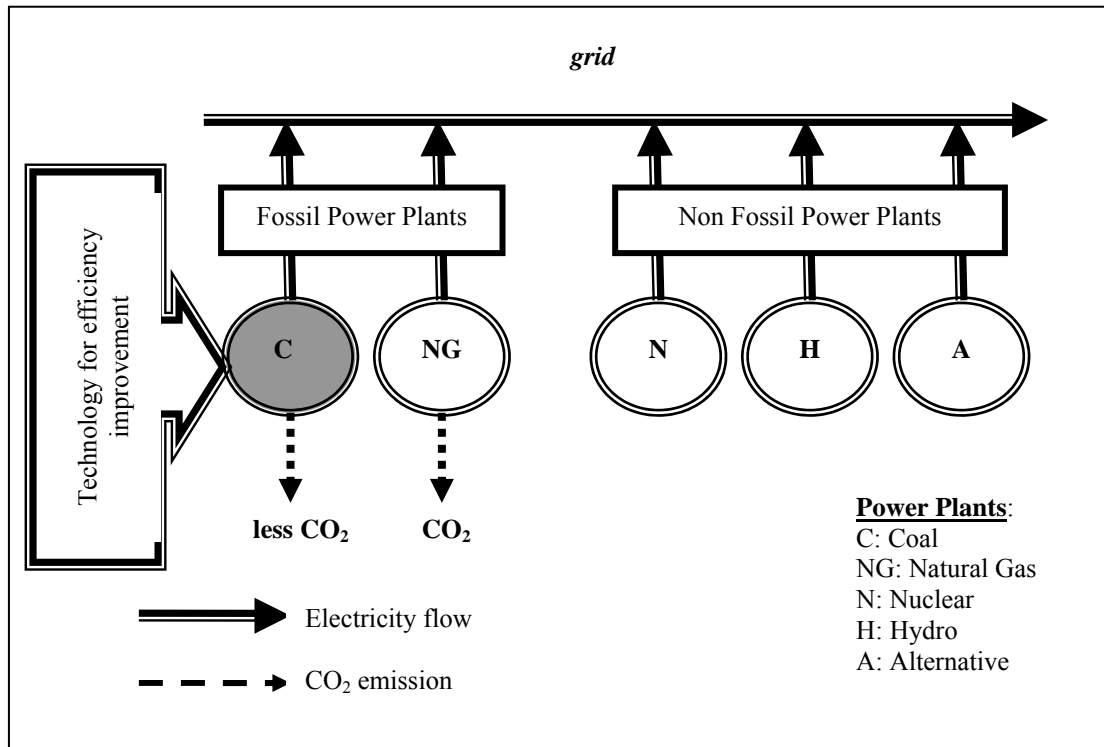
Figure 4.4. Superstructure for efficiency improvement technologies

4.3 Problem Description for This Case Study

CO_2 is the main greenhouse gas and is suspected to be the principal responsible for global warming and climate change. Fossil-fuel power-generation plants are being challenged to comply with the Kyoto Protocol developed by the United Nations Framework Convention on Climate Change (UNFCC). For Canada, the Kyoto Protocol prescribed a legally binding greenhouse gas emission reduction target of 6% below 1990 levels by 2008-2012.

OPG operates currently 6 fossil fuel power plants ($C_{i=1-6}$): five running on coal and one on natural gas, 69 hydroelectric ($H_{i=1-69}$), 3 nuclear ($N_{i=1-3}$) and one wind turbine ($A_{i=1}$). In 2003, OPG had a total installed capacity of 13,765 MWe and emitted about 36.5 Mt of CO_2, mainly from fossil fuel power plants. There are 27 fossil fuel boilers at the 6 fossil-fuel stations: 4 boilers at Lambton (L1-L4), 8 boilers at Nanticoke (N1-N8), 1 boiler at Atikokan (A1), 8 boilers at Lakeview (LV1-LV8), 4 boilers at Lennox (L1-L4), and 2 boilers at Thunder Bay (TB1-TB2). Figure 4.5 shows Ontario map and location of these fossil fuel power plants. Currently, the 4 boilers at Lennox are running on natural gas. Table 4.1 shows a general view of OPG fossil fuel generating stations. Since non fossil fuel power plants are assumed to emit no CO_2, the main focus is on electricity generated from the fossil fuel power plants. The operational costs for nuclear, hydroelectric, and wind turbine were estimated to be $32, $5, and $4/MWh, respectively. Cost is in US$.
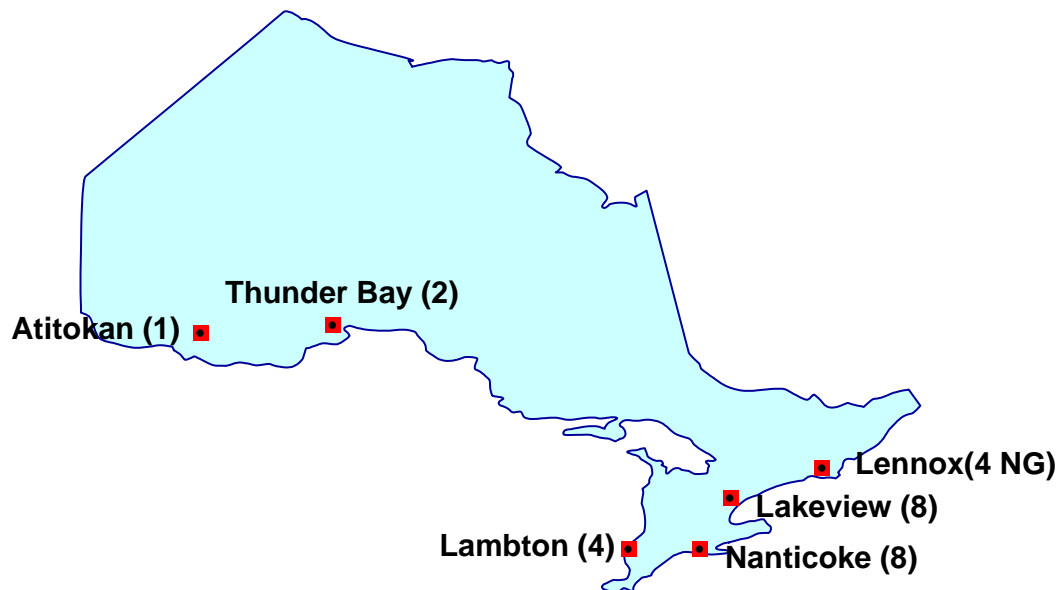
Figure 4.5. OPG fossil fuel power plants location

Table 4.1. Ontario Power Generation fossil fuel generating stations

Generating Station	Fuel	Installed Capacity (MW)	Number of units	Annual capacity factor	Operational cost ($/MWh)	CO_2 emission rate (tonne/MWh)
Lambton1 (L1)	Coal	500	2	0.75	25	0.9384
Lambton2 (L2)	Coal	500	2	0.5	34	0.9386
Nanticoke 1 (N1)	Coal	500	2	0.75	30	0.9300
Nanticoke2 (N2)	Coal	500	6	0.61	30	0.9300
Atikokan (A)	Coal	215	1	0.44	30	1.0230
Lakeview (LV)	Coal	142	8	0.25	35	0.9765
Lennox (LN)	Natural gas	535	4	0.15	50-70	0.6510
Thunder Bay (TB)	Coal	155	2	0.55	30	1.0230

The nominal conditions for OPG's existing fleet of power plants are [Hashim et al. 2005]:

Total electricity generation   : 13,765 MW

Total CO_2 emissions   : 36.57 x 10^6 tonne/yr

Total operational cost   : 2.808 x 10^9 US$ /yr

Figure 4.6 shows the existing OPG fossil fuel power plants (27 boilers) and their associated electricity generation. The non fossil fuel power plants are not shown since they do not emit CO_2.
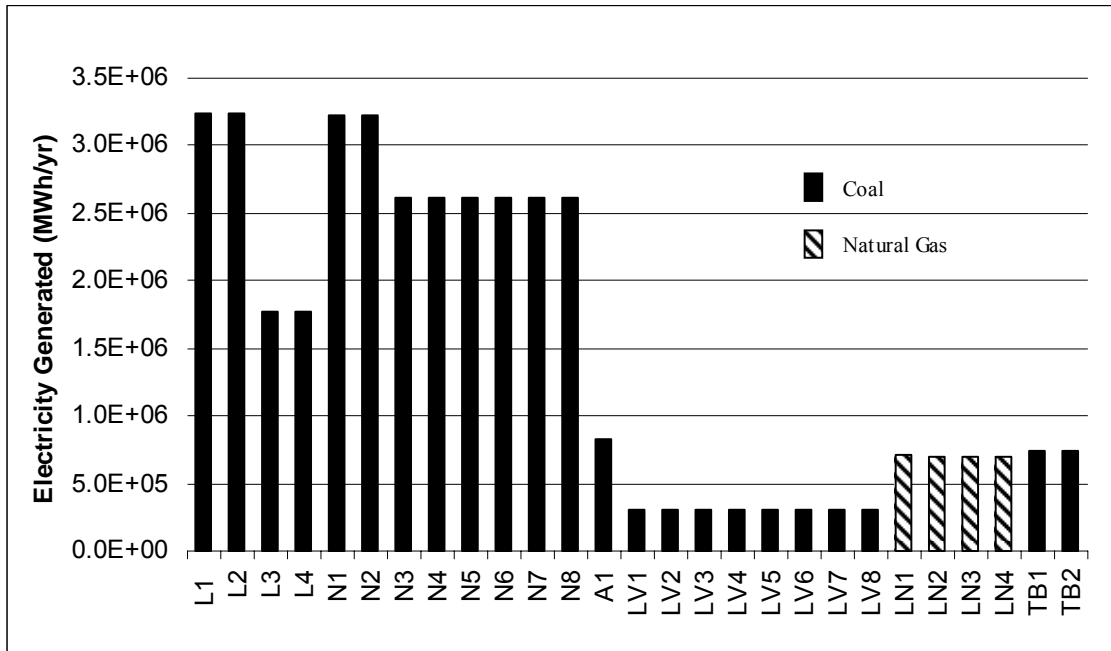
Figure 4.6. Electricity generated from OPG power plants in 2003 (27 boilers)

Three options to reduce CO_2 emission considered here are fuel balancing, fuel switching and efficiency improvement technologies for coal power plants. The efficiency improvement technologies being considered in this study are: install variable speed drive, with 1.5% efficiency improvement, and install high efficiency turbine blades with about 1% increase in efficiency. The actual cost for these technologies depends on the boiler capacity; estimates were obtained from Wisconsin Electric Power Company (WEPCO) (Wisconsin Electric Power Company, 2005) and they are US$2,000,000 and US$5,000,000 respectively for a 500 MW power plant capacity. The cost for each technology is amortized with a 20-year lifetime and a 10% annual interest.

4.4 Results and Discussion

This section presents the results for different CO_2 reduction targets. The options being considered for CO_2 reduction are fuel balancing, fuel switching and applying technology for efficiency improvement. The linearized model discussed earlier was coded into GAMS and solved using the MILP solver. The optimization results show that changing the electricity generated from the Nanticoke generating station, (the largest coal power plant in Ontario), will have a large impact on the CO_2 emissions. The overall effect of the adjustments in the capacity factors is to reduce the overall CO_2 emissions. The results show that all non fossil fuel power plants have to operate with 1% (maximum allowable value) higher than the nominal capacity factor. Table 4.2 shows the results for non fossil fuel power plants in which the production should be increased by 1% for 1% CO_2 reduction. This amount is the maximum allowable increase in production specified in the model.

Table 4.2. Capacity factor for each power plant before and after optimization

Power Plants	MWh/yr	Nominal capacity factor	Adjusted capacity factor
Fossil Fuel Power Plants			
Lambton	17292080	0.580	0.585
Nanticoke	34339200	0.645	0.652
Atitokan	1883400	0.437	0.441
Lakeview	9968880	0.246	0.220
Lennox	18746400	0.148	0.100
Thunder-Bay	2715600	0.549	0.554
Hydroelectric Plants			
NW-Caribou	347328	0.600	0.606
NW-Car	88128	0.600	0.606
NW-Manitou	373248	0.600	0.606
NW-Whitedog	352512	0.600	0.606
NW-Silver	248832	0.600	0.606
NW-Kababeka	129600	0.600	0.606
NW-Cameron	414720	0.600	0.606
NW-Pine	720576	0.600	0.606
NW-Alexander	347328	0.600	0.606
NW-Aquasaloon	243648	0.600	0.606
NW-Aubrey	851472	0.600	0.606
NW-Wells	1256184	0.600	0.606
NW-Rayner	241776	0.600	0.606
NW-Red-Rock	215496	0.600	0.606
NE-Kipling	741096	0.600	0.606
NE-Harmon	741096	0.600	0.606

Table 4.2. Continued

Power Plants	MWh/yr	Nominal capacity factor	Adjustable capacity factor
Hydroelectric plants			
NE-Otter	956592	0.600	0.606
NE-Smokey	273312	0.600	0.606
NE-Long	699048	0.600	0.606
NE-Abitibi	1629360	0.600	0.606
NE-Sturgeon	26280	0.600	0.606
NE-Sandy	15768	0.600	0.606
NE-Wawaitin	57816	0.600	0.606
NE-Indian	15768	0.600	0.606
NE-Hound	21024	0.600	0.606
NE-Notch	1440144	0.600	0.606
NE-Matabitchuan	52560	0.600	0.606
O-Hulden	1277208	0.600	0.606
O-Joachims	2254824	0.600	0.606
O-Chenaux	756864	0.600	0.606
O-Calabogie	26280	0.600	0.606
O-Barrett	925056	0.600	0.606
O-Mountain	893520	0.600	0.606
O-Stewartville	956592	0.600	0.606
O-Amprior	430992	0.600	0.606
O-Chats	504576	0.600	0.606
O-Saunders	5340096	0.600	0.606
N-DeCew	120888	0.600	0.606
N-DeCew2	756864	0.600	0.606
N-Beck1	2617488	0.600	0.606
N-Beck2	7384680	0.600	0.606
N-BeckPGS	914544	0.600	0.606
E-McVittie	15768	0.600	0.606
E-Coniston	26280	0.600	0.606
E-Crystal	42048	0.600	0.606
E-Nipissing	10512	0.600	0.606
E-Bingham	5256	0.600	0.606
E-Elliott	10512	0.600	0.606
E-Ragged	42048	0.600	0.606
E-Eddy	42048	0.600	0.606
E-Chute	52560	0.600	0.606
E-Hanna	5256	0.600	0.606
E-Trethewey	10512	0.600	0.606
E-South	21024	0.600	0.606
E-High	15768	0.600	0.606
E-Mernckville	10512	0.600	0.606
E-Lakefield	10512	0.600	0.606
E-Healey	63072	0.600	0.606
E-Seymour	31536	0.600	0.606
E-Ranney	47304	0.600	0.606
E-Auburn	10512	0.600	0.606
E-Eugenia	31536	0.600	0.606

Table 4.2. Continued

Power Plants	MWh/yr	Nominal capacity factor	Adjustable capacity factor
Hydroelectric plants			
E-Sills	10512	0.600	0.606
E-Hagues	21024	0.600	0.606
E-Frankford	15768	0.600	0.606
E-Sidney	21024	0.600	0.606
E-Meyersburg	21900	0.600	0.606
Nuclear Power Plants			
Pickering-A	0	0.000	0.000
Pickering-B	14300000	0.600	0.606
Darlington	27600000	0.600	0.606
Wind Turbine			
Tiverton	713000	0.250	0.253

The only plant for which the capacity factor decreased is the Lennox generating station (natural gas) in which the capacity factor decreased by about 10% which is the maximum allowable lower limit or the plant should be shut down. This result may seem to be counter intuitive since the Lennox generating station is fuelled by natural gas. However, the reason why the capacity factor of Lennox must be decreased is because this plant uses the most expensive fuel in OPG's fleet. The reduction in CO_2 emissions is accomplished by increasing slightly the capacity factor of the non-fossil fuel generating stations (hydro-electric, nuclear and wind) and by decreasing significantly the capacity factor of Lennox. The capacity factors of the other fossil fuel plants were increased by only a small increment as shown in Table 4.2 above.

Figure 4.7 shows the optimization results for the case of a 1% CO_2 reduction target. For this case, no fuel switching is needed. In other words, the objective can be obtained by adjusting the operation of existing boilers e.g. increasing load from existing non fossil power plants and decreasing load from some existing fossil power plants (fuel balancing). The results show that the capacity factor for all four natural gas boilers has been reduced. No efficiency improvement technologies were recommended. Therefore, a 1% CO_2 reduction target can be achieved by fuel balancing only.
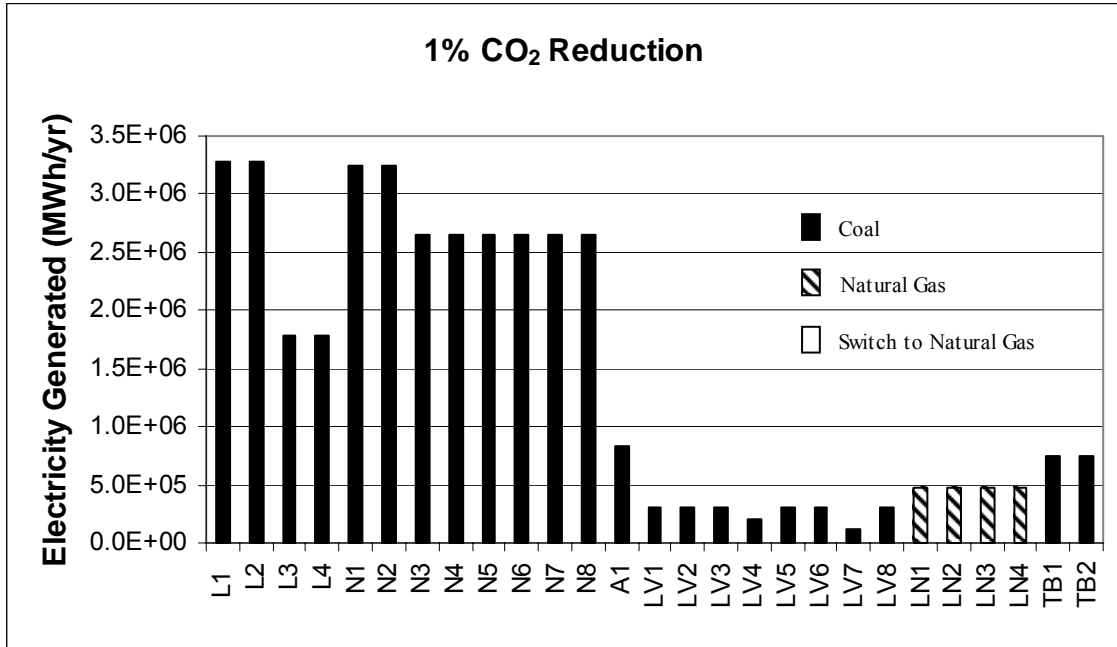
Figure 4.7. Electricity generation strategy for 1% CO_2 reduction

In order to achieve more than a 1% CO_2 reduction, it was found that fuel switching must be implemented. This involves fleet changes from coal to natural gas. As seen in Figure 4.8, the optimization results show, that in order to achieve a 5% CO_2 reduction while maintaining the nominal amount of electricity generated at minimum cost, the capacity factor of one of the natural gas boilers at Lennox (LN4) needs to be increased by 2%, and the one boiler at Atikokan, two boilers at Thunder Bay and one boiler, (LV5), at Lakeview need to be switched from coal to natural gas. The capacity factors for the non-fossil fuel generating stations should be increased by 1%. The model also showed that only one efficiency improvement technology (install variable speed drive) should be applied to the Nanticoke power plant and to three other boilers (L1, L3 and L4) at Lambton power plant.
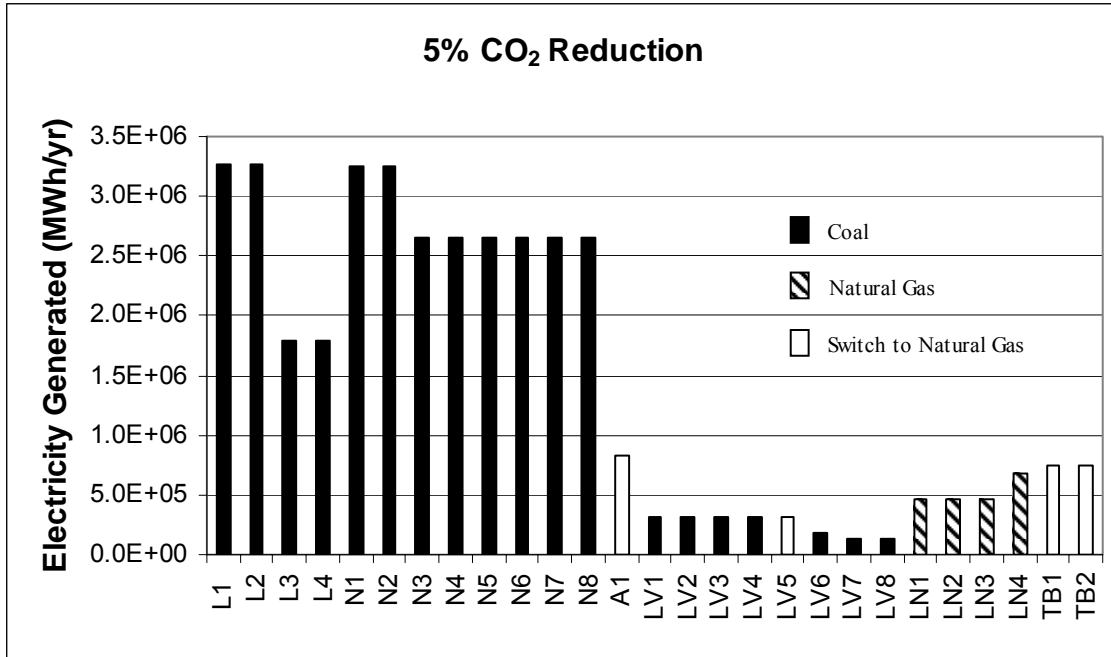
Figure 4.8. Electricity generation strategy for 5% CO_2 reduction

Higher CO_2 reduction targets require more coal boilers to be switched to natural gas. For a 10% reduction (see Figure 4.9) the results show that larger boilers - two boilers (L1 and L2) at Lambton, two boilers (LV5 and LV8) at Lakeview and one boiler (TB2) at Thunder Bay power plants should be switched to natural gas. The electricity generation from all non fossil fuel power plants have also been increased by 1%. The optimizer considered to install variable speed drive technology for efficiency improvement on two boilers (L3 and L4) at Lambton power plant and on all boilers except (N2) at the Nanticoke power plant.

As greater CO_2 targets are required, the optimizer will choose more fuel switching options. For a 30% reduction, the results show that only two boilers (L3 and L4) at Lambton, one boiler (N3) at Nanticoke and the whole Lakeview power plants should continue to operate with coal and the other remaining boilers should be switched to natural gas (Figure 4.10). The electricity generation from all non fossil fuel power plants should be increased by 1%. The optimizer recommended installing variable speed drives

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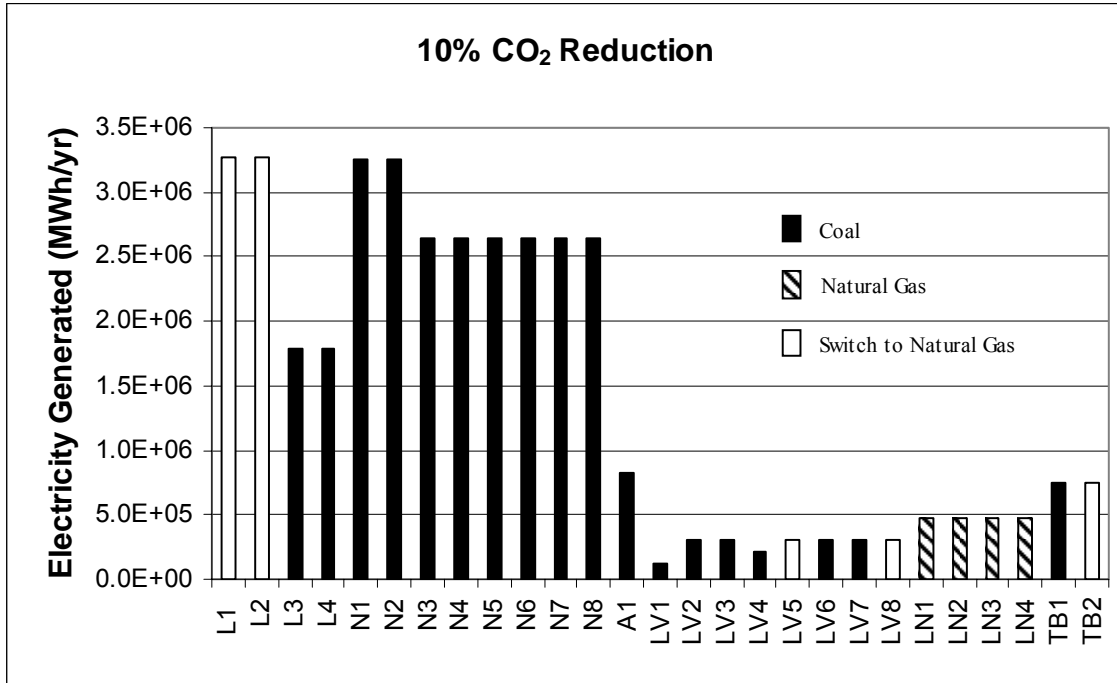
Figure 4.9. Electricity generation strategy for 10% CO_2 reduction
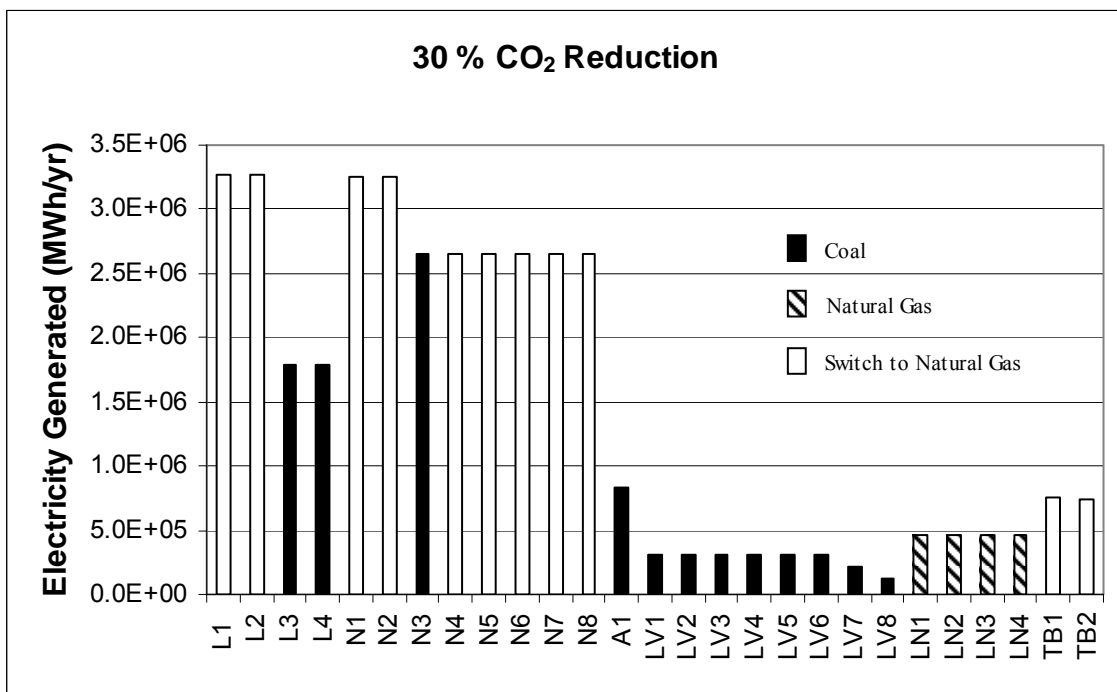
Figure 4.10. Electricity generation strategy for 30% CO_2 reduction

for efficiency improvement at only two boilers, one (L4) at Lambton and another one (N3) at Nanticoke power plant.

A summary of the results is shown in Table 4.3 with selection of technologies and whether the boiler needs to be switched to natural gas or not. The full black circles represent coal boilers while open circles represent natural gas boilers. Switching is represented by open squares and k1 and k2 represent the installation of efficiency improvement technologies, variable speed drives and high efficiency turbine blades, respectively. For all reduction targets, installation of high efficiency turbine blades is never applied since it is too expensive for the benefit gain.

Table 4.3. A summary of optimization results

plant	Base	1 % CO$_2$ Reduction			5 % CO$_2$ Reduction			10 % CO$_2$ Reduction			30%CO$_2$ Reduction		
		S	K1	k2	S	k1	k2	S	k1	k2	S	k1	k2
L1	●	●			●	√		□			□		
L2	●	●			●			□			□		
L3	●	●			●	√		●	√		●		
L4	●	●			●	√		●	√		●	√	
N1	●	●			●	√		●	√		□		
N2	●	●			●	√		●			□		
N3	●	●			●	√		●	√		●	√	
N4	●	●			●	√		●	√		□		
N5	●	●			●	√		●	√		□		
N6	●	●			●	√		●	√		□		
N7	●	●			●	√		●	√		□		
N8	●	●			●	√		●	√		□		
A1	●	●			□			●			●		
LV1	●	●			●			●			●		
LV2	●	●			●			●			●		
LV3	●	●			●			●			●		
LV4	●	●			●			●			●		
LV5	●	●			□			□			●		
LV6	●	●			●			●			●		
LV7	●	●			●			●			●		
LV8	●	●			●			□			●		
LN1	○	○			○			○			○		
LN2	○	○			○			○			○		
LN3	○	○			○			○			○		
LN4	○	○			○			○			○		
TB1	●	●			□			●			□		
TB2	●	●			□			□			□		

●		Coal	
○		Natural Gas	
□		Switch to NG	
k1		Install variable speed drive	
k2		Install high efficiency turbine blades	

Table 4.4 shows the cost and CO_2 emission for each reduction target with the cost of CO_2 avoided. The cost of CO_2 avoided ($/tonne CO_2 avoided) can be calculated from the following equation:

$$\text{Cost of } CO_2 \text{ avoided (\$/tonne } CO_2 \text{ avoided)} = \frac{COE - COE^{\text{Ref}}}{CO_2 - CO_2^{\text{Ref}}}$$

Where *COE* is overall cost of electricity generated in ($/MWh); COE^{Ref} is overall cost of electricity for the base case (current OPG situation) in ($/MWh); CO_2 is total amount of CO_2 emission from all plants in (tonne/MWh); CO_2^{Ref} is total CO_2 emission for the base case in (tonne/MWh).

It is shown that OPG could save money at 1% CO_2 reduction since the cost of CO_2 avoided is negative. This can be achieved as mentioned earlier by only increasing the capacity factor of non fossil fuel power plants and decreasing the capacity factor of the natural gas power plant without structural change to the fleet. Increasing the reduction target will lead to a higher cost of CO_2 avoided since it involves structural change such as switch some of the coal power plants to natural gas.

Table 4.4. CO_2 emission and cost of CO_2 avoided at different reduction target

Reduction target(%)	Cost (10^9 $/yr)	CO_2 emission (Mt/yr)	Cost of CO_2 avoided ($/tonne CO_2 avoided)
1	2.771	36.08	-88.1
5	2.817	34.74	5.0
10	2.886	32.91	21.7
30	3.167	25.59	33.0

4.5 Summary

The optimization of CO_2 emissions from the Ontario power grid was studied. In our calculations, a linearized MINLP model was used and was implemented in GAMS. The reduction options considered were fuel switching, fuel balancing and technologies for power plant efficiency improvement.

The results indicate that applying several strategies for increasing the power plant efficiency is an effective way for reducing CO_2 emissions up to a certain target. The optimization results show that overall CO_2 emissions can be reduced by 1% by adjusting OPG's current operational level without having to change the fleet structure (fuel balancing). Fuel balancing also results in a reduction of operating costs by about 1.3%. However, if CO_2 emissions are to be reduced further (e.g., by 6% below 1990 level, Canada's Kyoto target), it will be necessary to employ structural changes such as fuel switching.

Fuel switching involving structural changes to the fleet has been considered as the best option for CO_2 reduction especially if the reduction target is 10% or above within an upper limit around 35%. Applying technologies for efficiency improvement can be an attractive option to reduce CO_2 emissions especially at small reduction targets such as around 5%. As reduction increases, the best option is fuel switching in order to achieve that target.

The size of the problem was as follows:

Model: MILP

Solver: OSL

Number of variables: 342

Number of discrete variables: 108

CPU: 0.04 sec

CHAPTER 5

MODEL DEVELOPMENT FOR AN OIL REFINERY

5.1 Introduction

This chapter represents the mathematical model development for an oil refinery which has been divided into five main phases:

Phase 1 represents the word and mathematical statements.

Phase 2 presents the superstructure framework that features a number of feasible CO_2 mitigation options in an oil refinery. These include flow rate balancing, fuel switching; and CO_2 capture technologies.

Phase 3 focuses on development of sub-models for the refinery units under study and then the development of a master model that represents the whole refinery process under study. The objective of the planning model is to maximize the profit from selling the final products with specific quality constraints and to meet a certain CO_2 reduction target at a minimum cost.

Phase 4 gives a general method to calculate CO_2 emissions from combustion sources within an oil refinery and gives products blending correlations.

In phase 5, the mathematical model is coded in GAMS. Different case studies are discussed in details in chapter 6. Figure 5.1 shows the different phases discussed above.

Phase 1: Statement of problem
"given a CO_2 reduction target, what is the best strategy or combination of strategies among (flow rate balancing, fuel switching and CO_2 capture) for an oil refinery to pursue?"

Phase 2: Superstructure representation		
Flow rate balancing	Fuel switching	CO_2 capture

Phase 3: Mathematical model development	
• Development of sub-models (refinery units) • Development of master model (planning model)	
Objective Maximize the profit	Constraints Demand satisfaction, capacity constraints, emission constraints, fuel selection, product qualities.

Phase 4: CO_2 emissions estimation and products blending
Estimation of CO_2 emissions from combustion sources within an oil refinery and products blending correlations.

Phase 5: Model application and coding	
Case 1:	Planning model with/without properties and flow rate balancing
Case 2:	Planning model with properties, balancing and fuel switching.
Case 3:	Planning model, balancing, switching and CO_2 capture.
Case 4:	Planning model, balancing, switching, capture and sequestration.

Figure 5.1. Methodological approach for an oil refinery

5.2 Phase 1: Statement of Problem

The basic problem to be addressed in this part can be stated as follows, "For a given CO_2 reduction target, what is the best strategy or mix of strategies among flow rate balancing, fuel switching and CO_2 capture processes for an oil refinery to implement while maximizing profit".

The goal of this part is to help the decision maker within an oil refinery to maximize the profit while meeting a CO_2 reduction target at minimum cost. The emphasis is on combustion sources since they are the major contributors to CO_2 emissions within an oil refinery. The options being considered are:

- Flow rate balancing: this means manipulating the inlet flow rate for each unit since the fuel consumption of each unit is a function of processing flow rate. For example, if a unit is the major contributor to CO_2 emissions, decrease the inlet flow rate to that unit but without affecting the final product demand.
- Fuel switching: this means switching the fuel being used to another one with less carbon content.
- CO_2 capture: this means to apply CO_2 capture process such as MEA process.

Each of these options has a cost associated with it ranging from flow rate balancing as the cheapest option and the CO_2 capture process as the most expensive solution.

The mathematical statement of the word problem above consists of maximizing an objective function while observing equality and inequality constraints. The superstructure is modeled mathematically and can be written as the following MINLP (Mixed Integer Non-linear Programming):

$$\max_{x,y} f(x,y,p)$$

such that,

$$h(x,y,p) = 0$$
$$g(x,y,p) \leq 0$$

$$x \in X \leq R^n \qquad \text{(x is a vector of continuous variables)}$$
$$y \in Y = \{0,1\} \qquad \text{(y is a vector of binary variables)}$$
$$p \qquad\qquad\qquad \text{(p is a vector of parameters)}$$

Variables

Continuous variables, x, are real numbers that may represent flow rates of products produced from each unit, capacity of a unit, CO_2 emissions etc.

Binary variables, y, are assigned (0-1) to represent the existence or non-existence of CO_2 capture technology.

Objective Function

In this research, the objective for the oil refinery model is to maximize the profit from selling the final products and reduce CO_2 emission by a specified amount. f(x,y,p) is a single objective function which represents the profit including revenues from selling the final products minus the operating cost of each unit and retrofit costs for fuel switching and eventual other retrofit costs for implementing the CO_2 capture technology.

Constraints

h(x,y,p) =0, are the equality constraints; these equations include,

- Mass balances
- CO_2 emission balances

g(x,y) ≤ 0 are the inequality constraints which correspond to design specifications, restrictions and feasibility constraints.

a) Quality constraints: these represent product specifications (e.g. octane number, sulphur content, etc.)

b) CO_2 constraints: the total CO_2 emissions must be less than or equal to a given CO_2 reduction target.

c) Demand constraints: the total amount of each final product must be equal or greater than the demand.

Limitations of process/size: capacity for each unit must not exceed a certain limit.

Binary constraints: These are represented by two binary variables:

Switching or not in (0-1 base) and another binary variable for existence or non existence of CO_2 capture technology.

5.3 Phase 2: Superstructure Representation

In order to solve the MINLP model, a superstructure representing the main units within an oil refinery, flow rate balancing, fuel switching and CO_2 capture process will be illustrated. As one can imagine, a superstructure representing all possible alternatives will be very complex.

Four options are presented in this section and these are:

- Option 1: Base case without CO_2 mitigation options shown in Figure 5.2 and Figure 5.3 represents a simpler diagram of an oil refinery.

- Option 2: Flow rate balancing shown in Figure 5.4.

- Option 3: Fuel switching shown in Figure 5.5.

- Option 4: Existence of CO_2 capture technology shown in Figure 5.6.

The units considered in an oil refinery are summarized as follows (Figure 5.3):

- Fractionation: (crude distillation unit-atmospheric and vacuum).

- Hydrotreating: (naphtha, distillate, gas oil and residual hydrotreater).

- Upgrading: (reformer, hydrocracker and fluidized catalytic cracking unit).

- Blending pools (gasoline, kerosene, diesel and fuel oil).

Figure 5.2 represents a refinery layout with the units and a simple layout is given in Figure 5.3.
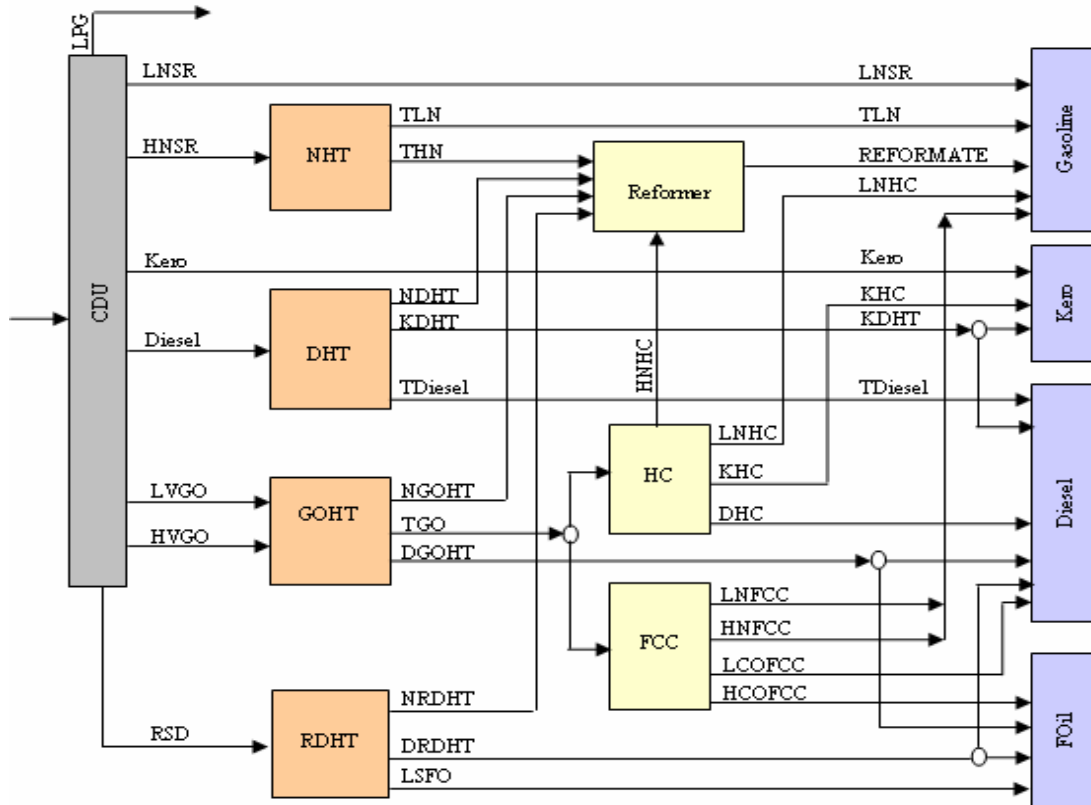
Figure 5.2. Basic refinery layout

The above figure can be simplified as follows:
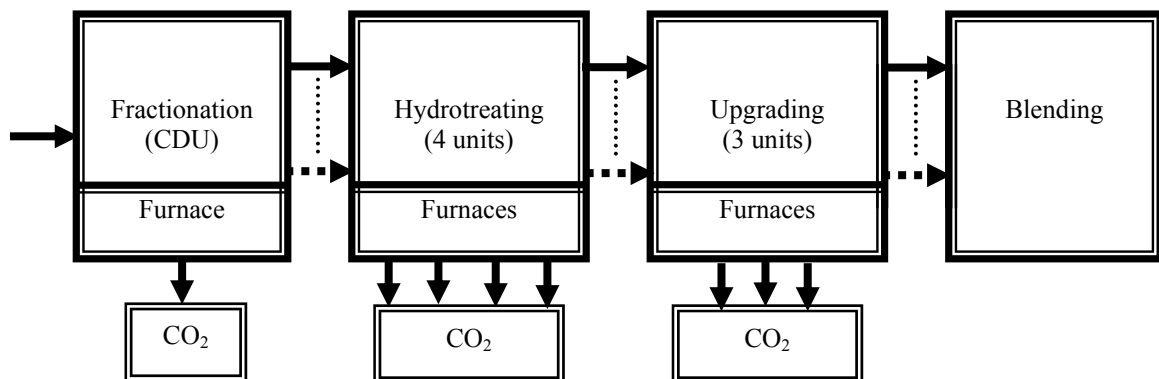
Figure 5.3. Simplified refinery layout

Figure 5.4 shows one possible option to reduce CO_2 emissions by decreasing the flow rates from units that emit more CO_2 emissions without affecting the product demand and quality. Fuel consumption for each unit is a function of inlet flow rate.
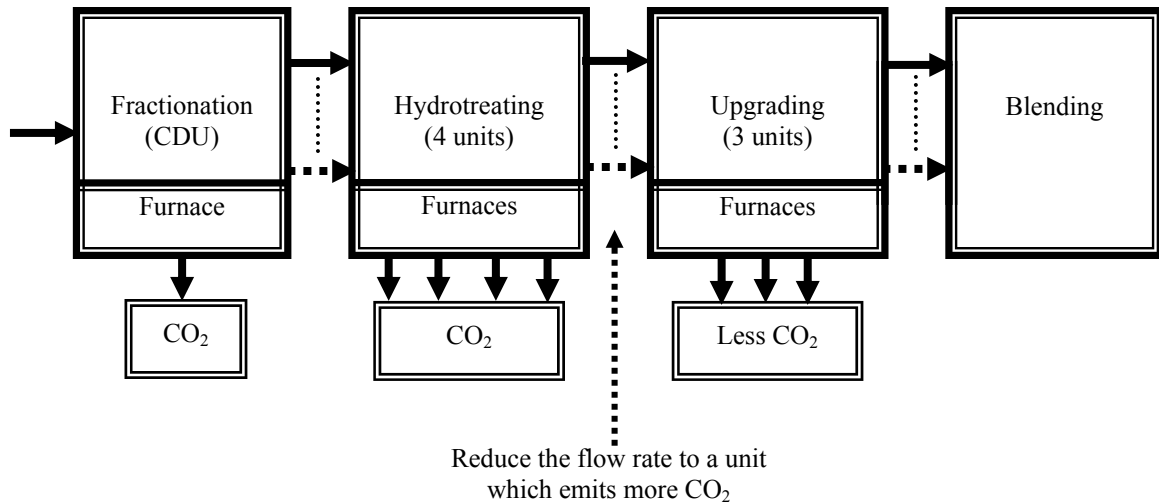
Figure 5.4. Superstructure for flow rate balancing

Option 3: Fuel Switching

The second option is by fuel switching. This is done by changing the current fuel with less carbon content fuel such as natural gas. Figure 5.5 shows this option.
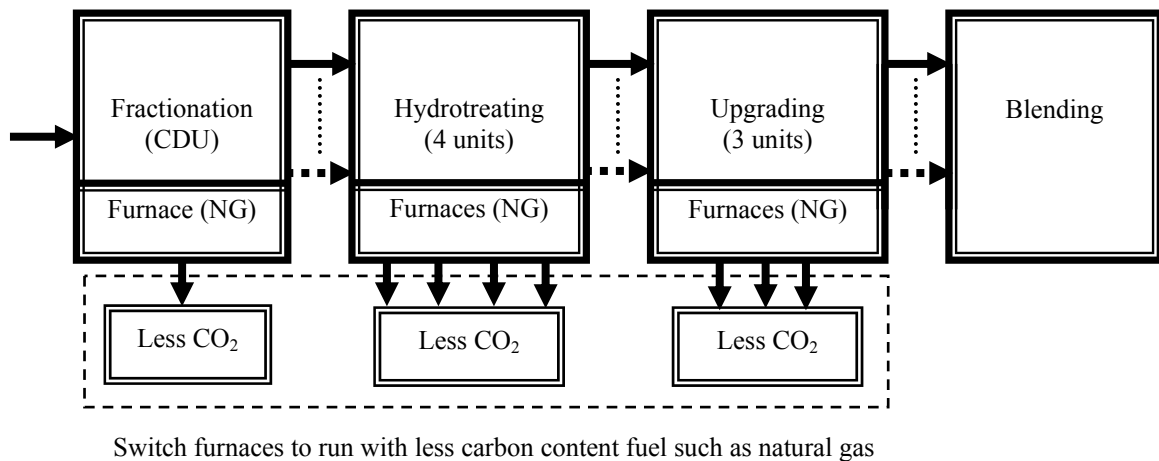
Figure 5.5. Superstructure for fuel switching

<u>Scenario 4:</u> CO_2 Capture

Figure 5.6 shows another option to reduce CO_2 emissions. This is the CO_2 capture and it is the most expensive option.

Apply CO_2 capture technologies
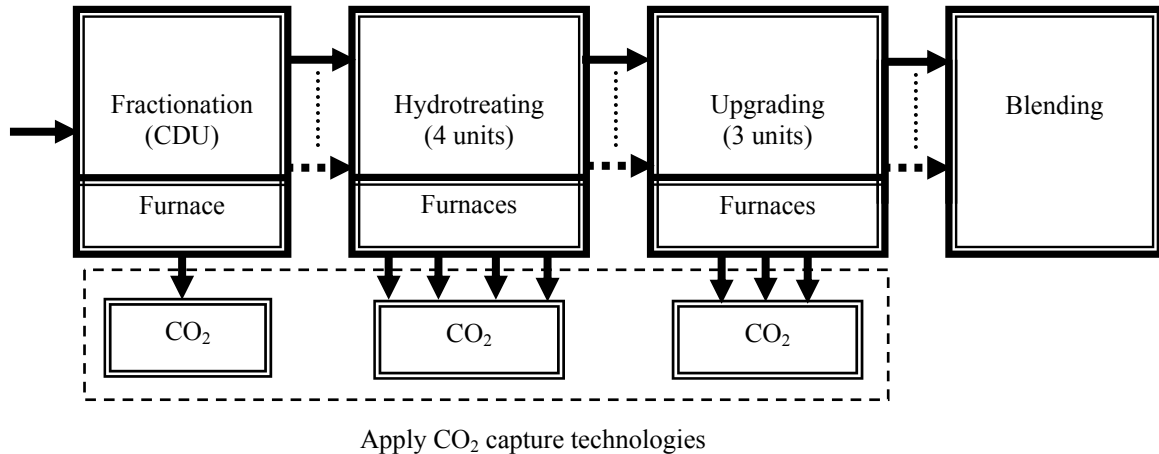
Figure 5.6. Superstructure for CO_2 capture

5.4 Phase 3: Mathematical Model Development

In this section, a general mathematical model for an oil refinery is developed. The objective of this model is to maximize profit from selling the final products with specifications subject to reducing CO_2 emissions to a certain target using the different mitigation options presented in the previous section.

Prior to the master model development which includes all units under consideration as shown in Figure 5.2, a model is developed for each unit (sub-models). Each unit under consideration falls into one of the four categories discussed earlier.

In total, there are eight major units and different blending pools. After developing the sub-model for each unit, they are connected together by specifying outlet of one unit as inlet for the following unit. For simplicity, only the CDU model is shown in details as an example and a general model is given after.

5.4.1 Sub-models Development

CDU model

The first major unit of any refinery is the crude distillation unit (CDU). Crude oil should be characterized before being fed to the CDU. One of the key attributes for characterizing the hydrocarbons composing crude oils is by boiling point. This attribute is determined through laboratory test methods by measuring the temperature at which the components of the crude oil will evaporate at a given pressure (typically atmospheric pressure unless stated to be a different pressure basis). The model development starts at having a certain crude assay that shows crude properties and volume % accumulated at each given temperature among all cuts or fractions that come out from the CDU. Table 5.1 gives an example of crude assay for Alaska crude. For each given cut temperature, the volume % accumulated is calculated by adding the volume % of the previous cut. For the first cut at temperature of $160^{o}F$ ($70^{o}C$), for example, the volume % accumulated is the summation of volume % given for that cut plus volume % of C_2, C_3, NC_4 and IC_4 in crude. For the following cut, the volume % accumulated will be the volume % accumulated for this cut added to the previous volume % accumulated. To find the properties of the outlet streams, a mid volume % needs to be defined since all properties are calculated at this mid volume %. The mid volume % is the average between the volume % accumulated from the previous cut and volume % accumulated from current cut. Table 5.2 gives data for the Alaska crude oil.

Table 5.1. Alaska crude oil assay (Gary, 1994)

Description	ALASKA
Temperature	F
Basis(Wt or Vol)	V
% C2 in crude	0.05
% C3 in crude	0.3
% IC4 in crude	0.13
% NC4 in crude	0.48

Cut final temp (°F)	160	220	300	360	450	525
Yld on crude,%	2.78	2.86	5.29	5.09	9.37	7.82
SG	0.6708	0.7491	0.7608	0.7878	0.818	0.8481
API	79.4	57.4	54.5	48.1	41.4	35.3
Sulphur	0.002	0.0026	0.0064	0.038	0.19	0.4
RON	72.9	66	59.7	52.3		
MON						
Aromatics,%		13.3	16.2	21.8	26.8	29.5
Naphthenes,%		38.3	38.8	37		
Smoke pt,mm					19.2	16.4
Cetane No					41.4	44.1
Nitrogen,%	0	0	0	0.0003	0.002	0.0057
Nickel,ppm						
Vanadium,ppm						
Property A						
Property B						

Cut final temp	650	1050	1300
Yld on crude,%	12.57	35.99	17.28
SG	0.881	0.9326	1.0289
API	29.1	20.2	6
Sulphur	0.64	1.21	2.93
RON			
MON			
Aromatics,%			
Naphthenes,%			
Smoke pt,mm			
Freeze point			
Pour point	9	92	130
Cetane No	44.4		
Nitrogen,%	0.0221	0.166	0.657
Nickel,ppm		0.43	61
Vanadium,ppm		0.53	151

Table 5.2. Volume % accumulated at different temperature (Alaska crude)

V%	T	mid V%	API	S	N2
0.96					
3.74	160	2.35	79.4	0.0020	0
6.60	220	5.17	57.4	0.0026	0
11.89	300	9.24	54.5	0.0064	0
16.98	360	14.43	48.1	0.0380	0.0003
26.35	450	21.66	41.4	0.19	0.0016
34.17	525	30.26	35.3	0.40	0.0057
46.74	650	40.45	29.1	0.64	0.0221
82.73	1050	64.73	20.2	1.21	0.1660
100.00	1300	91.37	6	2.93	0.6570

A plot of T vs. volume % accumulated is shown in Figure 5.7 and a 4th degree polynomial is used to fit the data in order to use it conveniently in the model for calculating volume % of such a product knowing the cut temperature. This is given by the following equation:

$$V\% = 8 \times 10^{-11} X^4 - 3 \times 10^{-7} X^3 + 0.0003 X^2 - 0.0473 X + 4.0406 \qquad (5.1)$$

where X is the cut temperature (^{o}F).
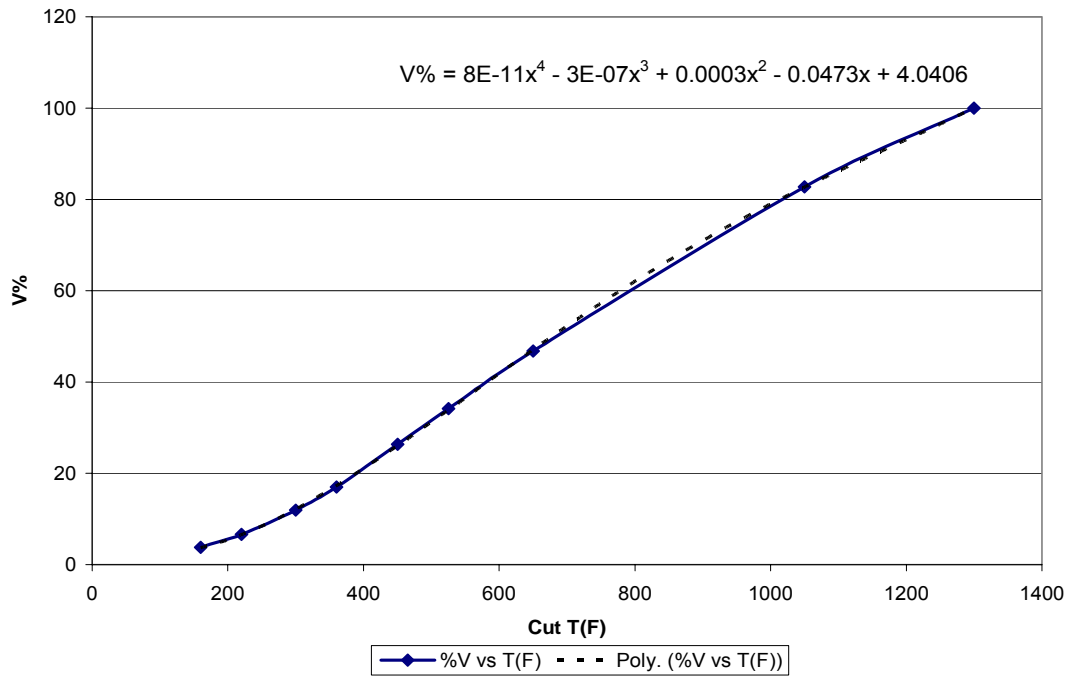
Figure 5.7. Volume % accumulated at different cut temperature

For a specified cut temperature, we can easily calculate the volume flow rate for the cut by multiplying volume % accumulated corresponding to this given cut temperature with the inlet flow rate to the CDU. For simplicity, both atmospheric and vacuum distillation units are incorporated into one model (CDU). The main products from CDU are:

- LPG (liquefied petroleum gas)
- LNSR (light naphtha straight run)
- HNSR (heavy naphtha straight run)
- Kerosene
- Diesel
- LVGO (light vacuum gas oil)
- HVGO (heavy vacuum gas oil)
- Residual

Taking any fraction as an example, if the cut temperature is predetermined, from Figure 5.7, or the equation given in the figure (equation 5.1), we can calculate the volume % accumulated at this given cut temperature. Then simply multiply this percent by inlet volume flow rate to the CDU. For the next fraction, the volume accumulated will be the current minus the previous accumulated volume.

For calculating the properties such as API, sulphur and nitrogen content, the mid volume % need to be calculated as shown in Table 5.2. For a given cut, mid volume % can be calculated as:

$$mid\ volume\% = \frac{cuurent\ cut\ volume\% + previous\ cut\ volume\%}{2} \qquad (5.2)$$

Figure 5.8 gives an equation to calculate API given mid volume %. API for a given cut can simply be calculated if the average volume % accumulated is known. It is given in this equation:

$$API = 7\times10^{-6}X^{4} - 0.0015X^{3} + 0.1133X^{2} - 3.778X + 81.848 \qquad (5.3)$$

Where X is the mid volume %.
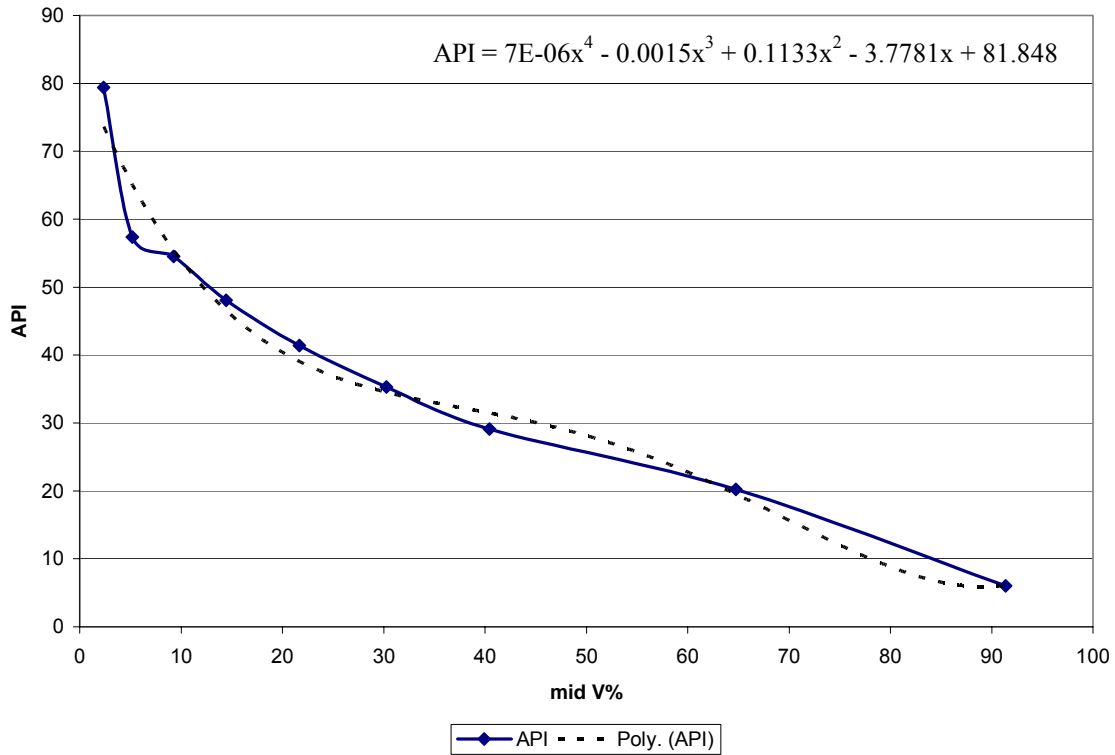
Figure 5.8. API as a function of mid volume %

For other properties such as sulphur and nitrogen content, the same procedure as for API is carried out. Figure 5.9 shows the sulphur content as a function of mid volume %. The equation to calculate sulphur content (%) is given as:

$$Sul(\%) = 7 \times 10^{-7} X^4 - 3 \times 10^{-5} X^3 + 0.0018 X^2 - 0.0204 X + 0.0506 \qquad (5.4)$$

Where X is the mid volume %.

For nitrogen content, Figure 5.10 gives a relation between mid volume % and nitrogen content (%). The equation is given as:

$$Nit(\%) = 2 \times 10^{-6} X^3 - 9 \times 10^{-5} X^2 + 0.0016 X - 0.0059 \qquad (5.5)$$

Where X is the mid volume %.
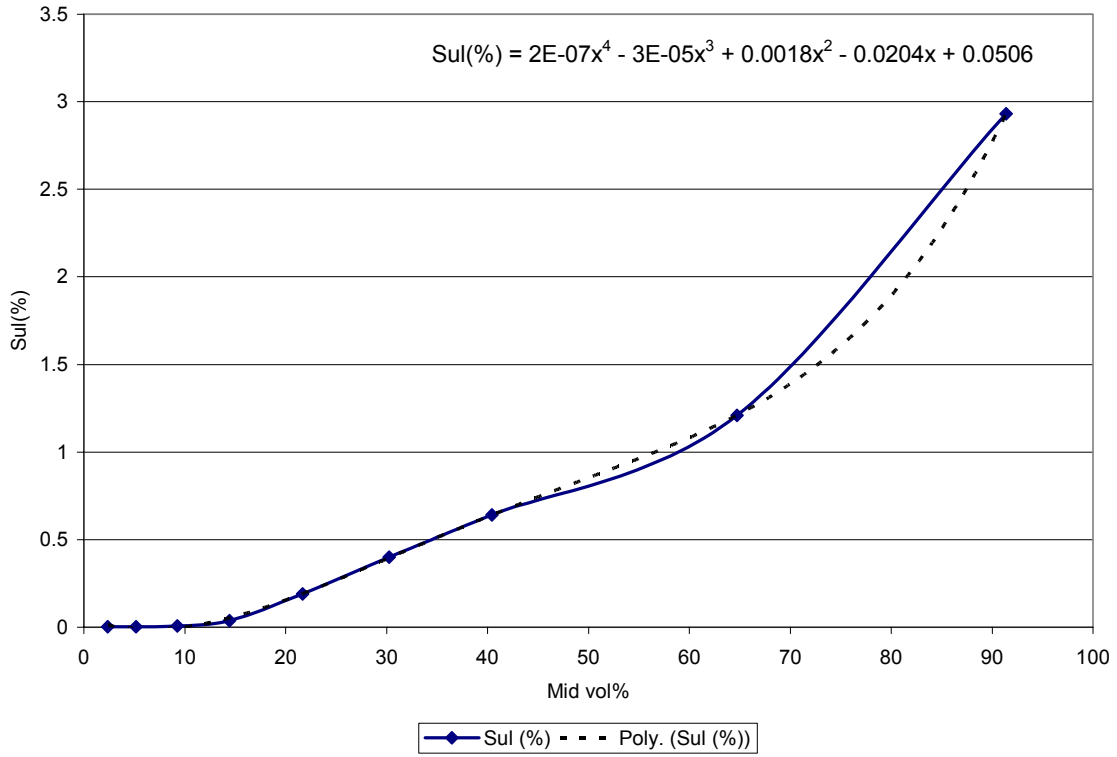
Figure 5.9. Sulphur contents as a function of mid volume %
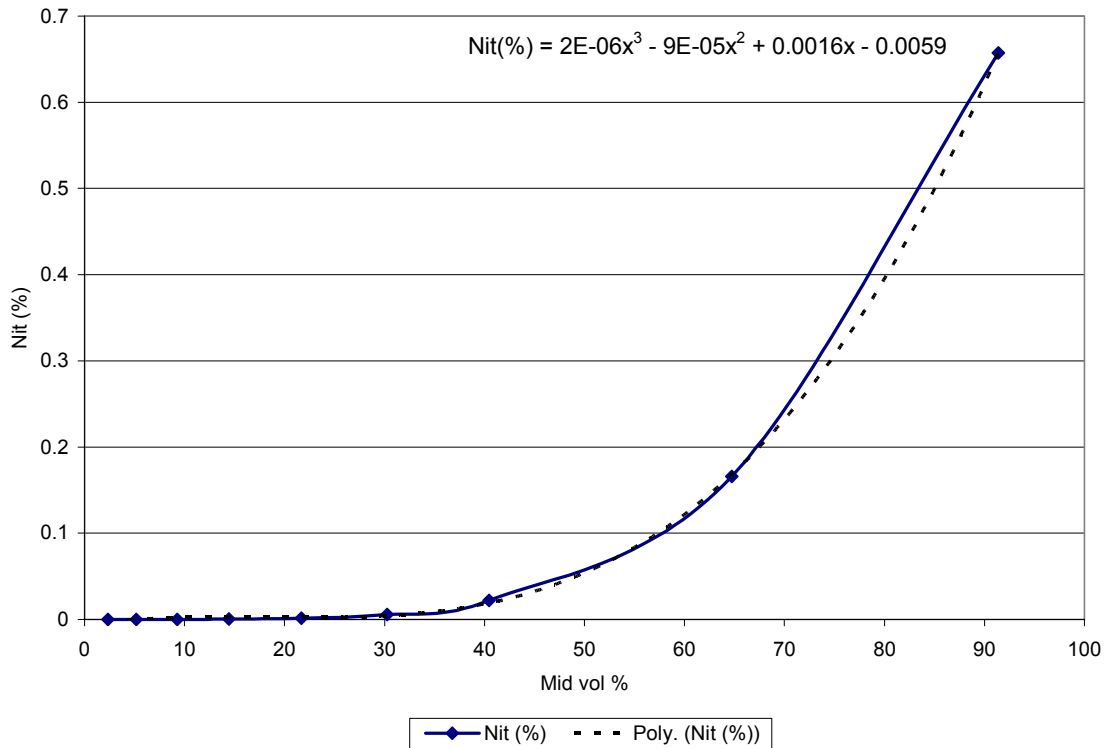
Figure 5.10. Nitrogen contents as a function of mid volume %

The CDU model can now be summarized as follows:

$$Cut_s = \sum_{k=0}^{4} a_k (TE_{CDU,s})^k \qquad \qquad \forall \ s \in S_{CDU} - \{Rsd\} \qquad \qquad (5.6)$$

Cut_s represent the volume percent vaporized (volume %) of all fractions (s), except the residue product, of the CDU unit (S_{CDU} is the set of all CDU products). The cuts are a polynomial function, as shown earlier, in product cut-point $TE_{CDU,s}$ which is equivalent to the end point temperatures (EP). The product cut-point $TE_{CDU,s}$ or end point temperature (EP) is the temperature at which a given fraction or cut will be vaporized.

Since the last cut is the residue of the crude, so it will be assumed that the accumulative vaporized percent will be 100%. The residual cut volume percent will be expressed as:

$$Cut_{CDU,s=Rsd} = 100 \qquad \qquad (5.7)$$

Each product, cut, volume flow rate is calculated from subtracting its volume percent vaporized from the previous cut and multiply the product with the crude feed to the CDU:

$$V_{CDU,s} = F_{CDU} * \left(\frac{Cut_s - Cut_{s-1}}{100} \right) \qquad \qquad \forall \ s \in S_{CDU} \qquad \qquad (5.8)$$

$V_{CDU,s}$ represents the volume flow rate of all the products (s) from the CDU unit. Where the F_{CDU} is the crude oil feed to the CDU unit.

Properties of each product from the CDU (API, sulphur etc.) are polynomial functions in each product mid-volume percent vaporized. Mid-volume for any product can be calculated from averaging the accumulative current cut volume percent with the previous cut volume percent vaporized as shown earlier in this section:

$$PV_{CDU,s,p} = \sum_{k=0}^{4} a_{k,p} \left(\frac{Cut_s + Cut_{s-1}}{2} \right)^k_p \qquad \forall\, s \in S_{CDU}, p \in P_s \qquad (5.9)$$

$PV_{CDU,s,p}$ represent different properties (p) for each product (s) from the CDU unit. P_s is the set of all the properties calculated for the specified stream (s).

$$V_{CDU,s} = \sum_{m \in M} VS_{CDU,s,m} \qquad \forall\, s \in S_{CDU} \qquad (5.10)$$

$VS_{CDU,s,m}$ represent the volume flow rate of all the streams split from the CDU products (s) to different destinations (m).

All fractions for the CDU, except the residue, have upper and lower limit for their cut-point:

$$TE^L_{CDU,s} \leq TE_{CDU,s} \leq TE^U_{CDU,s} \qquad \forall\, s \in S_{CDU} - \{Rsd\} \qquad (5.11)$$

$TE_{CDU,s}$ is the cut-point temperature for fraction (s) of CDU unit.

Also, the crude feed to the unit can not exceed its throughput capacity:

$$F_{CDU} \leq Umax_{CDU} \qquad (5.12)$$

Other sub-models for hydrotreaters, reformer, FCC and HC are developed with the aid of available correlations in the literature for the given units to calculate products amount with properties (Baird, 1987). Theses sub-models are coded in GAMS and are shown in Appendix C.

5.4.2 Master Model Development

This section describes the overall (master) model that involves all units under consideration in this study. It is written as an optimization problem. The objective function is to maximize a profit of selling the final products to meet the demand with quality specifications and reduce the CO_2 emissions while maximizing the profit. The main variables are the flows of each stream and products to be processed, intermediate products and finished products. These include also the properties of each stream such as API, sulphur content, octane number and others. Among the main equations, material balance equations are the most numerous. They usually express the equality between an available quantity of a given intermediate product (product yield at the exit of a unit multiplied by the quantity of feedstock processed) and the quantities used corresponding to the different possible destinations of this product. In this study, a sub-model for each unit, as discussed in the previous section, is developed. The model is non-linear since it involves the equations for product properties blending.

The demand equations reflect the fact that the sum of the quantities of intermediate products used in blends to produce a finished product should serve to meet the demand for this product.

Quality equations express the obligation, for each finished product, to meet the legal specification as well as a number of technical requirements. For automotive fuels, these are specific gravity, octane number, sulphur content; and for medium distillates and fuel oil, specific gravity, sulphur content, cetane number for engine diesel.

The capacity constraint reflects the capacity limitations of existing units. The CO_2 emissions constraints require that the overall refinery activity leads to CO_2 emissions that are less than current releases within a pre-specified percent level.

The main focus of this study is to provide methods of determining optimal production planning for a petroleum refinery processes. The most important variables will be the feed flow rate, feed properties, products flow rates, and the properties of the products.

The objective is to maximize the total profit of the refinery as follows:

$$profit \ = \ \sum_{i \in B} Cp_i \, F_i \ - \ \sum_{i \in E} Cf_i \, F_i \ - \ \sum_{i \in I} Cx_i \, F_i - \sum_{i \in IF} \sum_w Cs_{iw} X_{iw} - \sum_{i \in IF} \sum_k Cc_{ik} Y_{ik} \qquad (5.13)$$

The refinery profit is expressed as revenues from selling products minus the costs of purchasing feedstock and costs of operating the process units in the refinery. In equation 5.13 (B) represents the set of blending units for the final products and their sales price Cp_i (US$/bbl). The cost Cf_i (US$/bbl) of the feedstock purchased from external sources is defined under the set (E) for all the units that receive such material from outside. The third term represents the operating cost Cx_i (US$/bbl) for each processing unit (i) in the refinery where it is usually expressed as a function of the quantity fed to the running unit. The cost of applying fuel switching is shown in term 4 where X is a binary variable that represents which fuel w to select. Cs_{iw} (US$/yr) represents the cost of switching if fuel w is being chosen. Finally, the profit should be affected by applying CO_2 capture technology, k, with cost Cc_{ik} (US$/yr) if necessary to meet a given CO_2 reduction target.

A general model consists of the following sets of constraints:

- Feed flow rate of processing unit:

$$F_i = \sum_{j \in J} \sum_{s \in N} VS_{j,s,i} \qquad\qquad \forall i \in I \qquad\qquad (5.14)$$

The feeds for any processing unit i (i belongs to I the defined set for all the units in the refinery) are represented by F_i is summation of all the possible streams $VS_{j,s,i}$ that can be received by unit (i) from units (j), where (j) is defined as the set of all units that can send stream (s) to unit (i). Flow rates are in (bbl/yr).

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- Feed properties of processing units:

$$FP_{i,p} = f\left(VS_{j,s,i}, PV_{j,s,p}\right) \qquad \forall i \in I,\, p \in PF_i \qquad (5.15)$$

Properties (p) of the feed to unit (i) are represented by $FP_{i,p}$ and PF_i is the set of all feed properties to unit (i). The properties are functions of the streams quantities and properties from unit (j), $VS_{j,s,i}$ and $PV_{j,s,p}$ respectively.

- Product flow rates of processing units :

$$V_{i,s} = f\left(F_i, FP_{i,p}, OV_{i,ov}\right) \qquad \forall i \in I, s \in S_i \qquad (5.16)$$

Product flow rate from unit (i) for stream (s) is represented by $V_{i,s}$ (s belongs to S ; the set of all the streams produced from unit i) are functions of the feed quantity F_i and property $FP_{i,p}$ as well as the operating variables $OV_{i,ov}$ for unit (i).

- Products properties of processing units:

$$PV_{i,s,p} = f\left(FP_{i,p}, OV_{i,ov}\right) \qquad \forall i \in I, s \in S_i, p \in P_i \qquad (5.17)$$

$PV_{i,s,p}$ is the product property (p) for product stream (s) from unit (i) which is a function of feed properties of unit (i) and the operating variables of the unit (i) $FP_{i,p}$ and $OV_{i,ov}$ respectively.

- Processing unit capacity:

$$F_i \leq Umax_i \qquad \forall i \in I \qquad (5.18)$$

The feed of processing unit (i) can not exceed its maximum capacity, which is represented by $Umax_i$.

The possibility for each product from unit (i) to be split to many streams either as final product or feed to other processing unit:

$$V_{i,s} = \sum_{m \in M} VS_{i,s,m} \qquad\qquad \forall i \in I, s \in S_i \qquad\qquad (5.19)$$

Product stream (s) from unit (i) is represented by $V_{i,s}$ can be sent to different destinations (m) defined by streams $VS_{i,s,m}$ (m belongs to the set M defined as all the possible units or final products pool that can receive the splitted streams).

- Fuel switching

For each unit i, one fuel should be selected for each furnace of a unit. This constraint is represented by introducing a binary variable X_{iw} that represents the fuel selection (current or new fuel with less carbon content):

$$\sum_{w} X_{i,w} = 1 \qquad \forall i \in IF \qquad\qquad (5.20)$$

This means that each unit has to run with a specific fuel w. w is the set of fuels considered.

- CO_2 emissions

CO_2 emissions from each furnace of a unit i, α_i (tonne/yr) is defined as:

$$\alpha_i = \sum_{w} CO_{2iw} \, X_{iw} \qquad \forall i \in IF \qquad\qquad (5.21)$$

Where CO_{2iw} is the CO_2 emission for unit i using fuel w. CO_{2iw} is calculated by knowing the emission factor (EF) for fuel w multiplied by fuel consumption which is a function of the inlet flow rate of unit i.

$CO_{2iw} = (EF)_w * (FC)_i$

Where FC is fuel consumption and it is a function of inlet flow rate.

FC = f(F$_i$) and is different for every units. The relation is found from the literature (Gary, 1994).

In equation (5.21), CO_2 emissions from a unit i, α_i can be captured in capture process and in then defined as $\alpha_i^{cap}+\alpha_i^{released}$, where α_i^{cap} is the amount of CO_2 captured and $\alpha_i^{released}$ is amount of CO_2 emitted to the atmosphere. For the case of CO_2 capture with capture

$$\alpha_i^{released} = \alpha_i\left(1-\sum_k \varepsilon_{ik}\,Y_{ik}\right) \qquad \forall i \in IF \qquad (5.22)$$

$$\alpha_i^{cap} = \alpha_i\left(\sum_k \varepsilon_{ik}\,Y_{ik}\right) \qquad \forall i \in IF \qquad (5.23)$$

process, a binary variable Y_{ik} is defined to represent the application or not of a capture process on a unit i, if $Y_{ik} = 1$ and ε_{ik} is fraction of CO_2 captured using technology k,

If there is no CO_2 capture applied, $Y_{ik} = 0$, then all CO_2 emitted from the unit's furnace, α_i, is released to the atmosphere, which results to:

$$\alpha_i^{released} = \alpha_i \qquad \forall i \in IF \qquad (5.24)$$

$$\alpha_i^{cap} = 0 \qquad \forall i \in IF \qquad (5.25)$$

This case is also called carbon capture retrofit and the binary variable, Y_{ik}, indicates the existence/non existence of CO_2 capture process. The total CO_2 emissions (tonne per year) from existing units can be written as:

$$\sum \alpha_i^{released} = \sum_{i \in IF} \alpha_i\left(1-\sum_k \varepsilon_{ik}Y_{ik}\right) \qquad (5.26)$$

Substitution of equation (5.21) into equation (5.26) results in the following equation:

$$\sum \alpha_i^{released} = \sum_{i \in IF}\left[\left(\sum_w CO_{2iw}X_{iw}\right)\left(1-\sum_k \varepsilon_{ik}Y_{ik}\right)\right] \qquad (5.27)$$

The annual total CO_2 emissions from all units must satisfy a specific CO_2 reduction target, $\%CO_2$.

$$\sum_{i \in IF} \left[\left(\sum_w CO_{2iw} X_{iw} \right) \left(1 - \sum_k \varepsilon_{ik} Y_{ik} \right) \right] \leq (1 - \%CO_2) CO_2 \qquad (5.28)$$

In the above equation, the nonlinearity is due to the multiplication of continuous variable CO_{2iw} and binary variable, X_{iw} and also due to multiplication of two binaries X_{iw} and Y_{ik}.

- Fuel switching or CO_2 capture

For each unit i, if the model choose to switch a specific unit i, no capture technology will be applied on that unit.

$$\sum_k Y_{ik} + X_{iw \in NG} \leq 1 \qquad \forall i \in IF \qquad (5.29)$$

- Selection of CO_2 capture process to be installed

This constraint let the model select only one capture process for each unit i belongs to units furnaces set IF.

$$\sum_k Y_{ik} \leq 1 \qquad \forall i \in IF \qquad (5.30)$$

Equations (5.14) and (5.15) represent the feed quantity and properties of the processing unit model, which are playing an important role on the products flow rates and properties, defined by equation (5.16) and (5.17). Clearly, equations (5.14), (5.18) and (5.19) are linear functions. However, the mixing of the different streams properties coming to the unit as feed, and the calculating of the product flow rates and their properties, equations (5.15), (5.16) and (5.17), are nonlinear functions. All CO_2 emissions constraints are non linear.

The developed model for an oil refinery is applied to different case studies in the next chapter.

5.5 Phase 4: Estimation of CO$_2$ Emissions and Products Blending Correlations

This section gives a general procedure for the estimation of CO$_2$ from fuel combustion. Fuel combustion is responsible for about 90% of total CO$_2$ emissions within an oil refinery. Another section is devoted to different blending correlations for refinery final products specifications.

5.5.1 Estimation of CO$_2$ Emissions from Combustion

Fuel combustion CO$_2$ emissions depend upon the amount of fuel consumed and the carbon content of the fuel. To estimate emissions from fuel combustion, the following methodology has been adopted.

$$CO_2 \text{ emissions} = \text{Quantity of fuel combusted} \times \text{EF per physical unit of fuel}$$

EF is emission factor for a specific fuel. These factors have been obtained and developed from a number of studies conducted by Environment Canada, the United States Environmental Protection Agency (EPA) and other organizations. Table 5.3 gives emission factors for different fuels (Karin et al., 2005).

Table 5.3. Emission factor for different fuel (Karin et al., 2005)

Fuel	EF, (tonne CO$_2$/MBTU)
Crude oil	0.074
Diesel	0.073
Jet fuel	0.072
Gasoline	0.071
Natural gas	0.053
Fuel oil	0.081

5.5.2 Products Blending Correlations

Refinery products are typically the result of blending several components or streams. The purpose of the blending process is to obtain petroleum products from refined components that meet certain quality specification and market demand. Increased operating flexibility and profits result when refinery operations produce basic intermediate streams that can be blended to produce a variety of on-specification finished products. In this study, several blending properties are included in the master model. Blending index for each property is used through out this thesis. This blending index is reported in the literature for each property. Then, the blending index can be averaged to calculate the blending property value. The following steps are used for that calculation:

Find index value (IN) for each property (p) using appropriate equation. Then find the blending index (BI) for each property (p) by the following general equation:

$$BI_p = \sum_{s=1}^{S} IN_{p,s} X_s \qquad (5.31)$$

where BI_p represents the blending index for a property p. $IN_{p,s}$ is the index for a property p for stream s and x_s is either mass or volume fraction depends on the property. The properties covered in this study are as follows:

<u>API</u>

The density of petroleum oil is expressed in terms of API gravity rather than specific gravity. It is related to specific gravity in such a fashion that an increase in API gravity corresponds to a decrease in specific gravity. The blended API can be calculated by the following equation: (Gary, 1994)

$$API_{blended} = \frac{141.5}{sp.gr_{blended}} - 131.5 \qquad (5.32)$$

Where $sp.gr_{blend} = \dfrac{\displaystyle\sum_{s=1}^{S} RateV_s \times sp.gr_s}{\displaystyle\sum_{s=1}^{S} RateV_s}$

Where $RateV_s$ is volumetric flow rate of a stream s.

Specific gravity (sp.gr) can be averaged while API can not.

Sulphur content (wt%)

Sulphur content is an important property which has a major influence on the value of crude oil. The sulphur content for a blended stream is the average sulphur content for all coming streams and should be expressed in weight percent. It can be calculated from the following equation: (Gary, 1994)

$$Sul_{blended} = \dfrac{\displaystyle\sum_{s=1}^{S} RateW_s \times Sul_s}{\displaystyle\sum_{s=1}^{S} RateW_s} \tag{5.33}$$

Where $RateW_s$ is the mass flow rate for stream s being blended.

Octane number (ON)

Octane numbers are blended on a volumetric basis using the blending indexes of the components. True octane numbers do not blend linearly and it is necessary to use blending octane numbers in making calculations. Several blending approaches are provided in the literature and the simplest form has been converted to the following analytical relation (Riazi, 2005)

$$IN_{RON} = 651X^3 - 1552.9X^2 + 1272X - 299.5 \qquad 76 \le RON \le 103 \tag{5.34}$$

Where X = RON/100

$$BI_{blend} = \sum_{s=1}^{S} IN_{RON,s} X_s$$

Where X_s is the volume fraction and $IN_{RON,s}$ is the octane number blending index for stream s.

Reid Vapour Pressure (RVP)

The RVP is one of the important properties of gasoline and jet fuels and it is used as a criterion for blending products. The Reid vapour pressure is the absolute pressure exerted by a mixture at $100^{\circ}F$ ($38^{\circ}C$). There are two methods, shown below, for calculating the RVP of a blend when several components with different RVPs are blended. The first method is based on the simple mixing rule using mole fraction (X_s) of each stream. (Riazi, 2005)

$$RVP_{blend} = \sum_{s=1}^{S} (RVP)_s X_s \qquad (5.35)$$

Where $(RVP)_s$ is the RVP of stream s in bar or psia.

The second approach is to use blending index for RVP as:

$$(RVPBI)_s = (RVP)_s^{1.25} \qquad (5.36)$$

$$(RVPBI)_{blend} = \sum_{s=1}^{S} X_s (RVPBI)_s \qquad (5.37)$$

$$(RVP)_{blend} = \left[(RVPBI)_{blend} \right]^{0.8} \qquad (5.38)$$

Where $(RVPBI)_s$ is the blending index for $(RVP)_s$ and X_s is the volume fraction of stream s. Both units of bar or psia may be used in the above equation. This relation was originally developed by Chevron and is also recommended in other industrial manuals under Chevron blending number (Riazi, 2005).

Cetane Number and Diesel Index

For diesel engines, the fuel must have a characteristic that favors auto-ignition. The ignition delay period can be evaluated by the fuel characterization factor called cetane number (CN). The behavior of a diesel fuel is measured by comparing its performance with two pure hydrocarbons: n-cetane or n-hexadecane (n-$C_{16}H_{34}$) which is given the number 100 and α-methylnaphthalene which is given the cetane number of 0. A diesel fuel has a cetane number of 60 if it behaves like a binary mixture of 60 vol% cetane and

40 vol% α-methylnaphthalene. Another characteristic of diesel fuels is called diesel index (DI) defined as:

$$DI = \frac{(API)(1.8AP + 32)}{100}$$ (Riazi, 2005)   (5.39)

which is a function of API gravity and aniline point (AN) in ^oC. Products containing aromatics or naphthenes have lower aniline points than products containing paraffins. Cetane index (CI) is empirically correlated to DI and AP in the following form:

CI = 0.72DI+10

It is reported in the literature that cetane number can be blended by volume basis (Baird, 1987) as in the case of specific gravity.

Smoke point

Smoke point is a characterization of aviation turbine fuels and kerosene and indicates the tendency of a fuel to burn with a smoky flame. Higher amount of aromatics in a fuel causes a smoky characteristic for the flame and energy loss due to thermal radiation. The equation to calculate the smoke point index is (Riazi, 2005):

$$IN_{SP} = \frac{1}{SP}$$ (5.40)

The methodology of finding the blended smoke point is via the blending index and then by applying equation (5.31).

The previous blending correlations are implemented into the model for finding final product specifications.

5.6 Phase 5: Model Application and Coding

This section deals with implementing the refinery planning model, developed earlier, on different case studies. The objective is to maximize the profit and to meet the demand of each final product with quality specifications. The CO_2 emissions should be reduced up to a certain target while maximizing profit. This is achieved by selecting the best strategy or mix of strategies to meet the target. The mitigation options being considered

in this research are flow rate balancing, fuel switching and CO_2 capture technology. The case studies being considered are:

Base case: The refinery planning model is initially formulated as an NLP model (non-linearity due to blending correlations) to meet demand of each product with quality specifications. The objective is to maximize the profit and meet the products specifications without considering any CO_2 mitigation option.

Case 1: The refinery planning model with only flow rate balancing as an option to reduce CO_2 emissions is solved. Balancing simply reduces the inlet flow rate to a unit that emits more CO_2. Two different targets are set to see the effect of this mitigation option. The first target is to meet products demand without specifications. The second option is to meet products demand with specifications.

Case 2: The complete planning model with quality constraints and two CO_2 mitigation options are considered. The two options to reduce CO_2 are flow rate balancing (as in case 1) and fuel switching. The model is formulated as MINLP. A binary variable representing switching or not is introduced into the model.

Case 3: The third case study is basically an extension to case study 2. The model considered all three CO_2 mitigation options to meet further CO_2 reduction target. These are flow rate balancing, fuel switching and CO_2 capture. The model is MINLP since another binary variable is defined for existence or not of CO_2 capture process.

Case 4: The planning model is solved as in case 3 but sequestration cost is added to the model.

The mathematical models are coded into GAMS.

CHAPTER 6

CASE STUDIES: AN OPTIMIZATION APPROACH FOR INTEGRATING PLANNING AND CO_2 EMISSIONS REDUCTION IN THE PETROLEUM REFINING INDUSTRY

6.1 Introduction

The mathematical model developed in Chapter 5 for an oil refinery is illustrated on different case studies. This section considers the problem of reducing CO_2 emissions from unit heaters in an oil refinery by three different options. The first option is balancing in which the production from units that emit less CO_2 is increased with decrease in the production from units that emit more CO_2. This is because fuel consumption for each unit is a function of inlet flow rate. The second option for reducing CO_2 emissions is by switching in which the unit will be switched to operate with less carbon content fuel such as natural gas. The third option being considered in this section is applying CO_2 capture technologies. The objective of the model is to maximize the profit from selling final products while reducing CO_2 emission by a fixed target. The results for different case studies with sensitivity analysis are given at the end of this chapter. The cases under study are:

- Case 1: Planning model with properties (base case) and then add to it balancing as the only option to mitigate CO_2 emission.
- Case 2: Planning model with properties and two mitigation options. These are balancing and fuel switching.
- Case 3: Planning model with all three mitigation options. These are balancing, switching and capture.
- Case 4: Planning model with all three mitigation options and considering sequestration cost.

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6.2 Problem Description for these Case Studies

A petroleum refinery is an extremely complex entity. In general, a refinery is made up of various processing units that separate crude oil into different fractions or cuts, upgrade and purify some of these cuts, and convert heavy fractions to light, more useful, fractions. However, profitable operation of a refinery requires an optimization of streams flows and process feed. On the other hand, several trends in the oil refinery industry are leading to a tight production of different products because of new specifications and environmental regulations. The increased market for the heavier crude oils forces refineries to increase their use of conversion units, where hydrocracking as a way of upgrading heavy oils to more valuable products is employed. Tightening of air regulations continuously reduces the allowed sulphur content in fuel products (low sulphur gasoline and diesel fuel). The refinery sector also has to comply with the Kyoto accord to reduce CO_2 emissions. The major source of CO_2 emission within an oil refinery is combustion source such as furnaces. An efficient model for the refinery planning will represent production planning with different CO_2 mitigation options in order to meet a certain CO_2 emissions reduction. The model is illustrated for different case studies. The objective in the model is to maximize the profit of an oil refinery by producing certain amount of each product with specific quality and meet a CO_2 reduction target by implementing several mitigation options. The options being considered in this study are flow rate balancing, fuel switching (i.e. from fuel oil to natural gas) and CO_2 capture technology such as MEA.

The oil refinery described here (shown in Figure 6.1) consists of several processing units, splitters and mixers. The connections between these units, splitters and mixers draw the refinery network picture that general model aim to solve to meet the objective of planning model. Refinery intermediate streams with different properties are blended in order to feed for a processing unit or to be ready for sale as a final product. For both cases, the blended streams have to meet specified specifications. Nonlinear unit models, that describe more accurately product flow rates and properties than linear models assuming fixed yield, are presented and linked with nonlinear properties blending

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equations. The overall model is integrated with a CO_2 management model in order to reduce CO_2 emission from combustion source within an oil refinery.
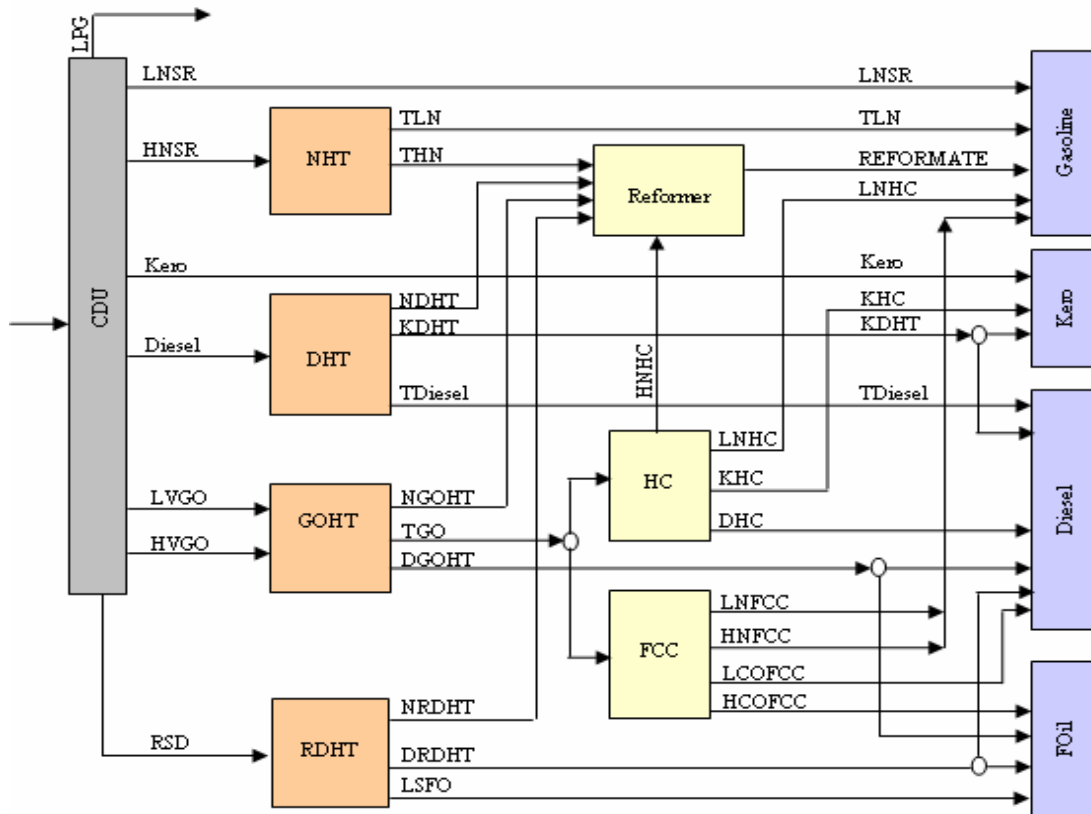
Figure 6.1. Refinery layout

The aim of the model is to optimize the flow rate and properties for each stream in order to maximize profit while reducing CO_2 emissions to a given target.

6.3 Model Formulation

The optimization problem to be studied in this chapter can be formulated in words as: "For a given CO_2 reduction target, what is the best strategy or mix of strategies, for an oil refinery, among the considered options (flow rate balancing, fuel switching and CO_2 capture) in order to meet the demand for each product with quality specifications while maximizing the profit?". The objective is to maximize the profit of selling the final

products to meet the demand with quality specifications and reduce the CO_2 emissions to a given level. The main variables are the flows of each stream and products to be processed, intermediate products and finished products. These include also the properties of each stream such as API, sulphur content, octane number, RVP, cetane number and smoke point. A binary variable X_{iw}, is introduced into the model that represents fuel switching or not. Another binary variable Y_{ik}, is introduced into the model to show existence or not of a capture process k.

Individual nonlinear mathematical models (sub-models) were developed for all units in the refinery, shown in Figure 6.1, prior to the development of the planning model (master model). The sub-models were developed for: the crude distillation unit (CDU), all the hydrotreaters, the reformer, the FCC and the HC.

The model is formulated as a MINLP since nonlinearity is present from the blending correlations and the binary variables introduced for the switching and capture options. In order to solve the MINLP model, a superstructure representing the main units within an oil refinery, flow rate balancing, fuel switching and CO_2 capture process was presented in the previous chapter.

Four different options are considered as discussed earlier and these are:
- Option 1: No CO_2 mitigation options
- Option 2: Flow rate balancing
- Option 3: Fuel switching
- Option 4: Existence of CO_2 capture technology

Fuel switching represents switching from current fuel (fuel oil) to natural gas. The CO_2 capture process used in this study is MEA. Economic data are given in Appendix D.

The model developed in chapter 5 is solved in this chapter and is applied to different case studies.

6.4 Results and Discussion

Four different cases in addition to the base case are considered:

Base case: Solve the planning model to meet demand and specifications without any CO_2 mitigation option.

Case1: Solve the planning model first and then consider only flow rate balancing as the CO_2 mitigation option with and without considering the quality constraints. This is just to show that balancing can affect the results. The model is still a NLP.

Case2: Solve the planning model with quality constraint considering flow rate balancing and fuel switching to meet certain CO_2 reduction target. The model is a MINLP since a binary variable is introduced for fuel switching.

Case3: Solve the planning model with quality constraints considering flow rate balancing, fuel switching and CO_2 capture technology. The model is a MINLP.

Case4: Solve the planning model with quality constraints considering flow rate balancing, fuel switching and CO_2 capture technologies with sequestration.

In order to illustrate the model, Figure 6.1 for a petroleum refinery process is used. A 100,000 bbl/day Alaska crude oil is selected to be the feed to the refinery. The refinery has to meet the market demands for different products (Table 6.1). The product price is given in the same table. Also, product specifications have to be met (Table 6.2) and a certain CO_2 emissions reduction target is set.

Table 6.1. Products demand

Final Product	Demand Bbl/day	Price US$/Bbl
Gasoline	25,000	88.2
Kerosene (Jet Fuel)	25,000	72.7
Diesel	25,000	66.0
Fuel Oil	18,000	39.5

The objective function will be to maximize the overall refinery revenue while meeting both market demand quantity and quality with certain CO_2 reduction target.

Table 6.2. Products specification

Final Product	Property	Specification requirement
Gasoline	S.Gr	≤0.8
	Sul%	≤0.05
	RON	≥89.0
	RVP, psi	≤9.0
Jet Fuel	S.Gr	≤0.85
	Sul%	≤0.25
	Smoke Point	≥20.0
Diesel	S.Gr	≤0.87
	Sul%	≤0.5
	CN	≥45
Fuel Oil	S.Gr	≤1.0
	Sul%	≤1.0

The model was written in the General Algebraic Modeling System (GAMS). The GAMS model optimizes all intermediate and final products streams across a crude oil refinery subject to connectivity, capacity, demand, and quality constraints with certain CO_2 reduction target. These constraints can be easily modified to either incorporate new data.

Base case:

First, the planning model is solved. The planning model is formulated as a NLP. A summary of every blending pool streams flow rates for the base case without CO_2 reduction target is illustrated in Table 6.3 with a total profit of 7.40×10^8 \$/yr (with quality constraints) and CO_2 emissions of 733,000 tonne/yr. Table 6.4 shows the product properties that the model is trying to satisfy while meeting the demand. The last column represents the model results.

It is clear from the two tables that the planning model tries to meet the demand requirement for each product and the properties required for meeting the quality constraint for each final product. The most profitable product among an oil refinery is gasoline. So, the model tends to produce more gasoline while meeting the demand for other products is also mandatory. For example, the kerosene produced by the diesel hydrotreater (KDHT) is selected to be blended with the kerosene pool rather than diesel since the kerosene selling price is higher than that for diesel fuel.

Table 6.3. Blending products flow rate

Product Stream	Flow Rate Bbl/day	Blending Pool	Final Product Bbl/day	Demand Bbl/day
LSRN	3530	**Gasoline**	**28,420**	**25,000**
TLN	1,530			
REFORMATE	15,300			
LNHC	1,558			
LNFCC	3,616			
HNFCC	2,886			
Kero (CDU)	13,360	**Kerosene**	**25,850**	**25,000**
KHC	10,230			
KDHT	2,260			
TDiesel	12,925	**Diesel**	**25,550**	**25,000**
KDHT	0			
DHC	10,665			
DGOHT	140			
LCOFCC	1,820			
DRDHT	0			
HCOFCC	685	**Fuel Oil**	**18,805**	**18,000**
DGHOT	1400			
DRDHT	1320			
LSFO	15,400			

Table 6.4. Product properties after running the model

Final Product	Property	Specification requirement	Model
Gasoline	S.Gr	≤0.8	0.795
	Sul%	≤0.05	0.003
	RON	≥89.0	91.5
	RVP, psi	≤9.0	8.9
Jet Fuel	S.Gr	≤0.85	0.835
	Sul%	≤0.25	0.2
	Smoke Point	≥20.0	20.8
Diesel	S.Gr	≤0.87	0.86
	Sul%	≤0.5	0.07
	CN	≥45	52
Fuel Oil	S.Gr	≤1.0	1.0
	Sul%	≤1.0	0.2

In the case of DGOHT and DRDHT; the model has a choice to send each stream to either the diesel pool or fuel oil pool. The model suggests sending these products to the fuel oil pool instead of the diesel pool although the diesel selling price is higher than fuel oil selling price. This is done in order to meet the demand for the fuel oil. If we could lower the demand for the fuel oil or if it could be met by other intermediate products, the model will blend that streams into the diesel pool.

For all products, the desired properties are met. Gasoline properties, for example are met. The specific gravity is near the desired value with sulphur content much lower than the specified range. None of the constraints, even octane number constraint is a binding constraint.

The properties for jet fuel are tighter than those for gasoline and they are all near the limit. For diesel, all properties are set away from the limit and they are all met. The fuel

oil property constraints are all satisfied with specific gravity constraint as the only binding one.

Figure 6.2 illustrates the CO_2 emissions from each unit (combustion source) without any mitigation options (Base case). The fuel used in combustion for all units is fuel oil. The profit is 7.40×10^8 \$/yr with the total CO_2 emission of 733,000 tonne/yr.
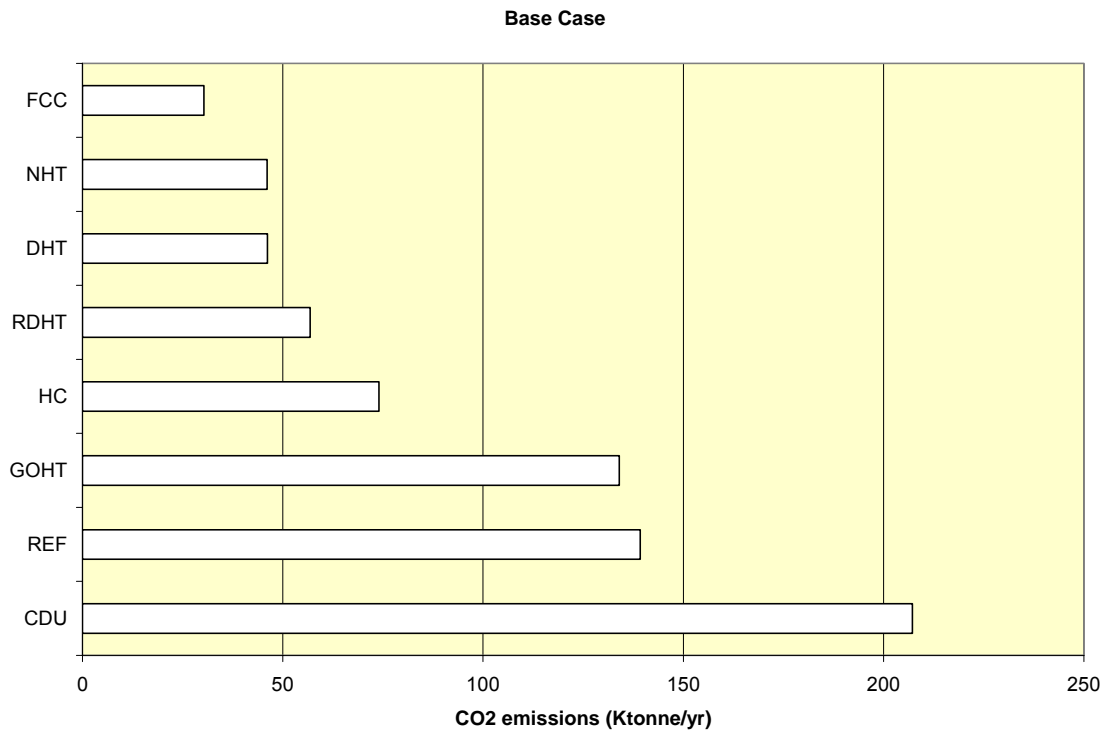
Base Case

Figure 6.2. Base case

Case 1:

In this case study, the planning model is solved with only one mitigation option and this is balancing. It is found that CO_2 balancing is a good option only when the product quality specifications are not considered in the model. A maximum of 3% CO_2 reduction can be achieved by simply decreasing the flow rate for the units that emit more CO_2 such as the reformer and the hydrocracker and increase production from units

that emit less CO_2 such as the FCC. The profit is about 7.44×10^8 \$/yr with no properties included. It decreases by four million when properties are added to the model.

Flow rate balancing can achieve only 0.4% CO_2 reduction and no more than that when the product specifications are added to the model (Base case). For that reduction target, it is achieved simply by increase production from the FCC (less CO_2) by 20% and decrease production from the hydrocracker (HC) by the same amount. This results in more gasoline and fuel oil production from the FCC unit and a decrease in jet fuel production but still the demand is met for each final product.

The results for this case study mean that for higher reduction target, such as above 1%, more CO_2 mitigation options need to be considered. These include fuel switching and CO_2 capture. These are shown in the following cases.

Case 2:
Planning model with quality constraint and CO_2 mitigation by balancing and fuel switching is studied in this case study. Only fuel switching to natural gas is considered here.
A retrofit cost , given in appendix D, is applied for each unit if it is switched to natural gas. A binary variable is introduced as shown in the model above.

$$X_{iw} = \begin{cases} 1 & \textit{if fuel w is selected} \\ 0 & \textit{otherwise} \end{cases}$$

Figure 6.3 shows the results for 1% CO_2 reduction targer. In this case, , the model chose to switch one unit to run with natural gas and this is the FCC unit. This unit is not considered a major contributor to CO_2 emissions. The base case is shown in each figure for comparison. The product quantity and quality remain almost unchanged except the profit which decreases with higher CO_2 reduction target due to the retrofit cost for switching. The natural gas cost and economic data are given in Appendix D.

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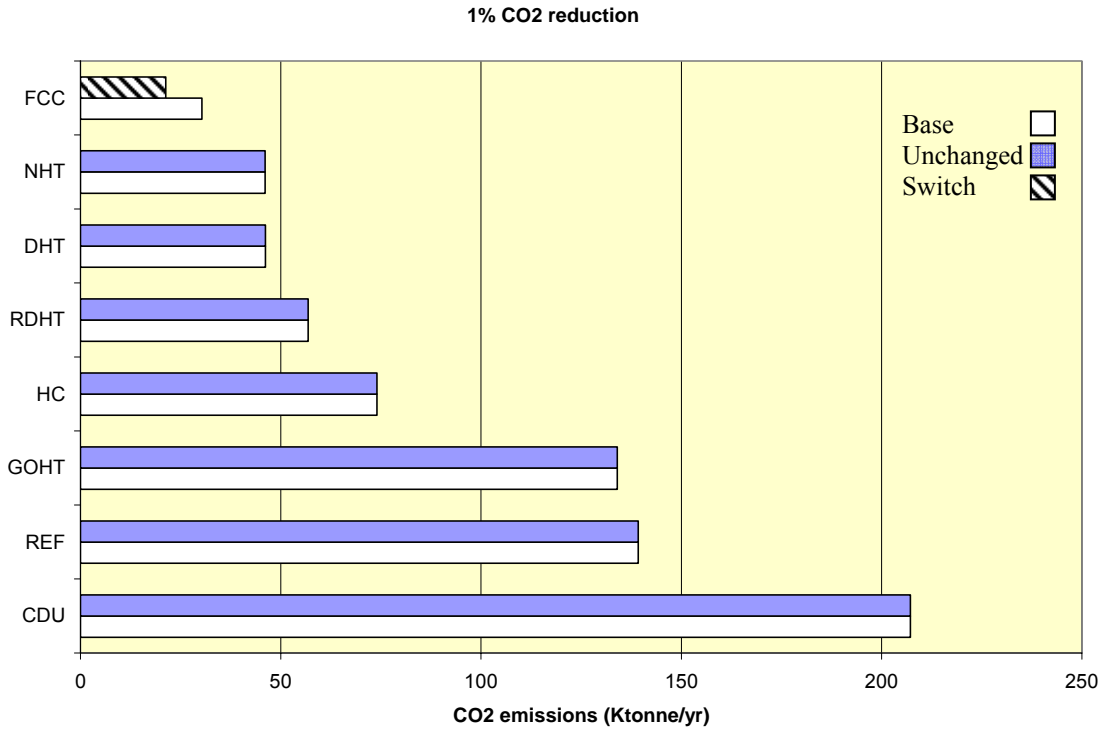
1% CO2 reduction

Figure 6.3.Case 2: 1% CO_2 reduction

For higher reduction target such as 10%. The model tends to switch more units to natural gas. Figure 6.4 shows the result for this case study.

As seen in Figure 6.5, for 20% reduction target, even more units should be switched to natural gas. Figure 6.5 shows that three major units are chosen to be switched and these are crude distillation unit (CDU), gas oil hydrotreater (GOHT) and the reformer. These units have the highest CO_2 emissions compared to other units. The products flow rate and product specification are all almost the same and only switching is considered as a good option to reduce CO_2 emission but the profit will decrease as shown later.
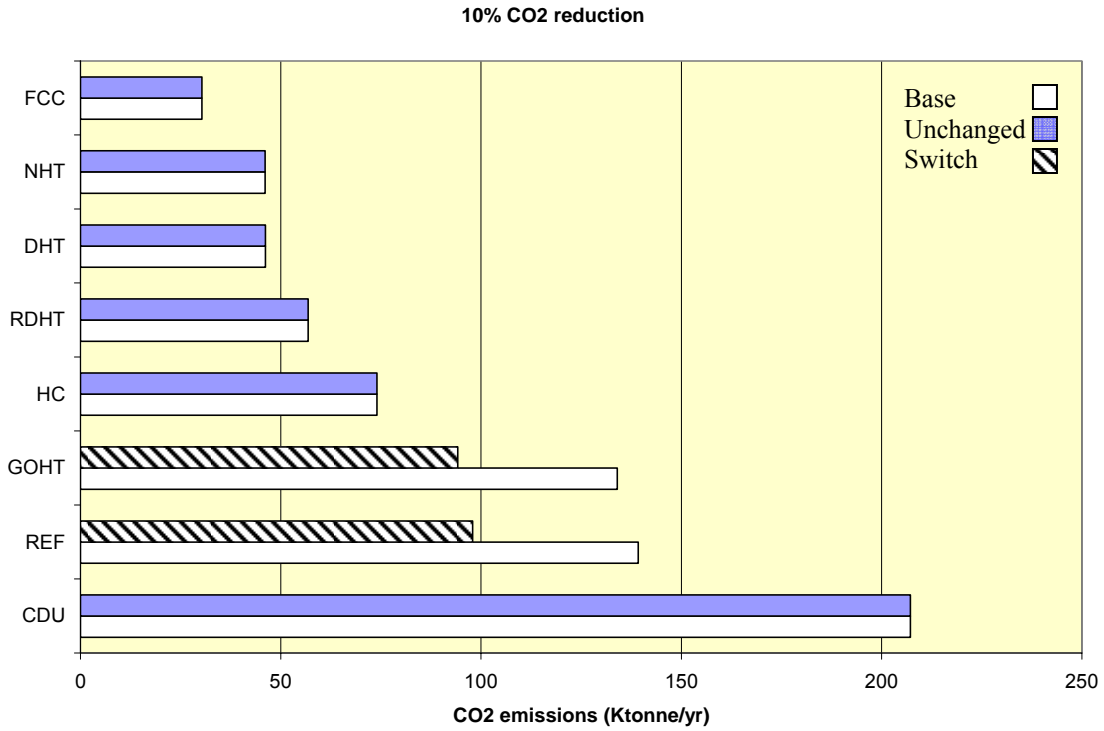
10% CO2 reduction

Figure 6.4. Case2: 10% CO_2 reduction
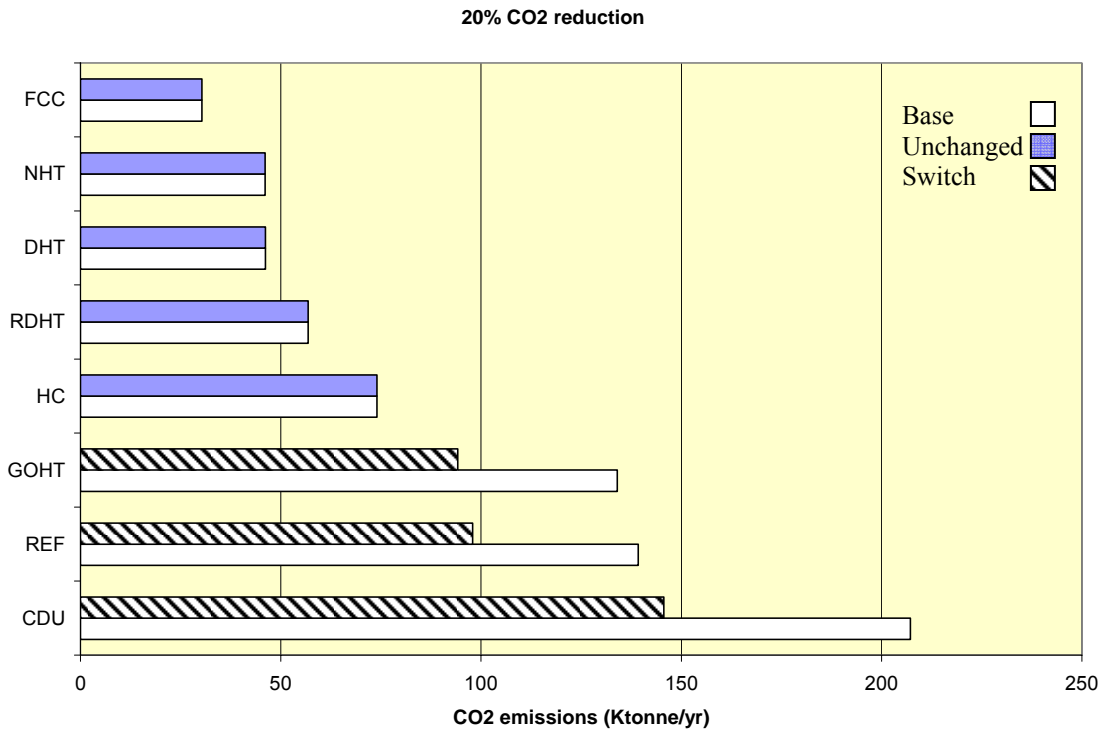
20% CO2 reduction

Figure 6.5. Case 2: 20% CO_2 reduction

Figure 6.6 shows the results for 30% reduction in CO_2 emissions with fuel switching. At this level of CO_2 reduction, all fuels have been switched to natural gas. To go beyond 30% reduction in CO_2 emissions, other mitigation options must be considered.
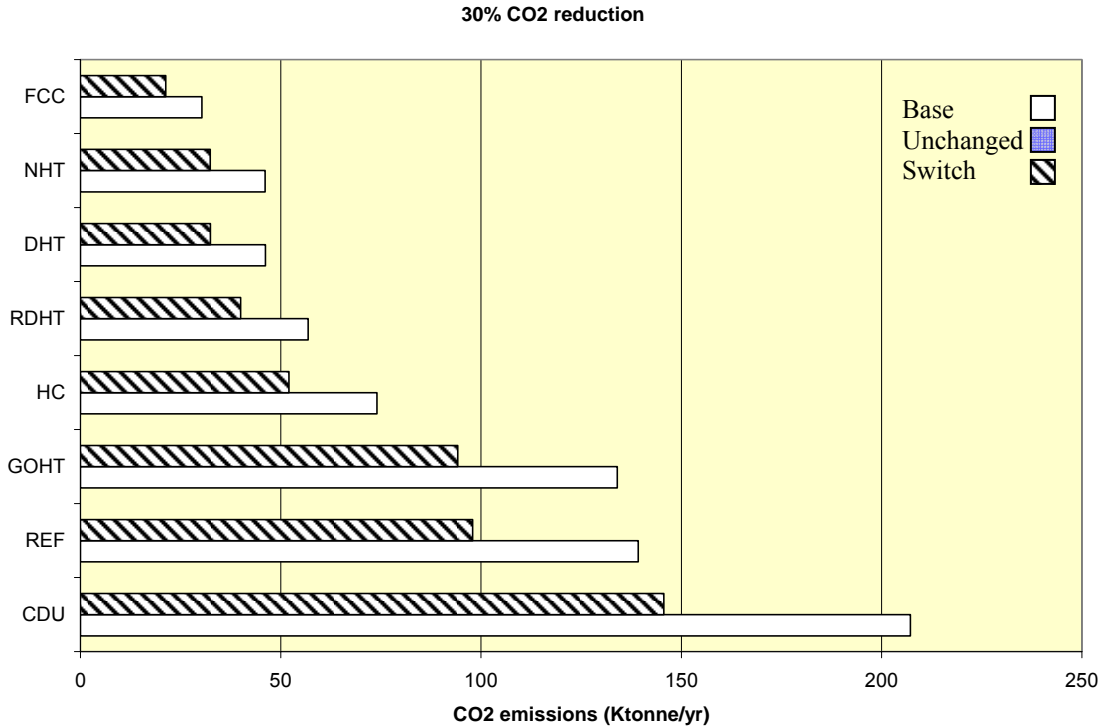
Figure 6.6. Case 2: 30% CO_2 reduction

Table 6.5 gives a summary of the results for this case. It shows the profit for each reduction target with % reduction in the profit. For 1% reduction, the profit decreases by only 0.14% since only one unit is switched to natural gas. As more units are switched to run with natural gas, the profit decreases by a noticeable percent. At 30% CO_2 reduction, for example, the profit decreases by about 3%.

Table 6.5. Summary of results for Case 2

% Reduction	Profit (million $/yr)	CO_2 emission (ktonne/yr)	% Reduction in Profit
Base	740	733.0	0
1	739	725.7	0.14
10	732	659.7	1.0
20	726	586.4	2.1
30	717	513.1	3.1

The next figure (Figure 6.7) shows the profit for each reduction target. As the reduction target increases, the profit decreases because more units are selected to run with natural gas. A decrease in profit seems more pronounced for CO_2 reduction target above 20%.
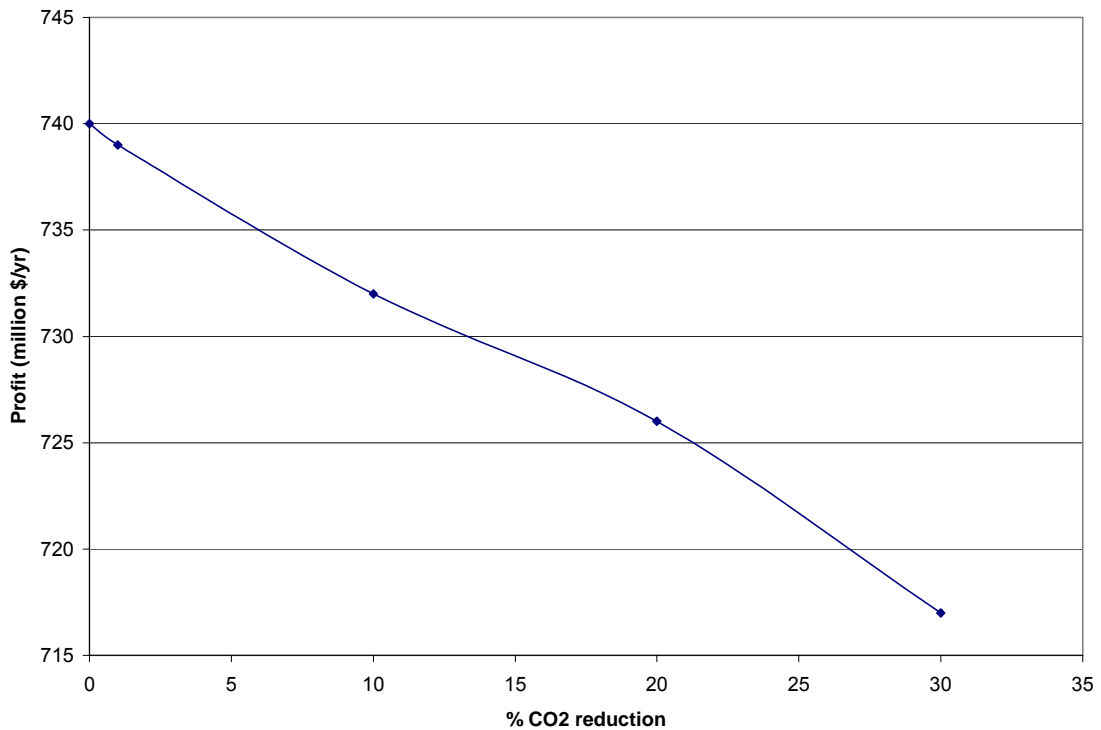
Figure 6.7. Profit vs. %CO_2 reduction target for case 2

Planning model with quality constraints and CO_2 mitigation by balancing, fuel switching and CO_2 capture process are considered in this case study. The capture process under consideration is MEA process since it is the only commercially available at this scale. The cost for capture process is implemented in the model. A binary variable, Y_{ik}, is introduced in the model to find existing or not of capture process k and also from which unit to capture.

$$Y_{ik} = \begin{cases} 1 & \textit{if capture process k applied} \\ 0 & \textit{otherwise} \end{cases}$$

Since up to 30% CO_2 reduction can be achieved by switching as shown in previous case, only higher reduction target will be shown in this case considering capture process. The capture process is a better alternative to achieve high percentage of CO_2 reduction. No capture process needs to be applied if the reduction target is 30% or less.

Figure 6.8 shows the results for 40% CO_2 reduction. The model chose then to switch four units (RDHT, GOHT, HC and REF) to natural gas and install capture process to the CDU since it is the major contributor to the overall CO_2 emissions. Note that now not all units have been switched to natural gas. Three units keep running with the old fuel (fuel oil). These units are DHT, NHT and FCC The quantity and quality of final products remain almost the same as the previous case (Case 2). The differences are only in the number of switched units and in the resulting profit which decreases as CO_2 reduction target increases. The base case is shown in each Figure for easy comparison.
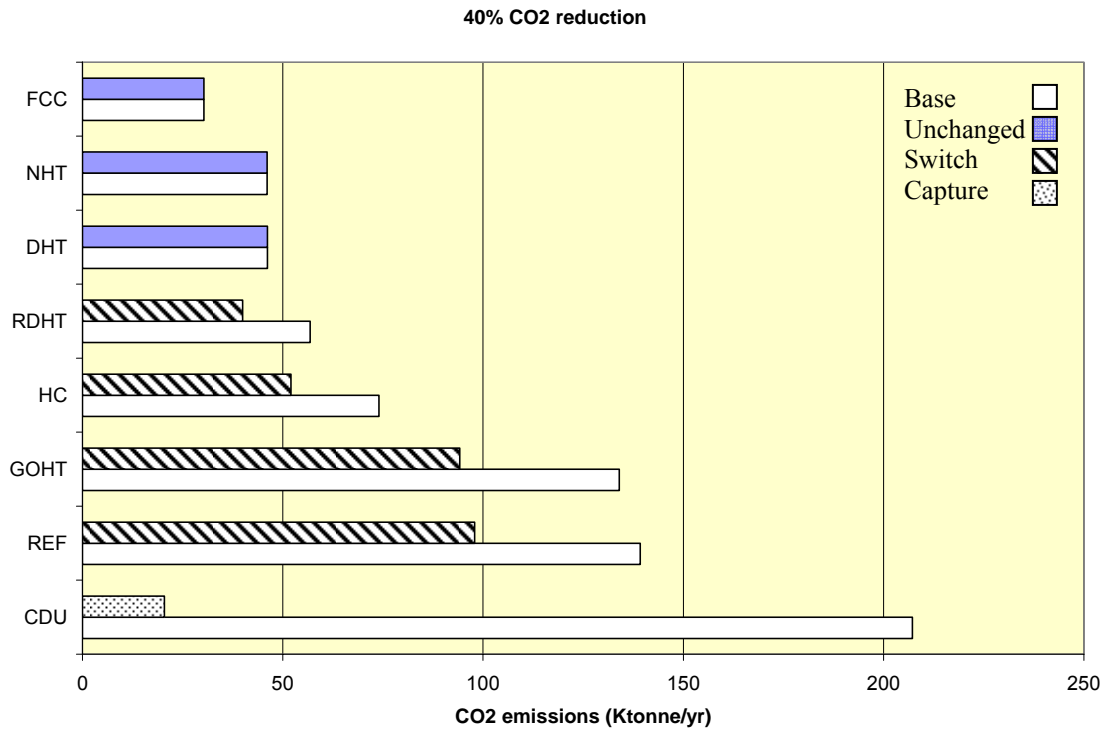
Figure 6.8. Case 3: 40% CO_2 reduction

For higher reduction targets, such as 60% (see Figure 6.9), more CO_2 needs to be captured from more units. The model chose to capture CO_2 from four different units. These units are CDU, RDHT, DHT and HC. These units have the highest impacts on the overall CO_2 emission. Three units are chosen to be switched to natural gas and these units are GOHT, NHT and REF. Only the FCC unit still runs with fuel oil.
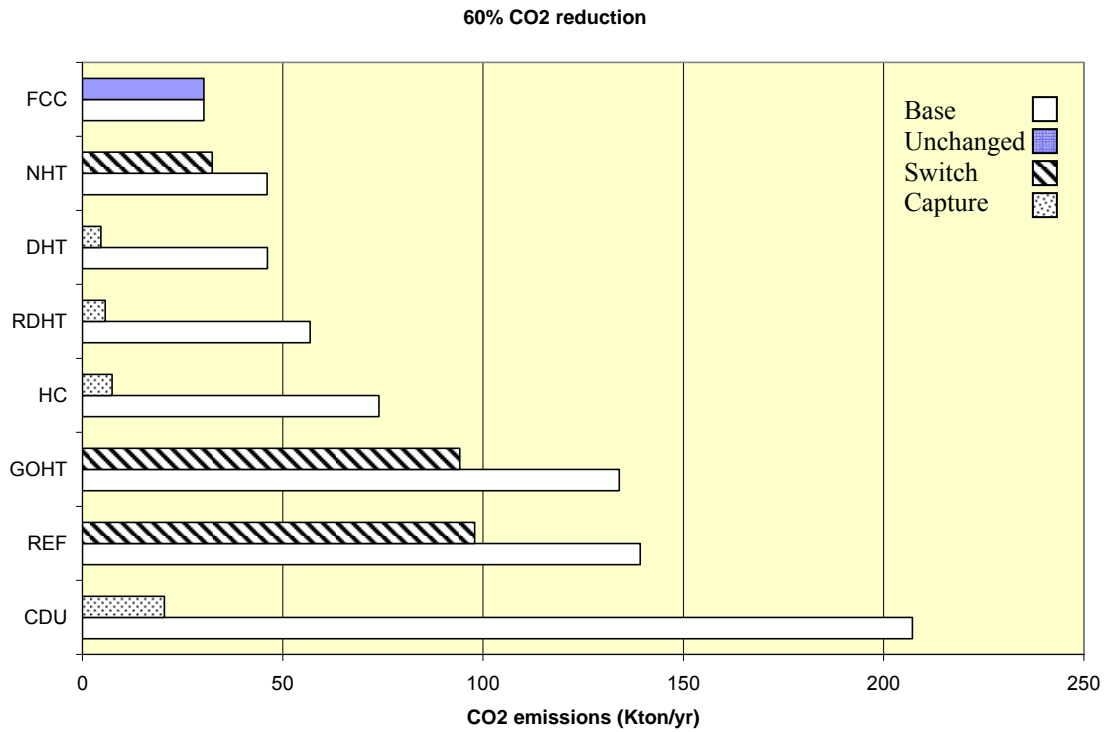
Figure 6.9. Case 3: 60% CO_2 reduction

Figure 6.10 shows the result for 80% reduction target. The results show that CO_2 emissions should be captured from six units and only NHT has to be switched and DHT remain unchanged. This is done to achieve the reduction target and maximizing the profit. However, it is found that 90% is the maximum possible reduction target when all CO_2 emissions from all units are captured. A summary of results for Case 3 is given in Table 6.6. It shows that the profit decreases by about 3.5% at 40% CO_2 reduction target. About 6% drop in profit is noticed at 90% CO_2 reduction when CO_2 emissions from all units are captured.
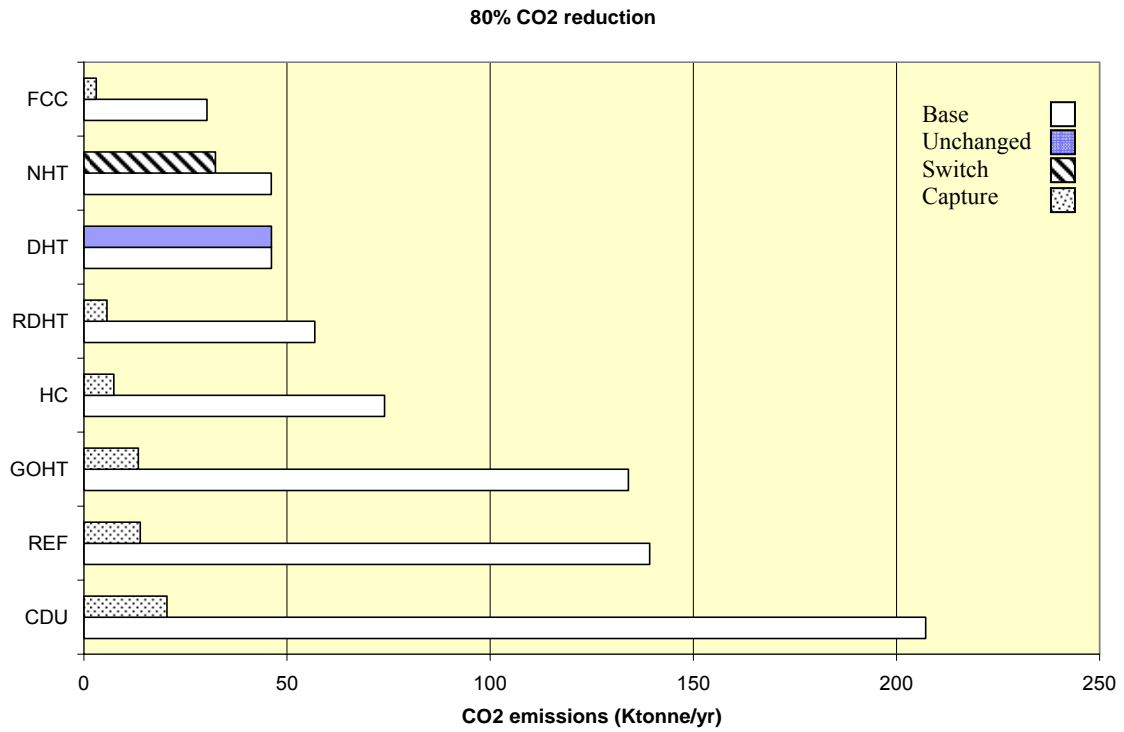
Figure 6.10. Case 3: 80% CO_2 reduction

Table 6.6. Summary of results for Case 3

% Reduction	Profit (million \$/yr)	CO_2 emission (ktonne/yr)	% Reduction in Profit
Base	740	733.0	0
40	715	440	3.5
60	710	293	4.0
80	702	147	5.3
90	698	73.3	5.8

Figure 6.11 shows the profit for each reduction target for this case study. Only higher reduction target is shown since no capture process is chosen to be applied at 30%

reduction target or less. The profit decreases as more CO_2 emissions are captured from more units.
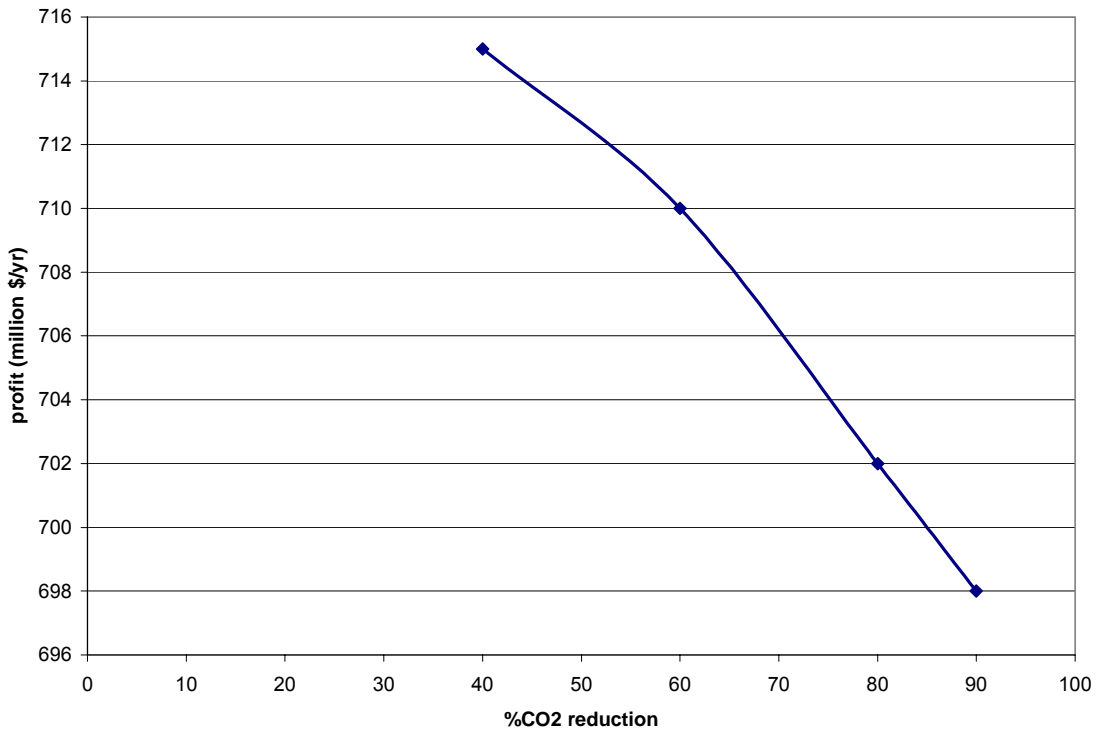
Figure 6.11. Profit vs. %CO_2 reduction target for case 3

Case 4: Planning model with quality constraint and CO_2 mitigation by balancing, fuel switching and CO_2 capture process with sequestration is considered in this case study. The only option considered in this study, for sequestration, is enhanced oil recovery. The results shown in the following table (Table 6.7) are for reduction target higher than 30% where CO_2 capture processes would be implemented. The model assumed existence of sequestration once capture process is applied. The cost of sequestration is implemented into the model. About 9% decrease in profit is noticed at 90% CO_2 reduction target. The cost data is given in appendix D.

Table 6.7. Summary of results for Case 4

% Reduction	Profit (million $/yr)	CO$_2$ emission (ktonne/yr)	% Reduction in Profit
Base	740	733.0	0
40	712	440	3.8
60	701	293	5.3
80	686	147	7.3
90	675	73.3	8.8

The profit as a function of reduction target for this case is shown in Figure 6.12.
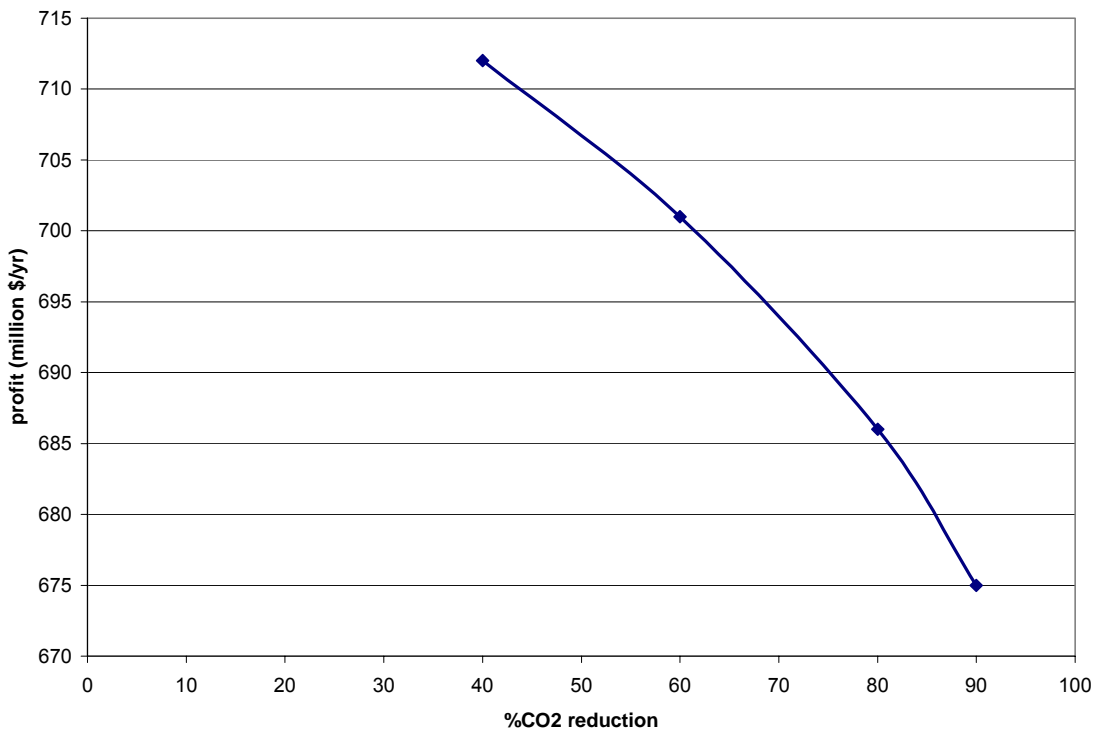
Figure 6.12. Profit vs. %CO$_2$ reduction target for case 4

6.5 Sensitivity Analysis

In this study, sensitivity analysis of final product prices, products demand, switching retrofit cost and CO_2 capture cost were performed to analyse the impact on the profit for the different case studies shown in the previous section.

Case 1:

Since for Case 1 only balancing was considered as the CO_2 mitigation option, only the effect of demand and final product prices are considered. Balancing can achieve up to 0.4% reduction by simply increase production from the FCC and decreasing production from the HC unit. Increasing demand of each final product will affect the final products quantity. However, the model tries to satisfy demand of each product by manipulating inlet flow rate for each unit to satisfy the demand and CO_2 reduction target. The results show, for higher demand, a decrease in jet fuel and an increase in diesel production. This will lead to a decrease in the profit of about 0.5 million $/yr. For an increase of 20% in final products price compared to the base case, the profit increases to about 885 (million $/yr) while it decreases to about 590 if the final products price decreases by 20%.

Case 2:

Two CO_2 mitigation options are considered in this case study and these are balancing and fuel switching. The effect of demand growth is also studied in this case study. Demand growth in each final product will make the model to incorporate flow rate balancing in order to achieve the desired demand and the reduction target. The demand is met for each product and the quantity of each product changes from the base case. Table 6.8 shows the sensitivity analysis results for Case 2. Gasoline and fuel oil change slightly where jet fuel is decreased and diesel production is increased leading to a profit decrease of about 1% for 1% reduction target. For higher reduction target, the optimizer implements balancing and switching in this case study to meet the demand even at higher target demand. The effect of final product selling price (increase by 20% in the price or decrease by 20%) is studied. In addition, effect of both an increase by 30% in

the switching cost to natural gas and decrease by 30% in the retrofit cost that involves switching is also investigated. It is noticed that any increase or decrease either on final product selling price or switching cost does not affect the number of units to be switched to run with natural gas. The amount of each final product does not change too. The only effected variable is the profit as shown in the table below. The profit obviously increases with increasing the price of selling final product or decreasing the retrofit cost of switching to natural gas.

Table 6.8. Sensitivity analysis results for Case 2

% CO_2 Reduction	Profit (million \$/yr)			
	20% increase in selling price of products	20% decrease in selling price of products	30% increase in switching cost	30% decrease in switching cost
1	884	589	739	739.4
10	880	585	731	735
20	877	582	727	732
30	857	568	713	724

Figure 6.13 shows these results for this case. The figure clearly shows that selling price of final products has the major effect on the profit. At low reduction target such as 1%, no major effect on the profit is noticed when increasing or decreasing switching cost since only one unit is chosen to be switched to natural gas. As the reduction target increases, switching cost starts to have significant effect on the profit.
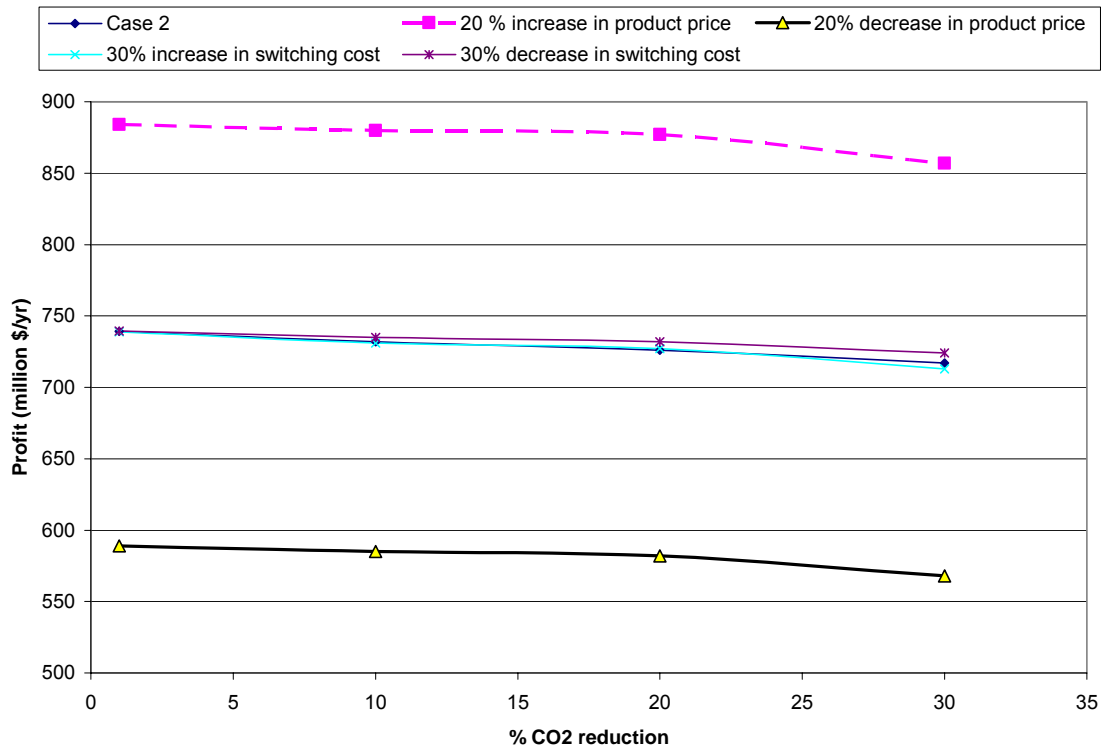
Figure 6.13. Sensitivity analysis results for Case 2

Case 3:

The effect of demand growth is studied and it is noticed that final products quantity is affected. Any increase in demand will lead to a change in flow rates which means that balancing is taking place in order to meet demand and a certain reduction target. The units chosen to be switched or captured do not change. The effect of final product selling price (increase by 20% in the price or decease by 20%) is studied as in the previous case. In addition, effect of an increase by 30% or decrease by 30% in the retrofit cost to natural gas and in capture process cost is investigated. As in case 2, it is noticed that any increase or decrease either on final product selling price or switching cost and capture process cost does not affect the number of units to be switched to run with natural gas or amount of CO_2 captured. The amount of each final product does not change much except when the demand change. The only affected variable is the profit as shown in the table below (Table 6.9). The profit obviously increases with increasing price of selling final product and decreases at higher cost of switching to natural gas or at higher cost of the capture process.

Table 6.9. Sensitivity analysis results for Case 3

% CO$_2$ Reduction	Profit (million $/yr)			
	20% increase in selling price of products	20% decrease in selling price of products	30% increase in switching and capture cost	30% decrease in switching and capture cost
40	868	573	712	723
60	858	563	703	719
80	848	554	690	712
90	841	546	682	706

Figure 6.14 shows the sensitivity analysis results. It is clear that final product price has the major effect on the profit. As the reduction target increases, the profit for the case of increase and decrease in the switching and capture cost start to change from the result of case 3. This is because the model chooses to apply capture on more units and the profit starts to be affected by the cost of switching and capture as more reduction target is set.

Case study 4:

As all previous cases, the effect of 20% increase or 20% decrease in product selling price on the objective function is studied. Also, 30% increase or 30% decrease in retrofit cost, CO$_2$ capture and sequestration cost and how it affects the objective function is shown. Table 6.10 shows this result. The maximum profit, for each reduction target, is noticed when there is an increase in final products selling price. Effect of retrofit cost for switching, capture and sequestration is noticed as CO$_2$ reduction target increases. Increase in demand leads to balancing to take place in order to meet the demand for each product. More diesel is produced than kerosene which leads to a significant decrease in the profit since the selling price for diesel is much lower than kerosene.
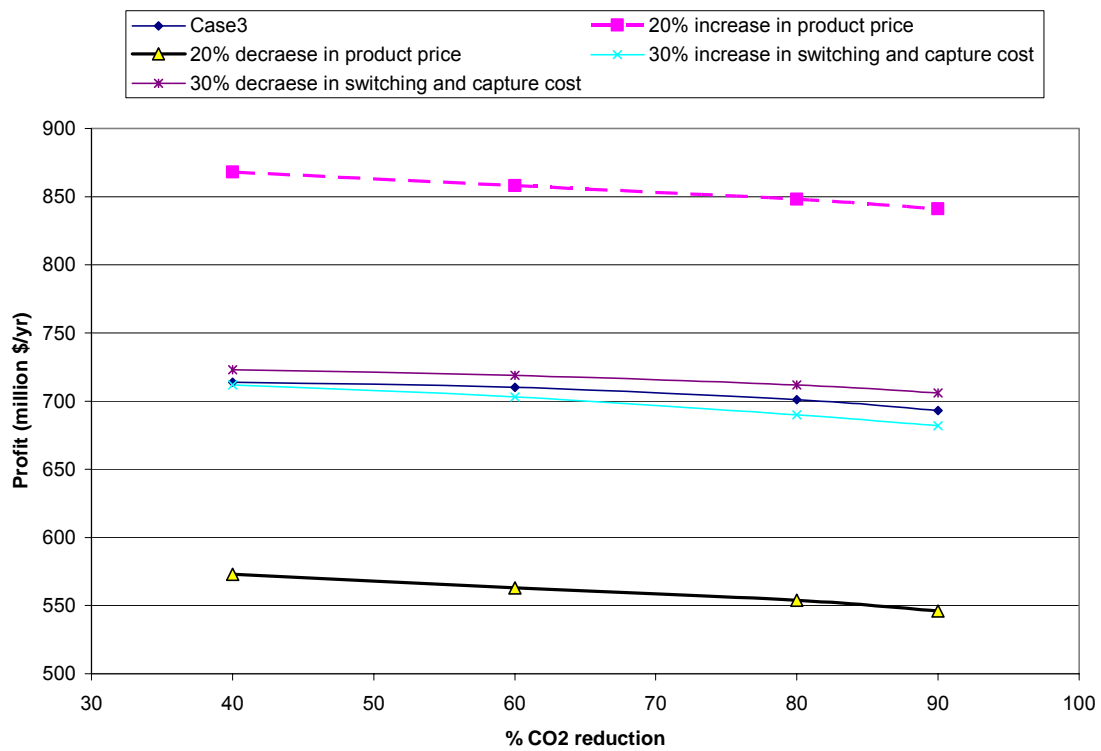
Figure 6.14. Sensitivity analysis results for Case 3

Table 6.10. Sensitivity analysis results for Case 4

% CO₂ Reduction	Profit (million $/yr)			
	20% increase in selling price of products	20% decrease in selling price of products	30% increase in switching, capture and sequestration cost	30% decrease in switching, capture and sequestration cost
40	860	567	709	721
60	848	553	690	711
80	833	538	671	702
90	822	528	658	693

Figure 6.15 shows the sensitivity results for this case study.
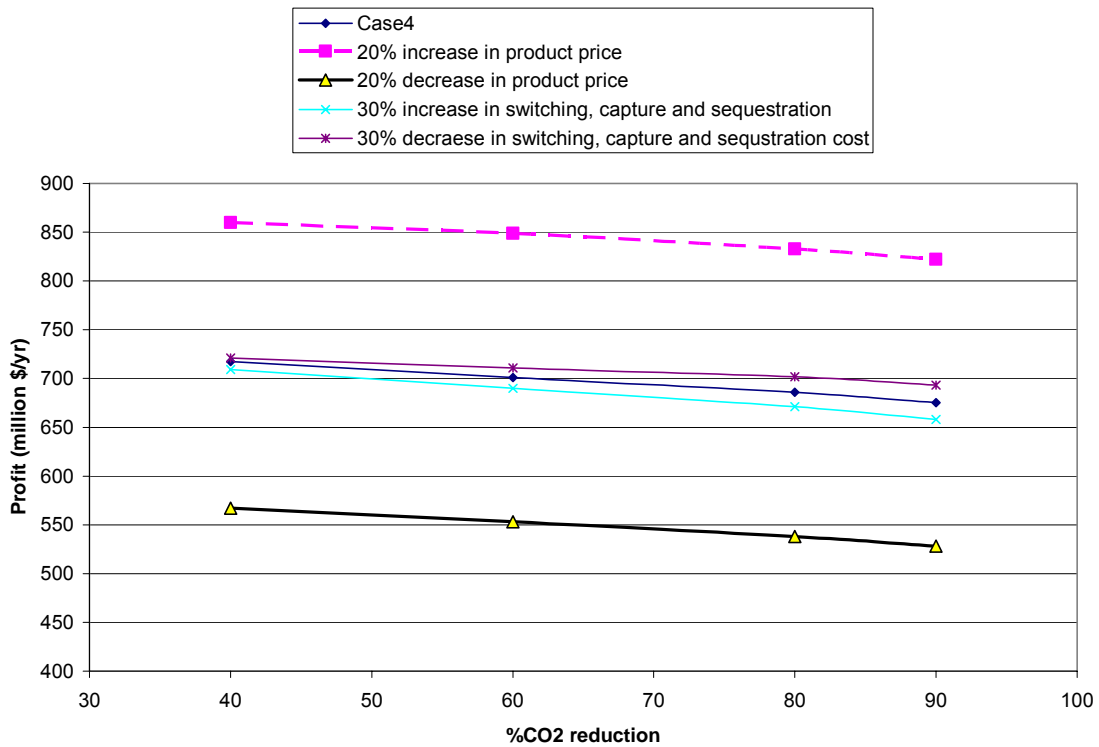
Figure 6.15. Sensitivity analysis results for Case 4

It is clear from above figure that the effect of CO_2 capture and sequestration is more significant on the profit at higher reduction target. This is expected because more CO_2 will be captured as more reduction is required. Table 6.11 gives a summary of all results for different reduction targets. The black circle represents that the unit is still using the current fuel which is fuel oil. The open circle represents switching to natural gas while the third symbol represents application of CO_2 capture technology.

Table 6.11. Summary of results

	CO$_2$ Reduction Target (%)							
Unit	1	10	20	30	40	60	80	90
CDU	●	●	○	○	☼	☼	☼	☼
RDHT	●	●	●	○	○	☼	☼	☼
GOHT	●	○	○	○	○	○	☼	☼
DHT	●	●	●	○	●	☼	●	☼
NHT	●	●	●	○	●	○	○	☼
HC	●	●	●	○	○	☼	☼	☼
FCC	○	●	●	○	●	●	☼	☼
REF	●	○	○	○	○	○	☼	☼

● Fuel oil   (current fuel)
○ NG   (switch)
☼ Capture   (MEA)

6.6 Summary

A general refinery planning model was developed to meet product demands with quality specifications and at the same time meet CO$_2$ reduction targets. Different CO$_2$ mitigation options were considered. These are flow rate balancing, fuel switching and CO$_2$ capture processes. It was shown that, in order to reduce CO$_2$ without fuel switching or CO$_2$ capture, the model tends to blend streams into the most profitable pool unless demand of such other product need to be met. This kind of flow rate balancing can achieve up to 3% reduction in CO$_2$ emissions without considering quality constraints. When product specifications are taken into account, only 0.4% reduction in CO$_2$ is achieved by decreasing slightly the inlet flow rate for the unit that emits more CO$_2$.

For higher reduction targets up to 30%, fuel switching is the option of choice. The final products quantity and quality remain unchanged. The profit is affected by the retrofit cost and natural gas price. The study shows also that any increase or decrease on final product selling price or retrofit cost affects the profit.

For CO_2 reduction of more than 30%, the CO_2 capture is a promising option since it can achieve up to 90% reduction. The profit is affected by this option because it is more expensive than fuel switching. The effect of increase or decrease on final product selling prices, retrofit cost and CO_2 capture cost is only noticed on the objective function and not on the configuration.

Sequestration adds more cost to the objective function and causes the profit to drop. For example, the maximum reduction in profit is about 9% for 90% reduction considering sequestration.

To sum up, the planning model tends to satisfy the product demand with quality specifications. Flow rate balancing is not a good option to reduce CO_2 emission if quality constraints are added into the model. Fuel switching can achieve up to 30% CO_2 reduction and beyond that, CO_2 capture processes should be applied.

The size of the problem was as follows:

Model: MINLP

Solver: SBB

Number of variables: 122

Number of discrete variables: 24

Number of nonlinear terms: 75

CPU: 0.52 sec

CHAPTER 7

CONCLUSIONS AND RECOMMENDATIONS

7.1 Conclusions

The electricity and refinery sectors were important contributors to greenhouse gas emissions, mainly CO_2, in Canada as of 2004. Optimization models were developed for the electricity and refinery sectors in order to meet demand at a given CO_2 reduction target. Three different mitigation options were considered for each sector. The model chose the best strategy or mix of strategies in order to meet a certain CO_2 reduction target with the least cost providing that the demand and other requirements were met. Each model was formulated as a MINLP and coded in GAMS. The mathematical model for each sector was illustrated through different case studies.

7.1.1 Electricity Sector

For the electricity sector, the objective was to meet the electricity demand with certain CO_2 reduction target at a minimum overall cost. The options considered for CO_2 reduction were fuel balancing (increase production from non fossil fuel and decrease production from fossil fuel power plants), fuel switching (switch from carbon intensive fuel such as coal to less carbon intensive fuel such as natural gas); and increase power plant efficiency through available technologies such as changing turbine blades. Binary variables representing existence or not of fuel switching and efficiency improvement technologies were introduced into the model. Due to nonlinear inequalities in CO_2 constraints, the model was a MINLP problem, and then reformulated as a Mixed Integer Linear programming (MILP).

The model was applied to the Ontario Power Generation (OPG) fleet. Three mitigation options for CO_2 reduction were considered as mentioned above. Different superstructure representations were used for the various options. The model was coded into GAMS and the following conclusions were drawn:

1. Fuel balancing could contribute up to 3% CO_2 reduction by increasing all non fossil fuel power plants by 1% above the nominal operating level, while reducing electricity generation from all four natural gas boilers (the most expensive fuel) by 34%. To meet the electricity demand, the optimization suggests then to increase all coal power plants by 1% above the nominal annual capacity factor. This results in a decrease of cost of electricity by about 1.3% when compared to OPG current optimal cost.

2. To achieve 5% CO_2 reduction, electricity generation from non fossil fuel power plants needed to be increased by 1% higher than nominal operational level. Four small boilers were switched to natural gas and these are: one at Atikokan (A1), two boilers at Thunder Bay and one boiler (LV5) at Lakeview power plant. The model showed also that only one efficiency improvement technology (install variable speed drive) should be applied to the Nanticoke power plant and to three other boilers (L1, L3 and L4) at Lambton power plant. The cost almost remains unchanged from the current OPG cost.

3. Higher CO_2 reduction targets required more coal-fired boilers to be switched to natural gas. To achieve 30% CO_2 reduction and generating current electricity demand, 11 coal-fired boilers were switched to natural gas compared to only 5 for 10% CO_2 emissions reduction. This resulted in an increase in cost of electricity generated by 13% and 2.8%, for 30% and 10% CO_2 reduction, respectively compared to that of the base case. The electricity generation from all non fossil fuel power plants should be increased by 1% as always the case. For 30% reduction, the optimizer recommended to install variable speed drives

for efficiency improvement at only two boilers, one (L4) at Lambton and another one (N3) at Nanticoke power plant.

4. For any reduction target, fuel balancing will be applied and all non fossil power plants will operate at a maximum specified level. Applying efficiency improvement technologies is a good option to reduce CO_2 especially for small reduction target. As more reduction is required, fuel switching becomes the best option to achieve the desired target. The cost will increase as more boilers are switched to natural gas since it is the most expensive fuel that OPG is using.

7.1.2 Oil Refinery Sector

The same general approach was applied to the refinery sector. The aim here was to maximize the profit from selling the final products with quality specifications and at the same time achieve a certain CO_2 reduction target by different mitigation options. The optimization process chose the best mitigation option that has the least effect on the profit for a given reduction target. The options being considered for CO_2 mitigation were balancing (i.e. changing the flow rates by decreasing production from units that emit more CO_2 and increasing production from units that emit less CO_2), fuel switching (switch from current fuel to another fuel that emits less CO_2 emissions such as natural gas); and CO_2 capture technologies.

The refinery planning model was first solved as a NLP before the introduction of binary variables for switching and capture. Nonlinearities in the model were mainly due to product blending correlations. The objective of the model was to meet the demand for each product with quality specifications. Then, binary variables were introduced into the model to indicate the selection of switching and capture technologies. The model was illustrated with different case studies. These included a base case without CO_2 mitigation options and another representing one mitigation option which is balancing only. Then, switching was added as an option to the previous case study followed by a

case study that included all three mitigation options. Sequestration was considered in the last case study. The following conclusions were drawn for that part of this dissertation:

1. The refinery planning model tends to blend products to the most profitable product pool unless the demand and quality specifications can not be satisfied for other final products. For example, the kerosene produced by the diesel hydrotreater (KDHT) is selected to be blended with the kerosene pool rather than diesel since the kerosene selling price is higher than that for diesel fuel. All properties for each final product are met within the specified target. Only one constraint was binding which was the specific gravity of fuel oil.

2. Balancing is a good option to reduce CO_2 emissions but up to a very small limit especially when quality constraints are added to the model. It can achieve only 0.4% reduction in CO_2 through a simple increase in the inlet flow rate to the FCC unit and a decrease in the inlet flow rate to the HC. This is done because CO_2 emissions from the HC are higher than that of the FCC. When higher reduction targets are set, other options should be applied.

3. Fuel switching (essentially from fuel oil to natural gas) can achieve a reduction target up to 30%. The profit decreases as the reduction target increases because more units are chosen to run with natural gas. For a 1% reduction, only one small unit need to be switched and this is the FCC unit. This unit has the least CO_2 emissions among the other units within the refinery. A reduction of about 0.14% is noticed in the profit. For higher reduction target such as 30% all units need to be switched to run with natural gas and this comes at a decreased profit of about 3.1%.

4. It is necessary for a reduction target higher than 30% to include CO_2 capture technology. For 60%, for example, the model chose to capture CO_2 from four different units. The four units had the highest CO_2 emissions among the remaining units. Three units were chosen also to be switched to natural gas. Only

one unit, which is the FCC, kept running with fuel oil. This was done because the FCC unit does not emit large amounts of CO_2. More CO_2 needed to be captured as the reduction target increased. Capture technology could achieve up to 90% reduction. This was achieved by capturing all CO_2 emissions coming from all units. Adding sequestration costs to the model and choosing to sequestrate captured CO_2 obviously further decreased the total profit.

5. Sensitivity analysis showed that the price of selling final products had the major impact on the profit. At high reduction target the profit starts to be affected by cost of capture technology since more CO_2 emissions are captured.

7.2 Recommendations

In order to improve the optimization model for each sector, a number of recommendations are proposed for further study:

1. The analysis used in this research for electricity sector was static in the sense that the electricity generation was held constant. However, in real situations, there is high variability in electricity demand. The demand should therefore be represented by load duration curves (LDC). The load duration curve is constructed for a particular consuming region by measuring the actual demand for power (MW) which occurs in each of the 8760 h in a given year. The model should therefore be expanded to take into account the variation in load demand.

2. Multi period planning should be considered for each sector under study. The current study did not address when to do switching or capture. So, time need to be incorporated into the model.

3. The same study can be extended to multi pollutants such as NO_x and SO_x in both the electricity and refinery sectors. The current approach considered only CO_2 emissions from fuel combustion.

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APPENDIX A: OPG EXISTING POWER PLANTS

The nominal conditions for OPG's existing fleet of power plants are:

Total electricity generation : 13,765 MWh/yr

Total CO_2 emissions : 36.57 x 10^6 tonne/yr

Total operational cost : 2.808 x 10^9 US$ /yr

Metric tonne is used throughout this thesis.

OPG has 6 fossil fuel power plants, 69 hydroelectric, three nuclear and one wind turbine power plant.

Table A1. OPG power plants production as of 2003.

Power Plants	MWh/yr
Fossil Fuel Power Plants	
Lambton	17292080
Nanticoke	34339200
Atitokan	1883400
Lakeview	9968880
Lennox	18746400
Thunder-Bay	2715600
Hydroelectric Plants	
NW-Caribou	347328
NW-Car	88128
NW-Manitou	373248
NW-Whitedog	352512
NW-Silver	248832
NW-Kababeka	129600
NW-Cameron	414720
NW-Pine	720576
NW-Alexander	347328
NW-Aquasaloon	243648
NW-Aubrey	851472
NW-Wells	1256184
NW-Rayner	241776
NW-Red-Rock	215496
NE-Kipling	741096

Power plant (Hydro)	(MWh/yr)
NE-Harmon	741096
NE-Otter	956592
NE-Smokey	273312
NE-Long	699048
NE-Abitibi	1629360
NE-Sturgeon	26280
NE-Sandy	15768
NE-Wawaitin	57816
NE-Indian	15768
NE-Hound	21024
NE-Notch	1440144
NE-Matabitchuan	52560
O-Hulden	1277208
O-Joachims	2254824
O-Chenaux	756864
O-Calabogie	26280
O-Barrett	925056
O-Mountain	893520
O-Stewartville	956592
O-Amprior	430992
O-Chats	504576
O-Saunders	5340096
N-DeCew	120888
N-DeCew2	756864
N-Beck1	2617488
N-Beck2	7384680
N-BeckPGS	914544
E-McVittie	15768
E-Coniston	26280
E-Crystal	42048
E-Nipissing	10512
E-Bingham	5256
E-Elliott	10512
E-Ragged	42048
E-Eddy	42048
E-Chute	52560

Power plant (Hydro)	(MWh/yr)
E-Hanna	5256
E-Trethewey	10512
E-South	21024
E-High	15768
E-Mernckville	10512
E-Lakefield	10512
E-Healey	63072
E-Seymour	31536
E-Ranney	47304
E-Auburn	10512
E-Eugenia	31536
E-Sills	10512
E-Hagues	21024
E-Frankford	15768
E-Sidney	21024
E-Meyersburg	21900
Nuclear Power Plants	
Pickering-A	0
Pickering-B	14300000
Darlington	27600000
Wind Turbine	
Tiverton	713000

Cost of efficiency improvement technologies for a 500 MW coal power plant (Wisconsin Electric Power Company, 2005):

1. Install variable speed drive : 2×10^6 US$
2. Install new turbine blades   : 6×10^6 US$

Each cost is amortized with a 20-year lifetime and a 10% annual interest.

APPENDIX B: GAMS CODE FOR POWER PLANTS

Title: Optimal CO_2 reduction strategies for OPG

*The objective of this model is to determine the best mix of power plants,
*fuels,annual capacity factor, improvement technology for increasing power
*plants efficiency to meet the electricity demand while satisfying the CO2
*reduction target at minimum cost.

```
$offtext
*
*.. list all sets
*
 Set i   plant type      /Fossil, nuclear, hydro, wind/
    F   fossil plants  /L1,L2,L3,L4,N1,N2,N3,N4,N5,N6,N7,N8,A1,
                 LV1,LV2,LV3,LV4,LV5,LV6,LV7,LV8,LN1,LN2,LN3,LN4
                 TB1,TB2/
    N   nuclear       /Pick-A,Pick-B,Darling/
    H   hydroelectric   /NW-Cari,NW-Car,NW-Mani,NW-White,NW-Silv,NW-Kaba,
                 NW-Came,NW-Pine,NW-Alex,NW-Aqua,NW-Aub,NW-WElls,
                 NW-Ray,NW-Red,NE-Kip,NE-Harm,NE-Otter,NE-Smok,
                 NE-Long,NE-Abi,NE-Sturg,NE-Sandy,NE-Wawai,NE-Ind,
                 NE-Hound,NE-Notch,NE-Mata,O-Huld,O-Joa,O-Chen,
                 O-Cala,O-Barr,O-Mount,O-Stew,O-Amp,O-Chats,O-Saund,
                 N-DeCew,N-DeCew2,N-Beck1,N-Beck2,N-Beck3,E-Mc,
                 E-Conis,E-Crys,E-Nipi,E-Bing,E-Elli,E-Ragg,E-Eddy,
                 E-Chute,E-Hanna,E-Treth,E-South,E-High,E-Mern,
                 E-Lake,E-Heal,E-Sey,E-Ran,E-Aub,E-Eugen,E-Sills,
                 E-Hag,E-Frank,E-Sid,E-Meyer/
    W   wind          /Tiverton/
    k   technology      /vr-spdr,blades/
    j   fuels          /coal,ng/;
*
*.. list all scalars
*
 Scalar MaxE     Electricity generated at peak time (MWe) /13765/;
 Scalar Optime   Annual operating time (hr per year) /8760/;
```

Scalar CO2   CO2 emission in tonne per year /36569055/;

Scalar CO2red   Percent of CO2 reduction /0.3/;

Scalar NucOpr   Operating cost for nuclear ($ per MWh) /32/;

Scalar HydOpr   Operating cost for hydroelectric ($ per MWh) /5/;

Scalar WindOpr Operating cost for wind ($ per MWh) /4/;

Scalar R   allowable electricity increment /0.01/;

Scalar L   ACF lower bound /0.1/;

Scalar nk   number of technology /2/;

*

*.. list all parameters

*

Parameters

Fmax(F)   Maximum fossil electricity generation(MWh per year)

/L1	4323020
L2	4323020
L3	4323020
L4	4323020
N1	4292400
N2	4292400
N3	4292400
N4	4292400
N5	4292400
N6	4292400
N7	4292400
N8	4292400
A1	1883400
LV1	1246110
LV2	1246110
LV3	1246110
LV4	1246110
LV5	1246110
LV6	1246110
LV7	1246110
LV8	1246110
LN1	4686600
LN2	4686600
LN3	4686600

164

LN4	4686600
TB1	1357800
TB2	1357800/

Efossil(F)   Electricity from fossil power plants in (MWh per year)

/L1	3242295
L2	3242295
L3	1768705
L4	1768705
N1	3219300
N2	3219300
N3	2619567
N4	2619567
N5	2619567
N6	2619567
N7	2619567
N8	2619567
A1	823000
LV1	306875
LV2	306875
LV3	306875
LV4	306875
LV5	306875
LV6	306875
LV7	306875
LV8	306875
LN1	690500
LN2	690500
LN3	690500
LN4	690500
TB1	745000
TB2	745000/

Enuclear(N)   Electricity from nuclear power plants in MWh per year

/Pick-A	0
Pick-B	14300000
Darling	27600000/

Ehydro(H)	Electricity from hydroelectric power plants in MWh per year
/NW-Cari	347328
NW-Car	88128
NW-Mani	373248
NW-White	352512
NW-Silv	248832
NW-Kaba	129600
NW-Came	414720
NW-Pine	720576
NW-Alex	347328
NW-Aqua	243648
NW-Aub	851472
NW-WElls	1256184
NW-Ray	241776
NW-Red	215496
NE-Kip	741096
NE-Harm	741096
NE-Otter	956592
NE-Smok	273312
NE-Long	699048
NE-Abi	1629360
NE-Sturg	26280
NE-Sandy	15768
NE-Wawai	57816
NE-Ind	15768
NE-Hound	21024
NE-Notch	1440144
NE-Mata	52560
O-Huld	1277208
O-Joa	2254824
O-Chen	756864
O-Cala	26280
O-Barr	925056
O-Mount	893520
O-Stew	956592
O-Amp	430992

```
O-Chats      504576
O-Saund      5340096
N-DeCew      120888
N-DeCew2     756864
N-Beck1      2617488
N-Beck2      7384680
N-Beck3      914544
E-Mc         15768
E-Conis      26280
E-Crys       42048
E-Nipi       10512
E-Bing       5256
E-Elli       10512
E-Ragg       42048
E-Eddy       42048
E-Chute      52560
E-Hanna      5256
E-Treth      10512
E-South      21024
E-High       15768
E-Mern       10512
E-Lake       10512
E-Heal       63072
E-Sey        31536
E-Ran        47304
E-Aub        10512
E-Eugen      31536
E-Sills      10512
E-Hag        21024
E-Frank      15768
E-Sid        21024
E-Meyer      21900/


Ewind(W)     Electricity from wind turbine power plants in MWh per year
/Tiverton    713000/
perRed(k)    reduction
/ vr-spdr    0.0053
```

blades   0.0035/;

Table FosOpr(F,j)   Operational cost ($ per MWh)

	coal	ng
L1	25.50	39.15
L2	25.50	39.15
L3	34.50	48.15
L4	34.50	48.15
N1	30	43.65
N2	30	43.65
N3	30	43.65
N4	30	43.65
N5	30	43.65
N6	30	43.65
N7	30	43.65
N8	30	43.65
A1	30	43.65
LV1	35	48.65
LV2	35	48.65
LV3	35	48.65
LV4	35	48.65
LV5	35	48.65
LV6	35	48.65
LV7	35	48.65
LV8	35	48.65
LN1	60	60
LN2	60	60
LN3	60	60
LN4	60	60
TB1	30	43.65
TB2	30	43.65;

parameter Rcost(F) retrofit cost (million $ per year)

/L1	1738995.3
L2	1738995.3
L3	1738995.3

L4	1738995.3	
N1	1726662	
N2	1726662	
N3	172666	
N4	172666	
N5	172666	
N6	172666	
N7	172666	
N8	172666	
A1	757617	
LV1	501436.7	
LV2	501436.7	
LV3	501436.7	
LV4	501436.7	
LV5	501436.7	
LV6	501436.7	
LV7	501436.7	
LV8	501436.7	
LN1	0	
LN2	0	
LN3	0	
LN4	0	
TB1	546189	
TB2	546189/;	

Table CO2emis(F,j) CO2 emission from fossil (tonne per MWh)

	coal	ng
L1	0.938	0.5628
L2	0.938	0.5628
L3	0.9385	0.5631
L4	0.9385	0.5631
N1	0.93	0.558
N2	0.93	0.558
N3	0.93	0.558
N4	0.93	0.558
N5	0.93	0.558
N6	0.93	0.558
N7	0.93	0.558

N8   0.93   0.558

A1   1.023   0.6138

LV1   0.9765 0.5859

LV2   0.9765 0.5859

LV3   0.9765 0.5859

LV4   0.9765 0.5859

LV5   0.9765 0.5859

LV6   0.9765 0.5859

LV7   0.9765 0.5859

LV8   0.9765 0.5859

LN1   0.651   0.651

LN2   0.651   0.651

LN3   0.651   0.651

LN4   0.651   0.651

TB1   1.023   0.6138

TB2   1.023   0.6138;

Table CO(F,k)

	vr-spdr	blades
L1	234920	587000
L2	234920	587000
L3	234920	587000
L4	234920	587000
N1	234920	587000
N2	234920	587000
N3	234920	587000
N4	234920	587000
N5	234920	587000
N6	234920	587000
N7	234920	587000
N8	234920	587000
A1	141580	353770
LV1	110390	275820
LV2	110390	275820
LV3	110390	275820
LV4	110390	275820

```
LV5   110390   275820
LV6   110390   275820
LV7   110390   275820
LV8   110390   275820
LN1   0        0
LN2   0        0
LN3   0        0
LN4   0        0
TB1   116350   290700
TB2   116350   290700;
parameter NomE   Nominal electricity generated in MW;
*
NomE    =(sum(F,Efossil(F))+sum(N,Enuclear(N))+sum(H,Ehydro(H))
     +sum(W,Ewind(W)))/(Optime);
*
Display NomE;
*
*.. list all variables
*
Positive Variables
  En(N)    adjusted electricity generation for nuclear power plants
  Eh(H)    adjusted electricity generation for hydroelectric power plants
  Ew(W)    adjusted electricity generation for wind power plants
  Efj(F,j) adjusted electricity generation for fossil power plants used j fuels
  v(F)   %   reduction
  gama(F,j,k)   new var for linearization;


Variables cost;


Binary variables
  X(F,j)  fuel selection
  Y(F,k) technology selection;


*.. list all the equations
*
Equations
  totcost total annual cost for all power generation stations ($ per year)
```

totCO2 total CO2 emission (tone per year)

totMW   total electricity generation (MWh per year)

te(F)

swi(F)

gas1

gas2

gas3

gas4

newF(F,j)

newN(N)

newH(H)

newW(W)

newcon1(F,j,k)

* newcon2(F,j,k)

newcon3(F,j,k)

newcon4(F,j,k)

low(F,j);

totcost.. cost =e=(sum((F,j),Efj(F,j)*FosOpr(F,j))+

          sum(F,Rcost(F)*X(F,'ng'))+sum(N,En(N)*NucOpr)+

          sum(H,Eh(H)*HydOpr)+ sum(W,Ew(W)*WindOpr)+

          sum((F,k),co(F,k)*y(F,k)));

totCO2.. sum((F,j),CO2emis(F,j)*Efj(F,j))- sum((F,j,k),co2emis(F,j)*perRed(k)

        *gama(F,j,k))=l= (1-CO2red)*CO2;

totMW.. (sum((F,j),Efj(F,j))+sum(N,En(N))+sum(H,Eh(H))+sum(W,Ew(W)))/Optime

        =g=1.00*NomE;

te(F).. sum(k,y(F,k))+nk*X(F,'ng')=l=nk;

swi(F).. sum(j,X(F,j)) =e= 1;

gas1..   X('LN1','ng') =e= 1;

gas2..   X('LN2','ng') =e= 1;

gas3..   X('LN3','ng') =e= 1;

gas4..   X('LN4','ng') =e= 1;

newF(F,j).. Efj(F,j) =l= (1+R)*Efossil(F)*X(F,j);

newN(N).. En(N) =l= (1+R)*Enuclear(N);

newH(H).. Eh(H) =l= (1+R)*Ehydro(H);

```
newW(W).. Ew(W) =l= (1+R)*Ewind(W);
newcon1(F,j,k).. gama(F,j,k)=l=Efj(F,j);
*newcon2(F,j,k).. gama(F,j,k)=l=Efj(F,j)-(L*Fmax(F)*(1-Y(F,k)));
newcon3(F,j,k).. gama(F,j,k)=g=Efj(F,j)-1e12*(1-Y(F,k));
newcon4(F,j,k).. gama(F,j,k)=l=1e12*Y(F,k);
low(F,j).. Efj(F,j) =g= (L*Fmax(F))*X(F,j);


 cost.l = 1;
*
*.. define model name
*
 Model  model1 /all /;
*
*.. more commands
*
 option LIMROW = 0;

 option LIMCOL = 0;
*option rminlp=minos;
option mip = osl;
*option nlp=conopt2;

 option iterlim = 100000000;


 Solve model1 using mip minimizing cost;
 display cost.l;
display totco2.l;
```

APPENDIX C: GAMS CODE FOR REFINERY SUB-MODELS

Sub-Models

RDHT

```
* RDHT.mod  -  Vacuum Residue Hydrotreater

* Use this submodel for hydrotreating with minimal cracking
* Products: Naphtha, Distillate, LSFO   $ Naph:375-F, Dist:375-650F, LSFO:+650F

* Feed (Residue from the CDU) properties
Parameter RateVRDHT Vol flowrate of feed from CDU Residue
      RateWRDHT   Mass flow rate from CDU Residue
      SGRDHT      Specific gravity of feed from CDU Residue
      APIRDHT     API of feed from CDU Residue
      SulRDHT     SULFUR CONTENT (%) of feed from CDU Residue
      NITRDHT     NITROGEN % of feed from CDU Residue
      VANRDHT     VANADIUM % of feed from CDU Residue
      NIRDHT      NICKEL of feed from CDU Residue
      CS122RDHT   Viscosity @122F of feed from CDU Residue
      CS210RDHT   Viscosity @210F of feed from CDU Residue
      PORRDHT     Pour point of feed from CDU Residue
      FlshRDHT    Flash point of feed from CDU Residue
      VABPRDHT    Volume average boiling point of feed from CDU Residue
      C5IRDHT     C5 insoluble of feed from CDU Residue
      CCRRDHT     mass% of Conradson carbon of feed from CDU Residue;
RateVRDHT = FRSD;
SGRDHT   = VRsdSG;
APIRDHT   = VRsdAPI;
RateWRDHT = RateVRDHT*SGRDHT*.3502;
SulRDHT   = VRsdS;
NITRDHT   = VRsdN;
VANRDHT   = VAN8;
NIRDHT    = NI8;
CS122RDHT = CS1228;
```

CS210RDHT = CS2108;

PORRDHT   = POR8;

FlshRDHT = Flsh8;

VABPRDHT = VABP8;

C5IRDHT   = C5I8;

CCRRDHT   = CCR8;

* Products Yeild

Parameter SCFHYDRDHT

    WTFRHYDRDHT   H2 mass fraction

    H2RDHT   H2 Mass flow rate

    H2SRDHT   H2S Mass flow rate

    GASRDHT   Gas mass flow rate

    C3SRDHT

    IC4RDHT

    NC4RDHT

    NAPH   Naphtha mass fraction

    RateW1RDHT   Naph mass flow rate

    Dist   Mid Distillate mass fraction

    RateW2RDHT   Distt mass flow rate

    RateW3RDHT   Residue mass flow rate

    RATEV1RDHT

    RATEV2RDHT

    RATEV3RDHT;

SCFHYDRDHT =(140*SGRDHT+0.39*(VANRDHT+NIRDHT)+91.5*NITRDHT)*(2.72*SGRDHT-1.61);

WTFRHYDRDHT=(1/658.29)*(SCFHYDRDHT/SGRDHT);

H2RDHT   =-WTFRHYDRDHT*RateWRDHT/100;

H2SRDHT   =0.85031*SulRDHT*RateWRDHT/100;

NAPH   =(0.12*SulRDHT+0.0063*(VANRDHT+NIRDHT))*(2.035*SGRDHT-0.95);

GASRDHT   =0.67*NAPH*RateWRDHT/100;

C3SRDHT   =0.27*GASRDHT;

IC4RDHT   =0.05*GASRDHT;

NC4RDHT   =0.23*GASRDHT;

RateW1RDHT =NAPH*RateWRDHT/100;

Dist   =3.56*NAPH-0.16*NAPH**2;

RateW2RDHT =Dist*RateWRDHT/100;

RateW3RDHT =RateWRDHT-H2RDHT-H2SRDHT-GasRDHT-RateW1RDHT-RateW2RDHT;

SulNRDHT =0.0085*SulRDHT;

NITNRDHT =0.07*NITRDHT;

* Distillate (375-650F)

SulDRDHT =0.02*SulRDHT;

NITDRDHT =0.16*NITRDHT;

* RESIDUE (LSFO:+650F)

SGLSFO =SGRDHT-0.0195*SGRDHT*WTFRHYDRDHT+0.012*WTFRHYDRDHT;

SulLSFO =(0.2*SulRDHT*RateWRDHT-SulNRDHT*RateW1RDHT-

SulDRDHT*RateW2RDHT)/RateW3RDHT;

NITLSFO =(0.69*NITRDHT*RateWRDHT-NITNRDHT*RateW1RDHT-

NITDRDHT*RateW2RDHT)/RateW3RDHT;

PORLSFO =PORRDHT/(0.6+0.0028*SulRDHT*PORRDHT);

VGCF =(SGRDHT-0.1244*LOG10(4.664*CS210RDHT-31))/(0.9255-

0.0979*LOG10(4.664*CS210RDHT-31))-0.0839;

VGCRsd=VGCF+0.56*(SGLSFO-SGRDHT);

CS210LSFO=(31+10**((0.9255*VGCRsd-SGLSFO+0.0776)/(0.0979*VGCRsd-0.1162)))/4.664;

CS122LSFO=.85*CS122RDHT;

NILSFO =1600*NIRDHT/RateWRDHT;

VANLSFO =1600*VANRDHT/RateWRDHT;

VABPLSFO=VABPRDHT-25;

FlshLSFO=FlshRDHT;

C5ILSFO =C5IRDHT;

CCRLSFO =CCRRDHT;

*Volumetric flow rates

Parameter FNRDHT RDHT Naph

    FDRDHT RDHT Distt

    FLSFO   RDHT VRD;

FNRDHT = RATEW1RDHT/(SGNRDHT*0.3502);

FDRDHT = RATEW2RDHT/(SGDRDHT*0.3502);

FLSFO = RATEW3RDHT/(SGLSFO*0.3502);

GOHT

GOHDS.mod - Gas Oil Hydrotreater

* Use this submodel for hydrotreating with minimal cracking
* Products: Naphtha, Distillate, HTGasOil
* Parameters: Severity(50)
* Severity 0=low pressure, high LHSV, 100=high pressure, low LHSV

*Feed Rate and Properties
Parameter
RateWGOHT,RateVGOHT,SGGOHT,APIGOHT,VABPGOHT,SULGOHT,NITGOHT,NIGOHT,VANGOHT

　　　CCRGOHT,FlshGOHT,V650GOHT,OLEGOHT,PorGOHT,CS122GOHT,CS210GOHT;

RATEVGOHT= FLVGO + FHVGO;

SGGOHT   = (FLVGO*HVGOSG+FHVGO*LVGOSG)/RATEVGOHT;

RATEWGOHT= RATEVGOHT*SGGOHT*.3502;

APIGOHT = 141.5/SGGOHT-131.5;

VABPGOHT = (VABP6*FLVGO+VABP7*FHVGO)/RATEVGOHT;

SULGOHT = (LVGOS*RATEWLVGO+HVGOS*RATEWHVGO)/RATEWGOHT;

NITGOHT = (LVGON*RATEWLVGO+HVGON*RATEWHVGO)/RATEWGOHT;

NIGOHT   = (NI6*RATEWLVGO+NI7*RATEWHVGO)/RATEWGOHT;

VANGOHT = (VAN6*RATEWLVGO+VAN7*RATEWHVGO)/RATEWGOHT;

CCRGOHT = (CCR6*RATEWLVGO+CCR7*RATEWHVGO)/RATEWGOHT;

FlshGOHT = (Flsh6*FLVGO+Flsh7*FHVGO)/RATEVGOHT;

V650GOHT = (V6506*FLVGO+V6507*FHVGO)/RATEVGOHT;

OLEGOHT = (OLE6*FLVGO+OLE7*FHVGO)/RATEVGOHT;

PorGOHT = (Por6*FLVGO+Por7*FHVGO)/RATEVGOHT;

CS122GOHT= (CS1226*RATEWLVGO+CS1227*RATEWHVGO)/RATEWGOHT;

CS210GOHT= (CS2106*RATEWLVGO+CS2107*RATEWHVGO)/RATEWGOHT;

* YIELDS
Parameter SeverityGOHT/50/

KGOHT,convGOHT,SCFHYDGOHT,wtfrhydGOHT,H2GOHT,H2SGOHT,GasGOHT,C3SGOHT,IC4GOHT

　　NC4GOHT,RateW1GOHT,APITGO,SGTGO,RateW3GOHT,RateW2GOHT;

KGOHT   =(VABPGOHT+460)**.3333/SGGOHT;

convGOHT   =4.5*SULGOHT;

SCFHYDGOHT =(290+20*convGOHT*(1-

V650GOHT/100))*(1+.01*SeverityGOHT)+15*OLEGOHT+(VABPGOHT-700)*0.5;

wtfrhydGOHT= SCFHYDGOHT/65800/SGGOHT;

H2GOHT   =-wtfrhydGOHT*RateWGOHT;

H2SGOHT   =0.010625*SULGOHT*RateWGOHT*(1-(1-convGOHT/100)*(.2-.0016*SeverityGOHT));

GasGOHT   =(.004+.00001*convGOHT*convGOHT)*RateWGOHT;

C3SGOHT   =0.49*GasGOHT;

IC4GOHT   =(.001+.00015*convGOHT)*RateWGOHT;

NC4GOHT   =IC4GOHT*.7;

RateW1GOHT =(.02+.001*convGOHT)*RateWGOHT;

APITGO   =APIGOHT+.004*SCFHYDGOHT;

SGTGO   =141.5/(131.5+APITGO);

RateW3GOHT =(1-V650GOHT/100)*(1-convGOHT/100)*RateWGOHT*SGTGO/SGGOHT;

RateW2GOHT = RateWGOHT-H2GOHT-H2SGOHT-GasGOHT-IC4GOHT-NC4GOHT-

RateW1GOHT-RateW3GOHT;

DHT

*Feed Rate and Properties

Parameter

RATEVDHT,RATEWDHT,SGDHT,APIDHT,SULDHT,NITDHT,OLEDHT,ARODHT,V300DHT
    V400DHT,V500DHT,V650DHT;

RATEVDHT= FDIESEL;

SGDHT   = SRDSG;

RATEWDHT= RATEVDHT*SGDHT*0.3502;

APIDHT = 141.5/SGDHT-131.5;

SULDHT = SRDS;

NITDHT = SRDN;

OLEDHT = OLE5;

ARODHT = ARO5;

V300DHT = V3005;

V400DHT = V4005;

V500DHT = V5005;

V650DHT = V6505;

* YIELDS

Parameter SEVERITYDHT/20/

Parameter SCFHYDDHT,WTFRHYDDHT,H2DHT,H2SDHT,GASDHT,C3SDHT,IC4DHT,NC4DHT
    RATEW1DHT,DISTTWDHT,FRACKERODHT,RATEW2DHT,RATEW3DHT;

SCFHydDHT
=(150+OLEDHT*10+0.9*SULDHT*60)+(100+0.1*SULDHT*60+ARODHT*20)*SeverityDHT/100;

WtFrHydDHT = SCFHydDHT/65800/SGDHT;

H2DHT   = -WtFrHydDHT*RateWDHT;

H2SDHT   = 0.010625*SULDHT*(0.95+SeverityDHT*0.0005)*RateWDHT;

GasDHT   = (0.005+0.000005*SeverityDHT*SeverityDHT)*RateWDHT;

C3SDHT   = 0.35*GasDHT;

IC4DHT   = 0.15*GasDHT;

NC4DHT   = 0.20*GasDHT;

RateW1DHT = (0.001+0.0004*SeverityDHT)*RateWDHT;

DisttWDHT = RateWDHT-H2DHT-H2SDHT-GasDHT-RateW1DHT;

FracKeroDHT= V500DHT*0.008 +V650DHT*0.002;

RateW2DHT = DisttWDHT*FracKeroDHT*0.94;

RateW3DHT = DisttWDHT -RateW2DHT;

HC

Parameter SGHC,APIHC,VABPHC,OLEHC,SULHC,NIHC,VANHC,CCRHC;

SGHC   = SGTGO;

APIHC = 141.5/SGHC-131.5;

VABPHC = VABPTGO;

OLEHC = OLETGO;

SULHC = SULTGO;

NIHC   = NITGO;

VANHC = VANTGO;

CCRHC = CCRTGO;

Variable RateWHC,RateVHC;

Equation RateWHC1,RateVHC1;

RATEVHC1.. RATEVHC=E= FTGOHC;

RATEWHC1.. RATEWHC=E= RATEVHC*SGHC*0.3502;

* YIELDS

Parameter

CONVHC/75/,ModeHC/1/,SCFHYDHC,WtFrHYDHC,LNapHC,HNHC,JetHC,DslHC,SubTotLQHC;

Variable H2HC,H2SHC,GasHC,C3SHC,IC4HC,NC4HC,SubTotLEHC,TotalHC,AdjFactHC

     RateWLNHC Light Naph,RateWHNHC Hvy Naph,RateWKEROHC Jet,RateWDIESELHC Disel;

Equation H2HC1,H2SHC1,GasHC1,C3SHC1,IC4HC1,NC4HC1,SubTotLEHC1,TotalHC1

     AdjFactHC1,RateWLNHC1,RateWHNHC1,RateWKEROHC1,RateWDIESELHC1;

SCFHYDHC = 1600+300*(ModeHC-1)+30*(32-APIHC)+15*OLEHC;

WtFrHYDHC= SCFHYDHC*.00001508/SGHC;

H2HC1..   H2HC   =E= -WtFrHYDHC*RateWHC;

H2SHC1..   H2SHC   =E= 0.010625*(SULHC-0.0281+.0102*ModeHC)*RateWHC;

GasHC1..   GasHC   =E= (.001+.007*ModeHC)*RateWHC;

C3SHC1..   C3SHC   =E= (.005+.002*ModeHC)*RateWHC;

IC4HC1..   IC4HC   =E=(.00682+.00347*ModeHC)*RateWHC;

NC4HC1..   NC4HC   =E=IC4HC*.818;

SubTotLEHC1..

SubTotLEHC=E=(H2HC+H2SHC+GasHC+C3SHC+IC4HC+NC4HC)/(RateWHC+.00001);

* Unnormalized LN, HN etc below

LNapHC   = 1.86+3.39*ModeHC;

HNHC   = 0.26+5.77*ModeHC;

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JetHC   = 6.91+34.86*ModeHC;

DslHC   = 91.16-45.58*ModeHC;

SubTotLQHC=(LNapHC+HNHC+JetHC+DslHC)/100;

TotalHC1..   TotalHC =E=SubTotLEHC+SubTotLQHC;

AdjFactHC1.. AdjFactHC=E=RateWHC/100*(SubTotLQHC-TotalHC+1)/SubTotLQHC;

RateWLNHC1.. RateWLNHC=E=LNapHC*AdjFactHC;

RateWHNHC1.. RateWHNHC=E=HNHC*AdjFactHC;

RateWKEROHC1.. RateWKEROHC=E=JetHC*AdjFactHC;

RateWDIESELHC1.. RateWDIESELHC=E=DslHC*AdjFactHC;

* PROPERTIES
* Light Naphtha
Parameter RVPLNHC/10/,RONLNHC/82/,MONLNHC/77/,V150LNHC/70/,V200LNHC/80/
     V300LNHC/100/,V400LNHC/100/,KHC,KLNapHC,KHNHC,KJetHC,KDslHC,SGLNHC;

KHC   =(VABPHC+460)**.3333/SGHC;

KLNapHC=12.4+.2*(KHC-11.5);

KHNHC =KLNapHC-.75;

KJetHC =11.8+.4*(KHC-11.5);

KDslHC =KJetHC;

SGLNHC =(135+460)**.3333/KLNapHC;

* Heavy Naphtha
Parameter RVPHNHC/3/,RONHNHC/70/,MONHNHC/65/,V150HNHC/0/,V200HNHC/10/,
     V300HNHC/60/,V400HNHC/95/,SGHNHC,NAPHHNHC,AROHNHC;

SGHNHC = (290+460)**.3333/KHNHC;

NAPHHNHC= 40+3*(11.6-KHNHC);

AROHNHC = 5+3*(11.6-KHNHC);

* Kero/Jet
* AROKEROHC IS DEFINED BY THE USER TO BE 18
Parameter SULKEROHC/.01/,FLSHKEROHC/165/,PORKEROHC/-70/,CETKEROHC/60/
     FRZKEROHC/-65/,CS122KEROHC/1.5/,AROKEROHC/18/,SGKEROHC,SMKKEROHC;

SGKEROHC = (465+460)**.3333/KJetHC;

SMKKEROHC= 28+4*(KJetHC-11.4);

* Diesel
* CS210DIESELHC/1.2/ IS PREDICTED BY USER FROM CS122DIESELHC/2.0/

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Parameter SGDIESELHC,SULDIESELHC/.03/,FLSHDIESELHC/200/,PORDIESELHC/-50/

      CETDIESELHC/62/,CS122DIESELHC/2.0/,CS210DIESELHC/1.2/,V650DIESELHC/90/;

SGDIESELHC= (600+460)**.3333/KDslHC;

*Volumetric Flowrates

Variable FLNHC,FHNHC,FKEROHC,FDIESELHC;

Equation RATEVLNHC1,RATEVHNHC1,RATEVKEROHC1,RATEVDIESELHC1;

RATEVLNHC1..   FLNHC   =E=RATEWLNHC/(SGLNHC*0.3502);

RATEVHNHC1..   FHNHC   =E=RATEWHNHC/(SGHNHC*0.3502);

RATEVKEROHC1..   FKEROHC =E=RATEWKEROHC/(SGKEROHC*0.3502);

RATEVDIESELHC1.. FDIESELHC=E=RATEWDIESELHC/(SGDIESELHC*0.3502);

<u>Ref</u>

*Feed Rate and Properties

Variable RATEVREF,SGREF,RATEWREF,NAPHREF,AROREF;

*,V150REF,V200REF,V300REF,V400REF;

Equation RATEVREF1,SGREF1,RATEWREF1,NAPHREF1,AROREF1;

*,V150REF1,V200REF1,V300REF1,V400REF1;

RATEVREF1.. RATEVREF =E= FTHN + FNDHT + FNGOHT + FNRDHT +FHNHC;

SGREF1.. SGREF*RATEVREF =E=
FTHN*SGTHN+FNDHT*SGNDHT+FNGOHT*SGNGOHT+FNRDHT*SGNRDHT
+FHNHC*SGHNHC;

RATEWREF1.. RATEWREF =E= RATEVREF*SGREF*0.3502;

NAPHREF1.. NAPHREF*RATEVREF=E=
FTHN*NAPHTHN+FNDHT*NAPHNDHT+FNGOHT*NAPHNGOHT+FNRDHT*NAPHNRDHT+FH
NHC*NAPHHNHC;

AROREF1.. AROREF *RATEVREF=E= FTHN*AROTHN +FNDHT*ARONDHT
+FNGOHT*ARONGOHT +FNRDHT*ARONRDHT +FHNHC*AROHNHC;

*V150REF1.. V150REF*RATEVREF=E=
FTHN*V150THN+FNDHT*V150NDHT+FNGOHT*V150NGOHT+FNRDHT*V150NRDHT+FHNHC
*V150HNHC;

*V200REF1.. V200REF*RATEVREF=E=
FTHN*V200THN+FNDHT*V200NDHT+FNGOHT*V200NGOHT+FNRDHT*V200NRDHT+FHNHC
*V200HNHC;

*V300REF1.. V300REF*RATEVREF=E=
FTHN*V300THN+FNDHT*V300NDHT+FNGOHT*V300NGOHT+FNRDHT*V300NRDHT+FHNHC
*V300HNHC;

*V400REF1.. V400REF*RATEVREF=E=
FTHN*V400THN+FNDHT*V400NDHT+FNGOHT*V400NGOHT+FNRDHT*V400NRDHT+FHNHC
*V400HNHC;

* YIELDS

Parameter SEVERITYREF/100/

    PressureREF psia/150/;

Variable LVYLDREF,H2REF,GASREF,C3SREF,IC4REF,NC4REF,RATEW1REF;

Equation LVYLDREF1,H2REF1,GASREF1,C3SREF1,IC4REF1,NC4REF1,RATEW1REF1;

LVyldREF1.. LVyldREF =E=81.8-0.035*(PressureREF-50)+0.2*(NAPHREF+2*AROREF-39)-
1.0*(SeverityREF-100);

H2REF1.. H2REF*100=E=RateWREF*(3.2-.0118*(PressureREF-50)-0.2*(LVyldREF-81.8));

SCFHYDREF1.. SCFHYDREF=E=(3.2-.0118(PressureREF-50)-0.2*(LVyldREF-81.8))*658*SGREF;

GasREF1.. GasREF =E=RateWREF*(2.2-0.19*(LVyldREF-81.8))/100;

C3SREF1.. C3SREF =E=RateWREF*(2.0-0.2*(LVyldREF-81.8))/100;

IC4REF1.. IC4REF =E=RateWREF*(1.3-.055*(LVyldREF-81.8))/100;

NC4REF1.. NC4REF =E=IC4REF*58/42;

RateW1REF1.. RateW1REF=E=RateWREF-H2REF-GasREF-C3SREF-IC4REF-NC4REF;

* Products properties

* Reformate

Parameter RVPREFORMAT/7/

    AroREFORMAT,RONREFORMAT,MONREFORMAT;

AroREFORMAT =58+1.5*(SeverityREF-100);

RONREFORMAT =SeverityREF;

MONREFORMAT =RONREFORMAT-9;

Variable SGREFORMAT,FREFORMATE;

*BENZREFORMAT;

*,V150REFORMAT,V200REFORMAT,V300REFORMAT,V400REFORMAT;

Equation SG1REFORMAT,RATEV1REFORMAT;

RATEV1REFORMAT.. FREFORMATE =E=RATEW1REF/(SGREFORMAT*0.3502);

APPENDIX D: ECONOMIC DATA OF RETROFIT COST AND CO$_2$ CAPTURE ON REFINERY UNITS

For refinery units, fuel switching represents switching from fuel oil to natural gas.

Natural gas price (NG): 5 US$/MBtu (www.eia.doe.gov)

Cost of MEA capture process: 55 US$/tonne CO$_2$

Sequestration (enhanced oil recovery) cost: 25 US$/tonne CO$_2$ (Keigo et al., 2004)

Metric tonne is used throughout this thesis.

Interest rate: 10%.

Project duration: 20 years.