

Delineating Base Flow Contribution Areas for Streams: A Model Comparison

by

Reynold Chow

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AUTHOR'S DECLARATION

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

This study extends the methodology for the delineation of capture zones to base flow contribution areas for stream reaches under the assumption of constant average annual base flow in the stream. The methodology is applied to the Alder Creek watershed in southwestern Ontario, using three different numerical models. The three numerical models chosen for this research were Visual Modflow, Watflow and HydroGeoSphere. Capture zones were delineated for three different stream segments with reverse particle tracking and reverse transport.

The modelling results showed that capture zones delineated for streams are sensitive to the discretization scheme and the different processes considered (i.e. unsaturated zone, surface flow). It is impossible to predict the size, shape and direction of the capture zones delineated based on the model selected. Also, capture zones for different stream segments will reach steady-state at different times. In addition, capture zones are highly sensitive to differences in hydraulic conductivity due to calibration. It was found that finite element based integrated groundwater - surface water models such as HydroGeoSphere are advantageous for the delineation of capture zones for streams.

Capture zones created for streams are subject to greater uncertainty than capture zones created for extraction wells. This is because the hydraulic gradients for natural features are very small compared to those for wells. Therefore, numerical and calibration errors can be the same order of magnitude as the gradients that are being modelled.

Because of this greater uncertainty, it is recommended that particle tracking and reverse transport always be used together when delineating capture zones for stream reaches. It is uncertain which probability contour to choose when the capture zone is delineated by reverse transport alone. The reverse particle tracks help choose the appropriate probability contour to represent the stream capture zone.

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Chapter 1

General Introduction and Objectives

A healthy stream depends on groundwater discharge for maintaining a steady base flow and for keeping temperature and chemical/biochemical constituents at a level that is amenable to support a healthy aquatic ecosystem, including a cold-water fishery. Groundwater discharge maintains the environmental sustainability of the stream. Water that becomes groundwater discharge originates as precipitation falling on the ground within the catchment; it is stored within the aquifer and slowly released into the stream as base flow.

The dynamics of groundwater discharge (amount, rate of discharge, quality) depends on the extent and characteristics of the groundwater storage area. For a smaller near-stream storage area, the cycle from precipitation to discharge might take a few days, while for a large watershed, it could take centuries. The length of residence time in the aquifer and the characteristics of the system will determine the groundwater discharge to the stream. Thus, in order to assess groundwater discharge to a stream, it is essential to have a good understanding of the extent and characteristics of the area contributing to the discharge.

It is also important to understand the threats, actual or potential, to a contributing area that may exist and that might impact the quality and quantity of the discharge to the stream. A major threat is land development for industrial, commercial, or residential purposes. Such development can render impervious much of the ground surface, cutting off the recharge to the groundwater, and can introduce potential sources of contamination such as gas stations. Instead of storing the water in the aquifer and releasing it gradually as base flow, storm water will then be released at once as storm runoff, unless engineering measures are taken. Under worst-case conditions, a stream may degenerate to a drainage ditch, dry most of the year, overflowing during storm events, and unable to support any sort of life.

On the other hand, municipalities hungry for tax revenue may desire more development. In order to strike a balance, it is crucially important to be able to identify, with some confidence, the areas that contribute to sensitive streams or stream reaches. Knowing the contributing area would allow the assessment of stream sensitivity and the potential economic cost of saving the stream.

To efficiently assess an area contributing to groundwater discharge, we may utilize much of the well-established methodology for delineating capture zones for drinking water wells. This methodology consists of a variety of numerical models with varying capabilities including flow and transport simulation, particle tracking, and capture probability assessment. In fact, the basic concepts of well capture zones and stream contributing areas are the same, with only some details being different. The equivalence between the two concepts is illustrated in Figure 1 from Winter et al. (1998), where the left part of the figure shows a pumped well with associated capture zone, while the right part shows a stream reach, also with associated capture zone.

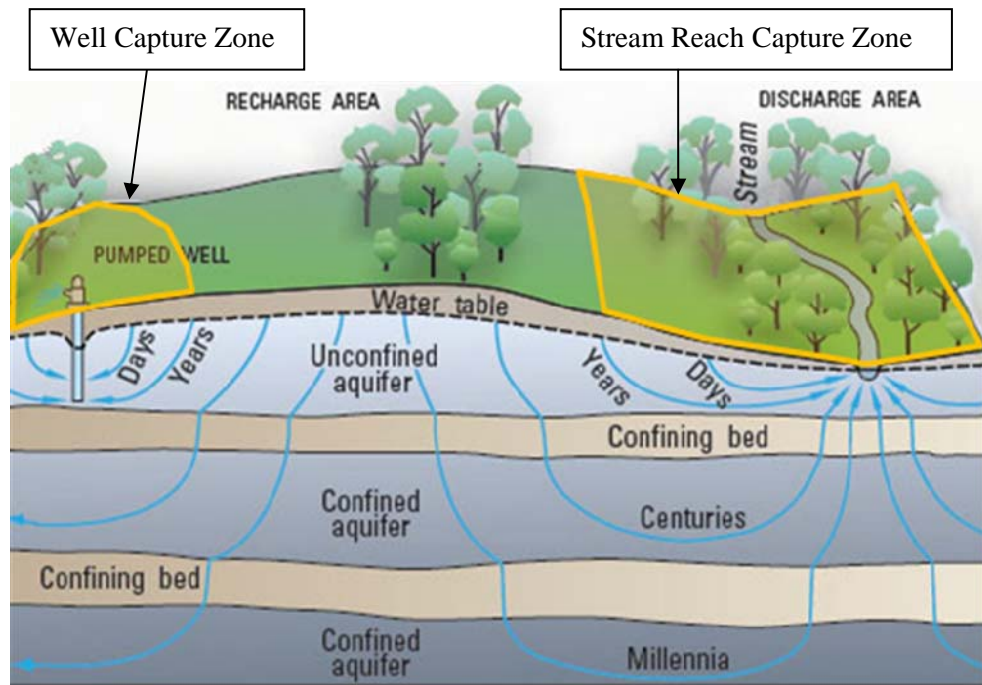


Figure 1: Groundwater flow paths, well capture zone and stream capture zone concept (from Winter et al., 1998)

One difference between the two types of capture zones is that for a water supply well, the pumping rate is generally constant for longer periods, while for a stream, it would be influenced by precipitation events and by the seasons. In the absence of precipitation, base flow would gradually decline as the water level in the aquifer drops. Thus stream discharge is more variable than water pumped from a well. Another difference is that at a well, the act of pumping induces a strong gradient toward the well, while at a stream, the gradient is due to natural causes at all times; this means that gradients near streams will be smaller than near wells, and data and numerical errors will be relatively more noticeable in the case of stream discharge. This also means that different models may give somewhat different results in terms of a stream discharge capture zone.

In well capture zone delineation, the standard assumption is that the flow system is at steady state. This is generally a reasonable assumption as well capture zones generally involve travel times of years to decades, and transient effects originating at the surface generally dampen out in the subsurface within a short distance and time. (Some groundwater models used for capture zone delineation (e.g. by means of particle tracking) do not even allow a capture zone analysis in transient flow mode.)

Accordingly, in order to be able to apply standard capture zone delineation methodology, the flow system should be taken to be at steady state. For the purposes of this study, we will therefore assume an average annual precipitation as well as an average annual base flow in the stream. All transients are assumed to dampen out in the groundwater system. A more complex transient analysis will have to await future study.

Thus the objective of this study is, first, to demonstrate the concept of the stream reach capture zone, and second, to show that the delineation of such capture zones may depend on the model being used. To achieve these objectives, a small number of well-known models will be applied to delineate capture zones for several stream reaches in the Alder Creek watershed within the Regional Municipality of Waterloo. In addition, two different capture zone delineation methods (reverse particle tracking and reverse transport) will be applied and the results compared.

In the following, for simplicity, we will use the term “capture zone” to mean “area contributing to stream base flow”.

Chapter 2

Background and Fundamental Concepts

2.1 Capture Zone Delineation Methodology

Identifying the source of groundwater recharge by delineating a capture zone is a proactive and preventative approach to protecting groundwater resources, both in the context of wells and stream discharge areas. Capture zone delineation is the first barrier in a multi-barrier system in ensuring the safety of water resources. As the saying goes, an ounce of prevention is worth a pound of cure. There are countless studies that have shown that protecting the resource is always more cost effective than remediating it after it has been contaminated. The implementation of an engineered groundwater remediation system is a reactive approach to treat groundwater contamination. Groundwater remediation systems are capital intensive, they take an extensive period of time and often fail to bring contamination levels back to pristine conditions. The additional costs of finding alternative water supplies, replacement of infrastructure, loss of public confidence and the cost of groundwater site assessments and remediation can be substantial. Therefore, preventative measures including the delineation of capture zones are a much more efficient use of capital.

European countries may have been the first to recognize the need to protect groundwater resources through the management and restriction of land use. In the 1930's, Germany imposed land use restriction around wells based on groundwater travel times (Schleyer et al., 1992). In 1986 the United States Environmental Protection Agency (EPA) amended the Safe Drinking Water Act, making it mandatory for states to develop Wellhead Protection Programs. The purpose of the program was to assure the quality of the water pumped from public wells. Wellhead protection areas are designed to protect wells from contaminants. The EPA identified several sources of contaminants that

can include but are not limited to: leaky tanks, industrial lagoons, landfills, road deicing chemicals, agricultural activities (pesticides and herbicides) and spills.

In 1989, a small town in southwestern Ontario by the name of Elmira faced a groundwater contamination crisis. The detection of a carcinogenic chemical by the name of DMNA was detected in the local municipal well (Cameron, 1995). The source of the contamination was from a chemical plant, then known as Uniroyal Chemical, which had been burying waste chemicals in the ground for disposal. Luckily nobody was harmed from the contamination, however Elmira's water supply was disrupted. The municipal well was shut down and a pipeline was built from the City of Waterloo to Elmira to support the city's drinking water demands.

This was an important lesson in southwestern Ontario which the Regional Municipality of Waterloo (RMOW) took to heart. The RMOW has been very proactive in its groundwater resource management, developing a comprehensive source water protection and management program (RMOW, 1994). The rest of Ontario however was slow to follow the RMOW's example, taking about a decade before actively protecting its groundwater resources by passing legislation. The lessons from Elmira had not fully hit home until groundwater was contaminated again in another small southwestern Ontario town. After this critical event, groundwater management was brought back into the spotlight and entered the forefront of public consciousness.

In 2000, another small southwestern Ontario town, Walkerton, was devastated when their drinking water was contaminated. What is known now as the Walkerton Tragedy occurred in May, 2000 when Walkerton's drinking water supply well became contaminated with E. coli. This happened after an intense rainfall event where approximately 134 mm of rain fell over 5 days. This intense rainfall event happened shortly after a period where fertilizer manure, believed to be the source of the E. coli, was applied to a nearby field. In addition, untrained operators of the water treatment facility

and local geological conditions (the well was under the direct influence of surface water) intensified the E. coli contamination. The E. coli contamination led to seven deaths and to this day more than 2,300 suffer from anemia, low platelet counts, and/or lasting damage to their kidneys.

Many lessons were learned from the Walkerton Tragedy. A comprehensive report prepared by The Honourable Dennis R. O'Connor was published in 2002 by the Ontario Ministry of the Attorney General, better known as the Walkerton Inquiry. The inquiry went into detail about the causes that led to groundwater contamination and recommendations to prevent groundwater contamination from happening again. The Walkerton Tragedy was a blessing in disguise since it motivated Ontario to become a leader in source water protection legislation in Canada. After the Walkerton inquiry in 2002 came the Ontario Clean Water Act (OMOE, 2006). This act specifies that "local communities, through local Source Protection Committees, assess existing and potential threats to their water, and that they set out and implement the actions needed to reduce or eliminate these threats." Numerical groundwater models and delineation of capture zones have become important components of source water protection methodology.

Numerical models have become the preferred tools for capture zone delineation. Numerical solution methods facilitate the modelling of heterogeneous, anisotropic hydrogeological systems with irregular three-dimensional geometries, and allow maximum flexibility and versatility in terms of modelling complex boundary conditions and hydrogeologic systems.

The process of delineating a capture zone starts with the creation of a conceptual model for the study area. A conceptual model is the mental picture created about the study area and is a simplification of the natural system to be modelled. Simplifying the natural system is a fine balancing act. On the one hand, simplification of the natural system allows us to create models that are nimble, quick to process and easy to use. On the other hand, we want to ensure that we take into account

enough significant processes so that we get physically realistic and useful results. The conceptual model identifies the boundaries surrounding the study area, the hydrostratigraphy of the study area, and any other significant hydrogeological features (i.e. lakes, rivers, significant fractures). Once the conceptual model is formed, a numerical model that has the capabilities of taking into account the major physical processes of the study area is selected.

Creating a groundwater model is a process that requires a great deal of information about the study area. Many parameters need to be determined and interpolated in the model in order to obtain results. These parameters include: hydraulic conductivity, recharge, aquifer storage coefficients, porosity and choosing appropriate boundary conditions. In most cases, detailed hydrologic data are scarce and obtaining more information is expensive. Therefore, many assumptions need to be made in order to create a workable model.

Groundwater models are also very useful in identifying areas where data gaps exist. This helps hydrogeologists make decisions when planning site characterization, such as determining the next monitoring well location and where to obtain more hydrostratigraphic data. In some cases it may be more useful to start off with a simplified conceptual model with a simple-to-run groundwater model of the study area and progressively add layers of complexity, as one uncovers more information. This approach is very cost effective in terms of giving insight into the study area.

Groundwater modelling has advanced rapidly over the last decade in terms of capability and usability. While the availability of easy-to-use groundwater modelling software has created better tools for hydrogeologists to investigate alternative scenarios and potential impacts of various plans affecting hydrogeological conditions, this has also opened the door to misuse of groundwater models when the limitations and assumptions of the groundwater models are not well understood. In some cases, groundwater modellers are trained by taking a weekend short course learning how to navigate the graphical user interface of a commercially available piece of groundwater modelling software.

This practice is conducive to selling more software licenses, but it inevitably leads to misunderstandings about the function of groundwater models and their place in decision making. With today's groundwater modelling software packages it can be easy for a user who has no hydrogeology background to create a fully functional groundwater model. A competent groundwater modeller must always be vigilant of this fact and question whether the results presented make logical sense.

New layers of complexity can be incorporated into more sophisticated groundwater models. Including the unsaturated zone allows the model to cover the entire subsurface up to the ground surface. Further including surface water flow allows for the representation of the complete terrestrial part of the water cycle; this type of model is known as an integrated groundwater - surface water model. The following section discusses the difficulties and assumptions made to conceptualize groundwater - surface water interactions necessary to delineate capture zones for stream segments.

2.2 Base Flow Contribution Areas for Stream Reaches

In a recent article by Sophocleous (2002) entitled "Interactions between groundwater and surface water: The state of the science", the author states that:

identification of stream reaches that interact intensively with groundwater would lead to better protection strategies of such systems. However, quantification of water fluxes in general, and specifically between groundwater and surface water, is still a major challenge, plagued by heterogeneity and scale problems.

With these issues in mind, some simplifying assumptions for the system must be made in order to quantify the exchange fluxes for streams at the watershed scale.

The interaction between the groundwater system and streams is a basic link in the hydrologic cycle. Streams that gain water from the inflow of groundwater through the streambed are called gaining streams [Figure 2A]. For this to occur, the elevation of the water table must be higher than the

level of the surface of the stream. Streams that lose water to the groundwater system by outflow through the streambed are called losing streams [Figure 2B]. A losing stream may also be disconnected from the water table [Figure 2C].

Throughout the year, streams can change from losing to gaining or vice versa, depending on the prevailing water table level. This can add increased complexity to a transient groundwater model and would change the capture zone over time, depending on the state of the stream. Since groundwater flow is slow relative to surface water flow, the capture zone delineated for gaining streams may not change quickly in response to seasonal changes in precipitation. Therefore, seasonal variability in precipitation would dampen out in the subsurface.

This study assumes an average annual base flow in the stream. Transient effects such as storm events are not considered. This assumption allows the focus to be placed on the groundwater system, with steady-state groundwater models used as a valid representation.

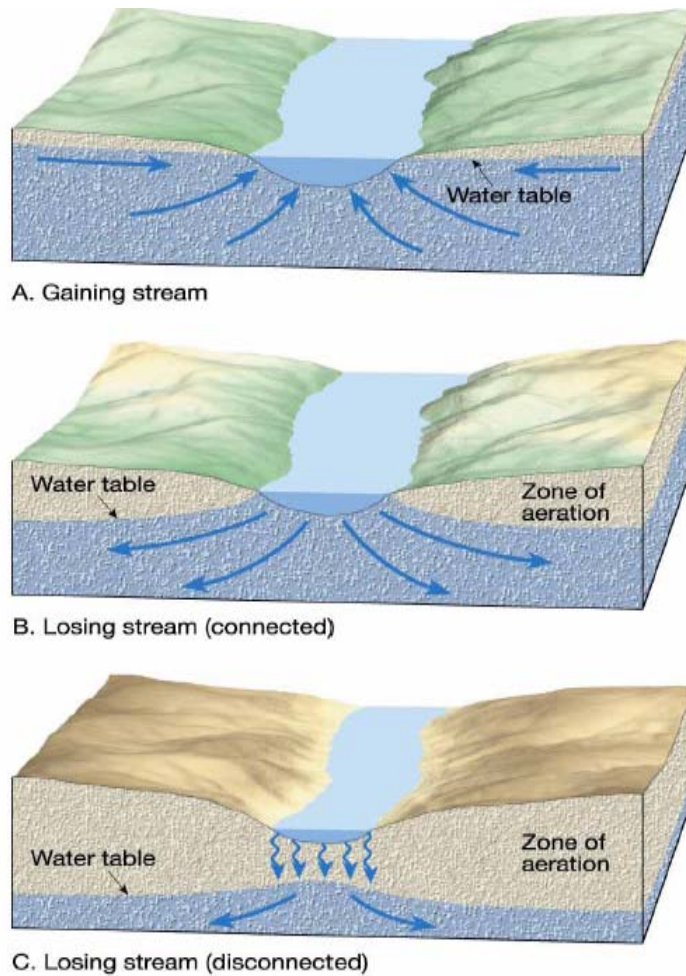


Figure 2: Interaction Between Groundwater Systems and Surface Water Streams (from Tarbuck et al., 2005)

Figure 3 shows schematically a segment just upstream of point A of a gaining stream within a watershed. The green area to both sides of the segment is the area contributing to the base flow entering the stream within that segment. If the remainder of the stream is also gaining then the area in yellow upstream of the marked segment also contributes base flow. Thus the total cumulative base flow measured at point A in Figure 3 will be the entire base flow contribution from the portion of the

watershed upstream of point A. This study will focus on the base flow contribution for a specific stream segment.

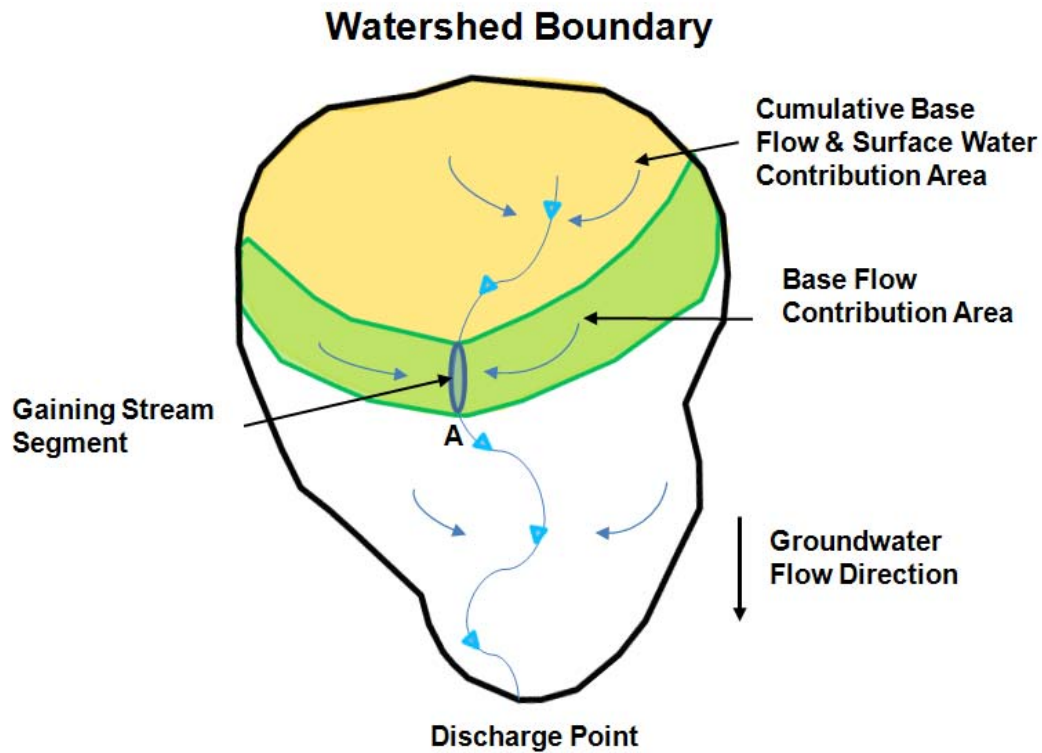


Figure 3: Areas Contributing to Base Flow

The streambed through which the groundwater enters the stream is known as the hyporheic zone [Figure 4]. This zone is composed of the upper few centimetres of sediments beneath surface water bodies. The hyporheic zone is known to have a profound effect on the water chemistry due to its richness in biochemical processes. It is a sensitive depositional environment where the constant flow of fluid causes the depositional characteristics to be variable in time. The chemical/biochemical processes, as well as changing depositional characteristics of the hyporheic zone are beyond the scope of this study and will not be considered here.

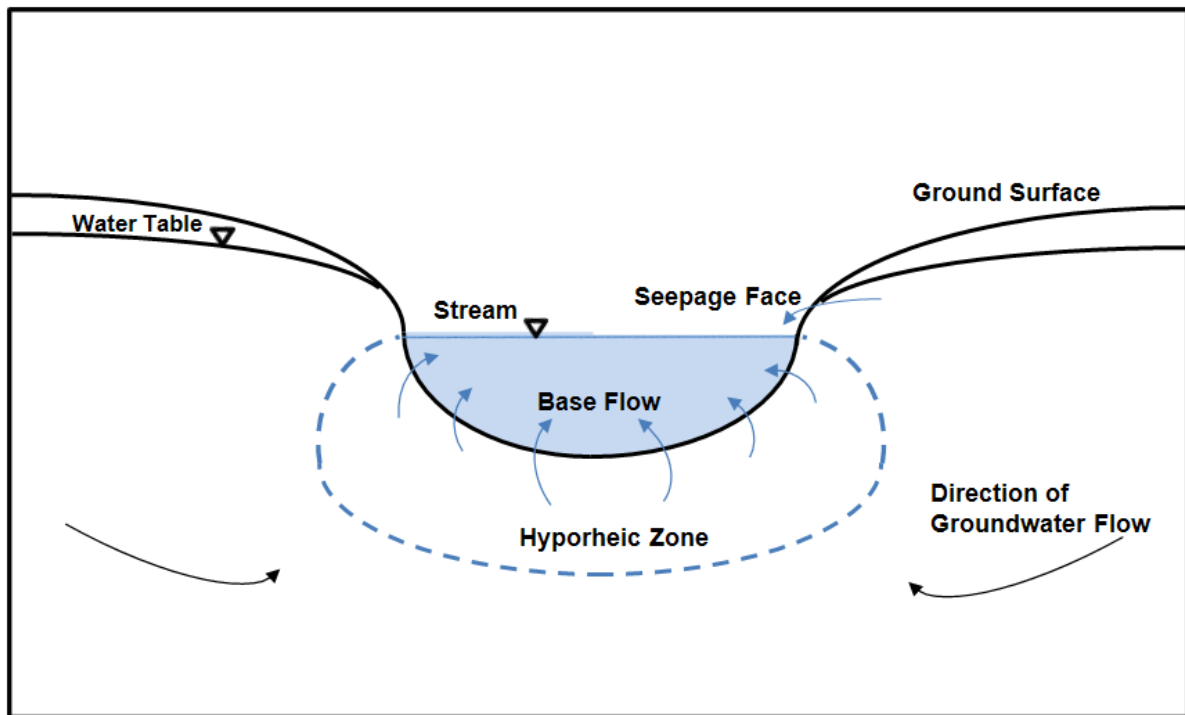


Figure 4: Base Flow through Streambed

2.3 Addressing Uncertainty in Capture Zone Delineation

Uncertainties from capture zone delineation can be classified as local-scale uncertainty or global-scale uncertainty. Local-scale uncertainty is defined as the uncertainty generated by unknown heterogeneities within a hydrogeological unit. Global-scale uncertainty (where the global scale is the scale of the study area) incorporates the shape of the aquifer and aquitard units, hydraulic connections between the aquifer units, boundary conditions, processes to be considered, uncertainties in conceptual model, as well as spatial and temporal discretization.

Local-scale uncertainty can be addressed by stochastic methods such as Monte Carlo analysis. Stochastic methods address uncertainty in groundwater modelling by representing heterogeneous porous media, with statistical distributions and delineating capture zones expressed in terms of confidence levels.

To determine the statistical parameters necessary to implement stochastic methods the study site must be very well characterized, such as the CFB Borden site in a classical study by Sudicky (1986) who sampled a sandy aquifer at the cm scale and developed statistical parameters in terms of variance of $\log(K)$ and correlation length. Sudicky applied the macrodispersion theory of Gelhar and Axness (1983) to derive effective macrodispersion coefficients that express the heterogeneity of the porous media. Frind et al. (1987) used micro-scale modelling to explain the physical processes underlying the macrodispersion theory.

The stochastic approach is a rigorous way of treating uncertainty; however, there are drawbacks. For example, Evers and Lerner (1998) state that under some conditions it may be difficult to specify statistical parameters necessary to utilize stochastic methods. In such cases it would be inappropriate to associate formal confidence levels with capture zones.

In addition, stochastic methods provide a way to address the uncertainty due to unknown parameters values, such as the properties of the porous media, but neglect uncertainties due to model structure (Refsgaard et al., 2005). Model structure includes: overall problem geometry, temporal and spatial discretization, the processes being considered, and different simplifying assumptions. Global uncertainties cannot usually be addressed stochastically because there may be little known about the statistical distribution of uncertain global-scale parameters.

Alternatively, a more pragmatic approach to address local-scale uncertainty is to apply reverse transport to generate a capture probability distribution (Frind et al., 2002), on the basis of macrodispersion theory (Gelhar and Axness, 1983). Conceptually, reverse transport determines the probable position and time of a particle upgradient from the receptor (Neupauer and Wilson, 1999). A backwards capture probability will not predict the actual impact on a well, it simply puts a number on the risk level. Thus, the higher the capture probability, the greater the risk.

The actual impact of a specific contaminant on a well can be determined by means of the well vulnerability method, which provides maximum concentrations to be expected at the well, plus arrival and exposure times from any source within the capture zone (Frind et al., 2006). Further details will be covered in Section 3.5.

A way to address global uncertainty is to compare results from different scenarios. Different scenarios can be generated by varying boundary conditions (Sousa et al., 2012), using different models, or calibration results with the same model. Scenario analysis is based on physical rather than statistical principles using a limited number of realistic conceptual model configurations. In this study, global uncertainty is investigated by comparing the results of three different models. The different models represent the physical system differently by taking into account different processes (i.e. fully integrated groundwater – surface water flow vs. saturated-only groundwater flow) and different discretization types (i.e. finite difference vs. finite element).

Another level of uncertainty exists in the model calibration. A groundwater model is typically calibrated by adjusting hydraulic conductivity values to match calculated head values to observed field measurements. Other calibration targets, such as stream flow, can be included. When calibrating a model there are more unknown variables than there are known variables, thus there are an infinite number of realizations that can provide a good calibration. Knowing hydrostratigraphic layers can help set constraints on hydraulic conductivity values that are adjusted, although the presence of discontinuities within hydrostratigraphic layers will not be recognized from calibration. In practice, once an acceptable fit is produced according to the calibration statistics, the model is considered to be valid. What is often not considered, however, is that there may be other realizations that could be equally valid. Thus an acceptable calibration fit does not mean that the model is unique. In fact, a successful calibration is just a necessary, but not a sufficient, condition for non-uniqueness. There is

also the possibility of over-calibration, which is calibration with insufficient data. Thus, calibration itself is subject to the judgment of the modeller.

Recent work by Sousa et al. (2012) sheds light on the uncertainty faced with delineating capture zones. In that study, three different recharge distributions were generated and applied to the same groundwater model, generating three different scenarios. The groundwater models for the three scenarios were calibrated separately and were then used for capture zone delineation for a municipal pumping well. The capture zones produced from each scenario were starkly different with no clues pointing towards the correct capture zone to choose. Since all three scenarios were based on a physically realistic conceptual model and deemed valid, it was proposed that the capture zones from the three different scenarios could be combined to form a final capture zone [Figure 5]. By taking the maximum extent capture zone from all three scenarios, a conservative capture zone was produced. This capture zone could be applied for conservative protection purposes to keep undesirable contaminants from reaching the well. Alternatively, the minimum extent could be chosen forming a capture zone with high probability of impacting the well. This capture zone could be applied for mitigation purposes, such as prioritizing areas for the implementation of Beneficial Management Practices to enhance water quality at the well.

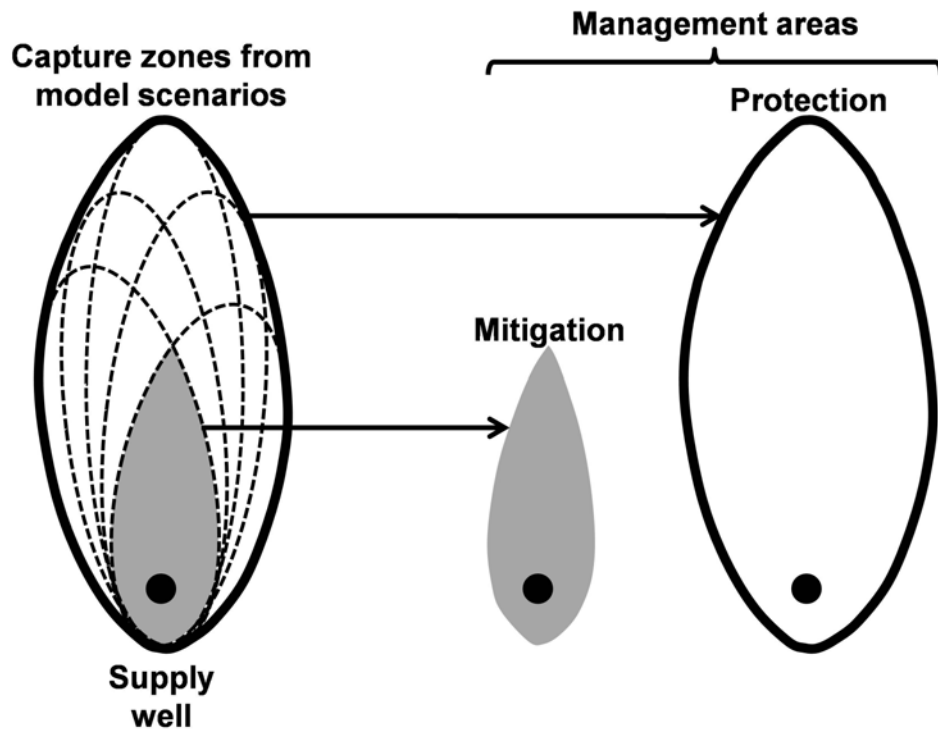


Figure 5: Conceptual Representation of Different Approaches for Protection and Mitigation Decisions (from Sousa et al., 2012)

Chapter 3

Groundwater Models Considered

Three models were used to compare the accuracy of modelling capture zones for streams. The three groundwater models chosen for this research are Modflow, Watflow and HydroGeoSphere. Modflow was selected because of its popularity in the consulting industry. Watflow was selected because it is capable of particle tracking, forward and reverse transport, and has a built-in autocalibration routine. HydroGeoSphere was chosen because it is a state-of-the-art fully integrated groundwater - surface water model and is believed to represent the physics of the hydrologic system with the greatest accuracy. HydroGeoSphere will also be used to generate the exchange fluxes for all three models in order to provide a common boundary condition for the top boundary. This choice also covers the two most important numerical modelling techniques, finite differences and finite elements. In addition, this research will consider two capture zone delineation methods, particle tracking and reverse transport.

3.1 Modflow

Modflow was originally developed by the United States Geological Survey (McDonald and Harbaugh, 1988). Subsequently a graphical user interface was added to Modflow by Waterloo Hydrogeologic Inc., giving it the name Visual Modflow (Schlumberger Water Services, 2009). With a graphical user interface and a highly credible scientific organization as the original developer, Modflow is considered to be the most widely used numerical model to simulate saturated groundwater flow (Brunner et al., 2010).

The governing equation for Modflow is a partial-differential equation of groundwater flow and is as follows (McDonald and Harbaugh, 1988):

$$\frac{\partial}{\partial x} \left(K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{yy} \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_{zz} \frac{\partial h}{\partial z} \right) + W = S_s \frac{\partial h}{\partial t}$$

Where:

K_{xx} , K_{yy} , and K_{zz} are values of hydraulic conductivity along the x, y, and z coordinate axes, which are

assumed to be parallel to the major axes of hydraulic conductivity (L/T);

h is the potentiometric head (L);

W is a volumetric flux per unit volume representing sources and/or sinks of water, with $W < 0.0$ for flow

out of the ground-water system, and $W > 0.0$ for flow in (T^{-1});

S_s is the specific storage of the porous material (L^{-1}); and

t is time (T).

This equation when combined with boundary and initial conditions, describes transient three-dimensional flow in a heterogeneous and anisotropic medium, provided that the principal axes of hydraulic conductivity are aligned with the coordinate directions. This would introduce an error when flow is at different angles to the major axes which may be encountered in fractured rock environments where there are sloping fracture planes.

Visual Modflow solves the saturated groundwater flow equation by using a finite-difference approximation. It does not take into account unsaturated groundwater flow (there are more current versions that have modules for unsaturated groundwater flow). Visual Modflow is capable of simulating irregularly shaped flow systems in which aquifer layers are confined, unconfined, or semi-confined. Hydraulic conductivities for differing layers may be heterogeneous and anisotropic.

The flow domain is divided up into finite blocks or a grid of cells where the properties of the porous medium are uniform. For each cell, the hydraulic head is calculated at the cell center. In the horizontal plan the cells are formed from a grid of perpendicular lines that can be variably spaced. In the vertical plane the model layers can vary in thickness. The flow equation is written for each cell and the equations are compiled to form a matrix.

A limitation is that the discretization of the finite difference grid makes it difficult to refine specific areas of interest such as areas surrounding pumping wells and stream reaches. The quadrilateral finite difference mesh generated in Visual Modflow requires adjacent cells to have the same length and width. Therefore to refine an area of interest (i.e. a well) all adjacent cells require refinement as well. Creating an extra fine mesh translates into a large matrix to solve, and hence a high computing cost.

3.2 Watflow

Watflow is a non-commercial finite element groundwater model developed at the University of Waterloo and is written in Fortran/77. Watflow uses triangular prismatic finite elements which facilitates a flexible grid refinement in the horizontal plane (e.g. around wells and along streams) and allows the grid to be deformed to fit irregular boundaries. Finite element discretization also allows for sloping stratigraphic contacts with variable layer thicknesses. A major advantage of using a finite element mesh compared with finite difference discretization is that grid refinement can be made only where necessary, thus minimizing the matrix size that is computed.

The governing equation for Watflow is based on the transient equation for 3D groundwater flow which can be expressed as (Bear, 1972):

$$\frac{\partial}{\partial x_i} \left[K_{ij} \left(\frac{\partial h}{\partial x_j} \right) \right] - \sum_{k=1}^N Q_k(t) \cdot \delta(x_k, y_k, z_k) = S_s \frac{\partial h}{\partial t}$$

Where:

K_{ij} is the hydraulic conductivity tensor (L/T);

h is the hydraulic head (L);

Q_k is the fluid volume flux for a source or sink located at x_k, y_k, z_k (L³/T);

S_s is the specific storage (L⁻¹); and

t is the time (T).

The governing equations are discretized using the Galerkin finite element method (Huyakorn and Pinder, 1983). Watflow has an extremely efficient pre-conditioned conjugate gradient solver to solve the matrix equations.

A 2D finite element grid is first generated in the horizontal plane using GRID-BUILDER (McLaren, 1997); this grid is then extended to 3D by a subroutine in Watflow. Watflow's triangular prisms are arranged in a "layer cake" formation. The triangles are oriented within the horizontal plane, and are joined to nodes above and below by vertical columns. A schematic of element layering and 3D node numbering scheme is provided in Figure 6.

Watflow is capable of solving three-dimensional or two-dimensional flow problems in confined/unconfined aquifer systems. Watflow can simulate transient or steady-state saturated flow and simplified unsaturated flow for steady-state flow conditions. Watflow is capable of simulating heterogeneous and/or anisotropic porous media, and it can accommodate multiple sources and sinks. It is versatile in terms of boundary conditions, where boundaries can be a mix of specified head (Dirichlet) and specified flux (Neumann) conditions. The recharge rate at the top of the model boundary can either be specified as a uniform value or may vary spatially.

Watflow assumes that the porous medium is non-deforming and non-fractured. Fractured porous media can only be modelled as equivalent porous media assuming the problem is appropriately scaled. The fluid is assumed to be isothermal and incompressible. Well bore storage is naturally accommodated by 1D line elements (Sudicky et al., 1995).

The following table from the Watflow Manual v4.0 summarizes the capabilities, as well as the assumptions and limitations of Watflow (Molson et al., 2002):

Table 1: Capabilities and Assumptions of Watflow

Capabilities	Assumptions and Limitations
<ul style="list-style-type: none"> • 3D or 2D domains. • Full transient or steady-state flow domain can be heterogeneous and anisotropic. • Multiple sources and sinks can be accommodated. • 1D line elements can accommodate well bore storage. • Versatile boundary conditions options. • Spatially variable recharge. 	<ul style="list-style-type: none"> • Non-deforming, non-fractured or equivalent porous medium. • Isothermal aquifer fluid is incompressible. • Fully saturated flow domain (transient/steady-state) or simplified unsaturated zone representations (steady-state only).

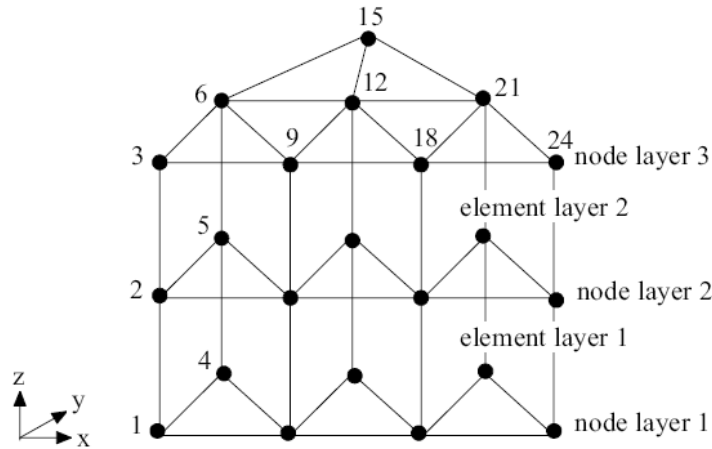


Figure 6: Schematic Layout of the 3D Prismatic Grid and Node Numbering Scheme used in Watflow (from Molson et al., 2002)

3.3 HydroGeoSphere

HydroGeoSphere is a control volume finite element model developed by a group of researchers at the University of Laval, the University of Waterloo and HydroGeologic Inc., Herndon, Virginia. Therrien et al. (2006) describes HydroGeoSphere’s fully integrated nature as being:

a unique feature... when the flow of water is simulated in fully-integrated mode, water derived from rainfall inputs is allowed to

partition in to components such as overland and stream flow, evaporation, infiltration, recharge and subsurface discharge into surface water features such as lakes and streams in a natural, physically-based fashion.

HydroGeoSphere is capable of complete hydrologic cycle modelling using detailed physics of surface and subsurface flow in one integrated code. The surface regime can be represented as a 2D areal flow for the entire surface or as 2D runoff into 1D channels. The subsurface regime consists of 3D unsaturated/saturated flow. Both surface water and groundwater flow regimes interact with each other through considerations of the physics of flow between them. HydroGeoSphere is capable of simulating a combination of porous, discretely-fractured, dual-porosity and dual-permeability media for the subsurface. Well bore storage is naturally accommodated by 1D line elements (Sudicky et al., 1995).

The governing equation in HGS for subsurface flow is the modified form of Richards' equation used to describe 3D transient subsurface flow in a variably-saturated porous medium (Therrien et al., 2006):

$$-\nabla \cdot (w_m q) + \Sigma \Gamma_{ex} \pm Q = w_m \frac{\partial}{\partial t} (\theta_s S_w)$$

Where:

w_m is the volumetric fraction of the total porosity occupied by the porous medium (dimensionless);

q is the fluid flux (L/T);

Γ_{ex} is the volumetric fluid exchange rate (L³L⁻³T⁻¹);

Q is the source sink term (L³/T);

θ_s is the saturated water content (dimensionless);

S_w is the water saturation (dimensionless).

The governing equation in HGS for surface runoff is the Saint Venant equation for unsteady shallow flow which assumes depth-averaged flow velocities, hydrostatic pressure distribution

vertically, mild slope, dominant bottom shear stress, and neglects inertial forces. Furthermore, it is assumed that the Manning, Chezy, and Darcy-Weisbach formulae are valid to calculate frictional resistance forces for unsteady flow. The Saint Venant equation is represented by the diffusion wave approximation (Therrien et al., 2006):

$$\frac{\partial \Phi_0 h_0}{\partial t} - \frac{\partial}{\partial x} \left(d_0 K_{0x} \frac{\partial h_0}{\partial x} \right) - \frac{\partial}{\partial y} \left(d_0 K_{0y} \frac{\partial h_0}{\partial y} \right) + d_0 \Gamma_0 \pm Q_0 = 0$$

Where:

Φ is a surface flow domain porosity which is unity for flow over a flat plane;

h is the water surface elevation (L);

d is the depth of water flow (L);

K is the surface conductance that depends on the equation used to approximate the friction slopes (L);

Q is a volumetric flow rate per unit area representing external sources and sinks (L^3/T);

and

t is the time (T).

For further detail on governing equations for surface flow (i.e. channel flow) and flow coupling refer to the User's Guide (Therrien et al., 2006).

HydroGeoSphere has a preprocessor by the name of *grok* that is capable of generating grids composed of either hexahedral blocks or triangular prisms. HydroGeoSphere is capable of using the same finite element mesh used in Watflow, however the node numbering becomes slightly different. In this study, HydroGeoSphere will use the same finite element mesh as Watflow, which is composed of triangular prisms and was generated using GRID-BUILDER.

It is important to note the limitations of the models used in this study. HydroGeoSphere is capable of simulating groundwater - surface water interactions, but does not have a particle tracking module. It also does not have a built-in calibration tool and can only be calibrated through manual adjustments, or the model could be linked to a calibration tool such as PEST (Doherty, 2005), but a

linked version is not yet available. Watflow has a built-in calibration tool, particle tracking and reverse transport, but does not have integrated surface water flow and only a simplified linearized representation of the unsaturated zone.

3.4 Particle Tracking

Particle tracking is a method whereby a particle is released and the advective groundwater flow field carries the particle through the flow system. The particle can either be released at the surface and tracked forward in time through the subsurface, or released at the point of interest (well screen or groundwater discharge area) and allowed to travel backwards until it reaches the surface or some other boundary. The two options are referred to as forward particle tracking or reverse particle tracking. Particle tracking only takes into account advective transport, generating a deterministic capture zone. The capture zones created are extremely sensitive to slight changes in the hydraulic head field (Franke et al, 1998).

The best-known particle tracking routine today is Modpath (Pollock, 1989), which is available as a module in Modflow. Modpath uses a semi-analytic solution method to calculate three-dimensional particle tracks from the steady-state flow solution generated by Modflow. This method requires the interfacial fluxes between cells and assumes that, the velocity varies linearly within a cell in order to calculate the average velocity components. Given the entry point of a particle, the exit face is selected based on the shortest travel time between entry and exit points. After choosing the exit face for the particle, the exit position on the selected face is calculated. This method avoids interpolating velocities between cells, producing physically realistic particle tracks for heterogeneous conditions. These considerations are important, without them the particle tracks tend to smear through low hydraulic conductivity layers rather than deviating around them when encountering sharply contrasting hydraulic conductivities.

A particle tracking program following a similar approach called Watrac was developed for unstructured finite element grids by Frind and Molson (2004). This program uses the steady-state hydraulic head distribution generated by Watflow to delineate its particle tracks. Watrac is capable of forward and reverse particle tracking.

HGS does not have particle tracking capabilities, in order to delineate capture zones in HGS it is necessary to convert the steady-state hydraulic head values generated by HGS into a format that can be run in Watrac.

When placing particles in Modpath and Watrac, the user specifies the x-y coordinates of the particle and the layer of the starting position. The particle can be placed anywhere within a cell or element; however, the vertical placement of the particle is always in the centre of the chosen layer in both Modpath and Watrac.

It is important to note that the direction, size and shape of these capture zones can change dramatically due to small differences in gradients. The hydraulic heads calculated in the domain are a product of boundary conditions, processes taken into consideration and material properties of the subsurface. The material property that is subject to the greatest uncertainty is hydraulic conductivity; this parameter can vary orders of magnitude.

3.5 Advective-Dispersive Transport

As discussed in the Section 2.3, one of the ways in which we can address local uncertainty is by delineating capture zones by reverse transport. Reverse transport is similar to reverse particle tracking, however it also takes into account dispersion and diffusion leading to the creation of capture probability plumes. Currently there is a module available in Visual Modflow to simulate forward transport, but not reverse transport. The model Watflow has the capability of simulating both forward and reverse transport. The transport code for Watflow is known as WTC (Molson and Frind, 2004) and was developed at the University of Waterloo.

The governing equation for WTC is based on the 3D advection-dispersion equation which can be expressed as:

$$\frac{\partial}{\partial x_i} \left[\left(\frac{D_{i,j}}{R} \right) \frac{\partial c}{\partial x_j} \right] - \frac{\partial}{\partial x_i} \left(\frac{v_i}{R} c \right) - \lambda c + \sum_{k=1}^N \frac{Q_k(t) c_k(t)}{R\theta} \delta(x_{k'}, y_{k'}, z_{k'}) = \frac{\partial c}{\partial t}$$

Where:

D_{ij} is the hydrodynamic dispersion tensor (L²/T);

V_i is the average linear groundwater velocity (L/T);

λ is the first-order decay term given by $\lambda = \frac{\ln(2)}{t_{1/2}}$ [Where $t_{1/2}$ is the half-life](T⁻¹);

R is retardation factor defined by $R = 1 + \frac{\rho_b K_d}{\theta}$ [Where ρ_b is the bulk density and K_d is

the distribution coefficient that governs the partitioning of the solute into dissolved and adsorbed phases (Freeze and Cherry 1979)] (dimensionless);

c_k is the source concentration for an injection well;

c is the unknown aquifer concentration.

WTC is capable of simulating transport in 1D, 2D and 3D domains, which can be heterogeneous and anisotropic. The elements used to discretize physical systems can be made to fit complex geometries. WTC can accommodate multiple sources and sinks, including variable pumping or injection rates over time. Boundary conditions can be set to first type (specified concentration), second type (default Neumann zero-gradient), or third type (specified mass flux). WTC incorporates linear retardation and first order decay. WTC can compute concentration breakthrough curves at selected points.

WTC assumes that the porous medium is non-deforming, isothermal and non-fractured or equivalent porous medium. The fluid is assumed to be incompressible. WTC can only simulate one contaminant species at a time, considers only the aqueous phase, and neglects chemical reactions.

The following is a summary table from the WTC Manual which lists capabilities, assumptions and limitations of WTC (Molson and Frind, 2004):

Table 2: Capabilities and Assumptions of WTC

Capabilities	Assumptions and Limitations
<ul style="list-style-type: none"> • 3D, 2D or 1D domains. • Domain can be heterogeneous and anisotropic. • Deformable elements can conform to complex geometry. • Multiple sources and sinks can be accommodated including a variable pumping history. • Versatile boundary condition options. • Includes linear retardation and first-order decay • Computes concentration breakthrough data (concentration vs. time) at selected points. 	<ul style="list-style-type: none"> • Non-deforming, isothermal aquifer • Fluid is incompressible. • Well bore storage and well losses are neglected • Single contaminant species • Chemical reactions are neglected • Aqueous phase contaminants • Non-fractured or equivalent porous media

Reverse transport is accounted for in WTC by reversing the sign on the advective term and the Type 3 boundary term. The following equation from Frind et al. (2002) expresses the concept of reverse transport:

$$\frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial p}{\partial x_j} \right) + v_i \frac{\partial p}{\partial x_i} = \frac{\partial p}{\partial \tau} \quad i, j = x, y, z$$

Where:

τ is backward time.

$p = p(x, y, z, \tau)$ is the probability that a particle arriving at a receptor at a given time τ has originated at location (x, y, z) in the aquifer, or the backward travel time probability density function.

D_{ij} is the dispersion coefficient, which is spatially variable and velocity dependent. Here it represents the dispersion of capture probability due to random uncertainties in the travel paths.

To implement reverse transport, a type 1 – constant probability of 1 is set at the point of interest and allowed to be transported in reverse. The capture probability plume travels backwards in relation to groundwater flow direction and varies between 0 and 1, where 1 represents 100% probability of capture by the groundwater sink and 0 representing 0% probability of capture by the groundwater sink.

The boundary and initial conditions for the reverse transport simulations for a stream reach are as follows. The capture probability p is assigned as 1 at the streambed, and zero throughout the entire domain:

$$p(\text{streambed}, \tau) = 1$$

$$p(x, y, z, \tau = 0) = 0$$

Capture zones delineated by particle tracking will be compared across all three models. Reverse transport capture zones will be delineated using the hydraulic head distribution from Watflow and will be compared to the reverse particle tracking capture zones in Watflow. The following chapter discusses the setting in which all the modelling will be based on.

Chapter 4

The Alder Creek Watershed

4.1 Setting

The Alder Creek Watershed is embedded within the south central area of the Waterloo Moraine [Figure 7]. The watershed covers an area of approximately 79 km², with Alder Creek at its core meandering through areas of open fields and residential areas [Figure 8]. The watershed boundaries are placed on the basis of topographic highs. The Alder Creek is a tributary of the Nith River within the Grand River Basin. The Alder Creek Watershed is situated in close proximity to the cities of Kitchener and Waterloo. The cities of Kitchener-Waterloo have developed over time along the eastern edge of the Waterloo Moraine, which is an important relief feature in the Region. Because of this the Alder Creek Watershed is under a great deal of development pressure. The western half of the Waterloo Moraine is a regionally significant groundwater recharge area for the Region's municipal well fields.

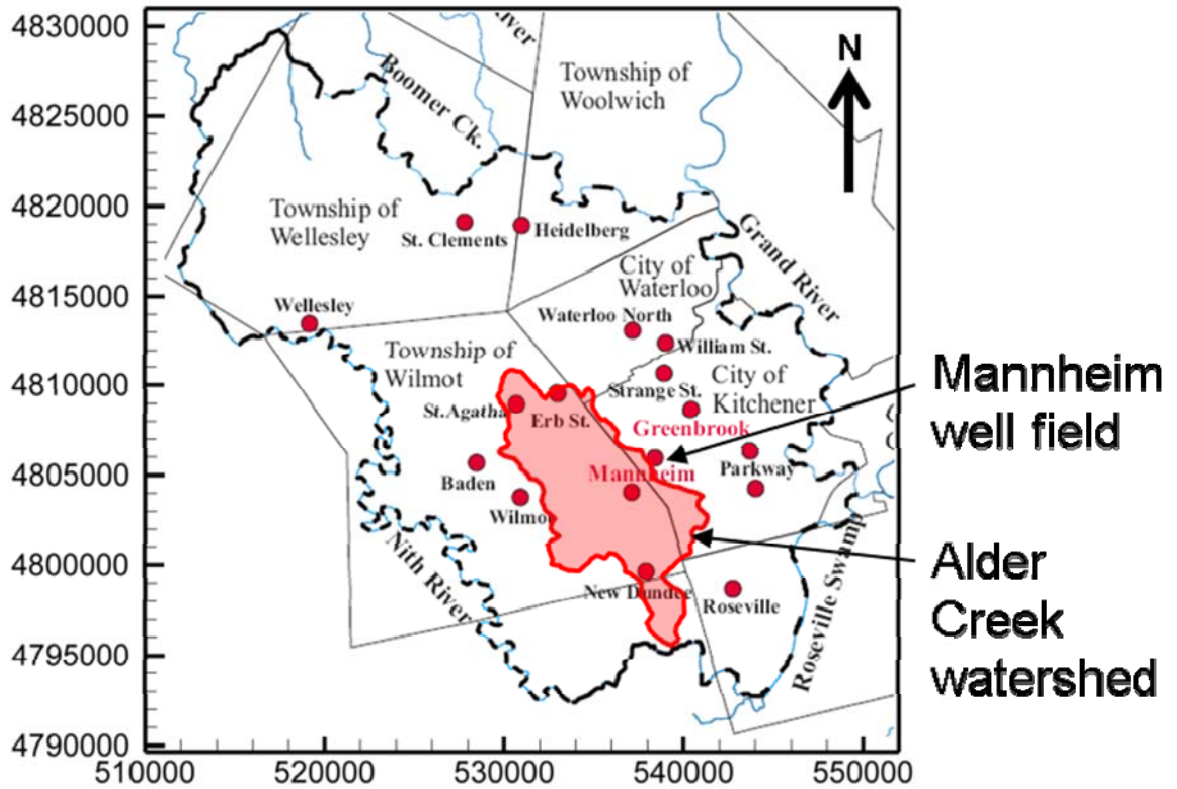


Figure 7: Alder Creek Watershed within Waterloo Moraine Model (from Frind et al., 2009)

Precipitation that reaches the water table within the Alder Creek Watershed recharges the Mannheim Aquifer. This aquifer contributes to the base flow of Alder Creek, as well as water to the Mannheim municipal well fields. Aquatic habitats and wildlife in the Alder Creek Watershed are heavily dependent on groundwater discharge to creeks, lakes and ponds.

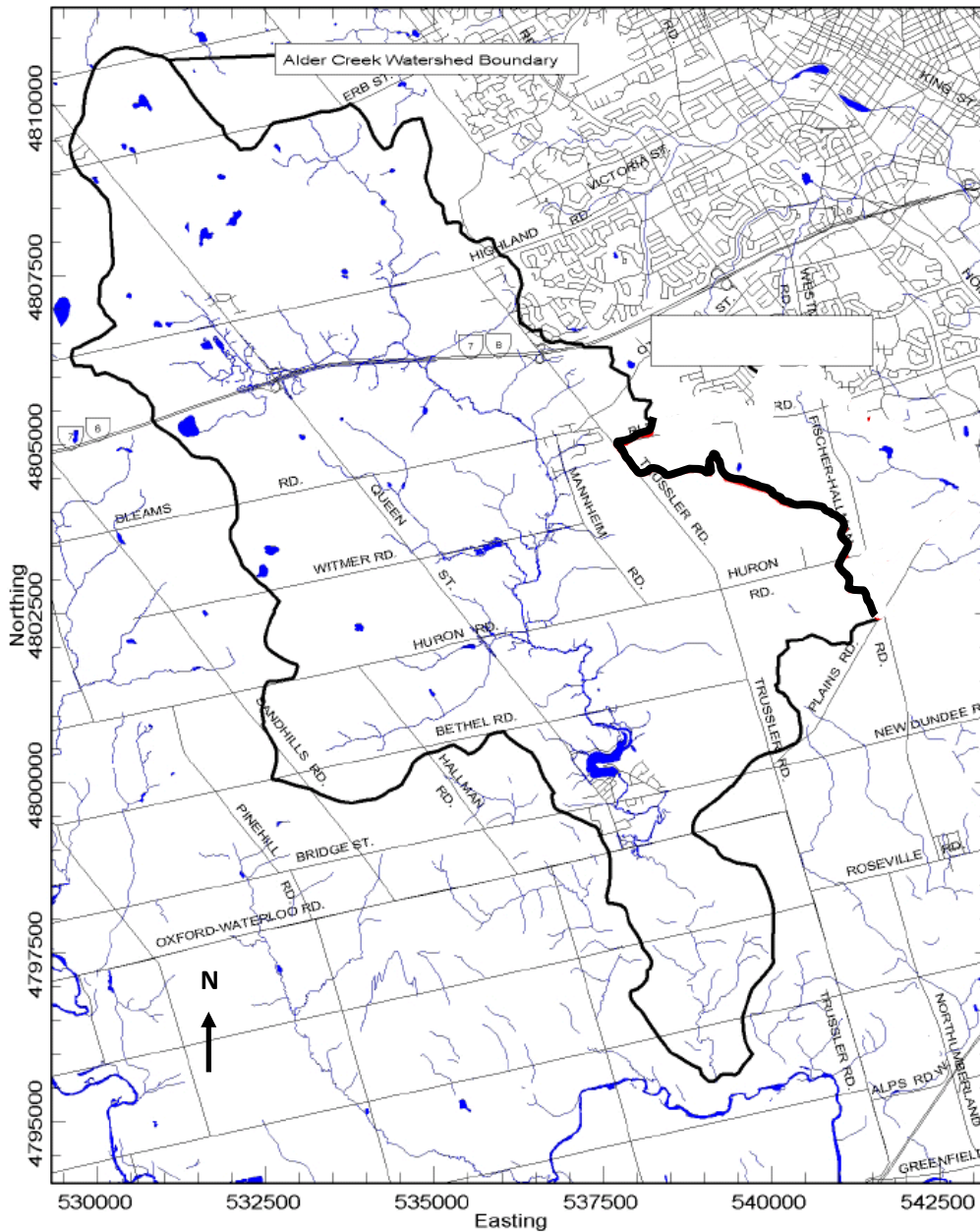


Figure 8: Alder Creek Watershed Boundary (from CH2MHILL and North-South Environmental Inc., 2008)

The land use within the Alder Creek watershed is mostly agricultural with some areas of aggregate extraction. There are five towns within the watershed, which include: New Dundee,

Mannheim, Petersburg, St. Agatha, and Shingletown. These towns primarily use individual septic tanks and tile beds as their sewage disposal systems. Agricultural activities and sewage disposal systems in the area may be contributors to nutrient loading to the local groundwater system, Alder Lake and Alder Creek (Grand River Conservation Authority, 2001).

The eastern fringe of the Alder Creek watershed includes portions of the City of Kitchener and a portion of the Erb Street Landfill in the City of Waterloo. There are networks of rural highways that run through the watershed as well as a major highway, Highway 7/8, that cuts through the watershed. These urban features and road-ways may be potential threats to groundwater resources. The Erb Street Landfill's leachate may be a source of contaminants, while road salt for deicing along major roadways during winter can be a non-point source contaminant.

4.2 Hydrogeology

The Waterloo Moraine is well characterized hydrogeologically because of its value as a water source to the local communities. The Waterloo Moraine is predominantly of hummocky relief, mainly composed of sand and gravel with intervening till layers and has been interpreted to be an interlobate kame moraine (Karrow, 1993).

The stratigraphy of the Waterloo Moraine is complex with a heterogeneous and anisotropic distribution of hydraulic conductivity. Three relatively continuous till units, the Port Stanly/Tavistock, Maryhill, and Catfish Creek tills have been identified throughout the Moraine and are seen as aquitards. Glaciofluvial sand and gravel deposits located between the major till units form the major aquifers in the system. The upper aquifer (Aquifer 1), thought to be reworked Maryhill till, is the most extensive and regionally continuous unit; it is also the most productive water source. The two lower aquifers (Aquifer 2 and 3) are discontinuous sand and gravel units and productive locally. The underlying bedrock consists of the Salina Formation, a Silurian dolomitic limestone (Karrow, 1993).

In 1998, Martin and Frind modelled the complex multi-aquifer system of the Waterloo Moraine in 3D. To accomplish this monumental task required the development of a hydrostratigraphic database. 4500 Waterloo Moraine boreholes logs from The Ministry of the Environment in Ontario were screened for quality, leading to the selection of 2044 borehole logs. Groups of boreholes were linked into 317 local-scale cross sections to allow continuous interpretation of the stratigraphy [Figure 9]. A typical cross section is depicted in Figure 10 showing the hydrostratigraphic interpretation of the borehole data. The lithologies of the boreholes were grouped into categories with hydraulic conductivity values based on literature and field data. By joining all the information together a conceptual model of the Waterloo Moraine's complex hydrostratigraphy was formed [Figure 11].

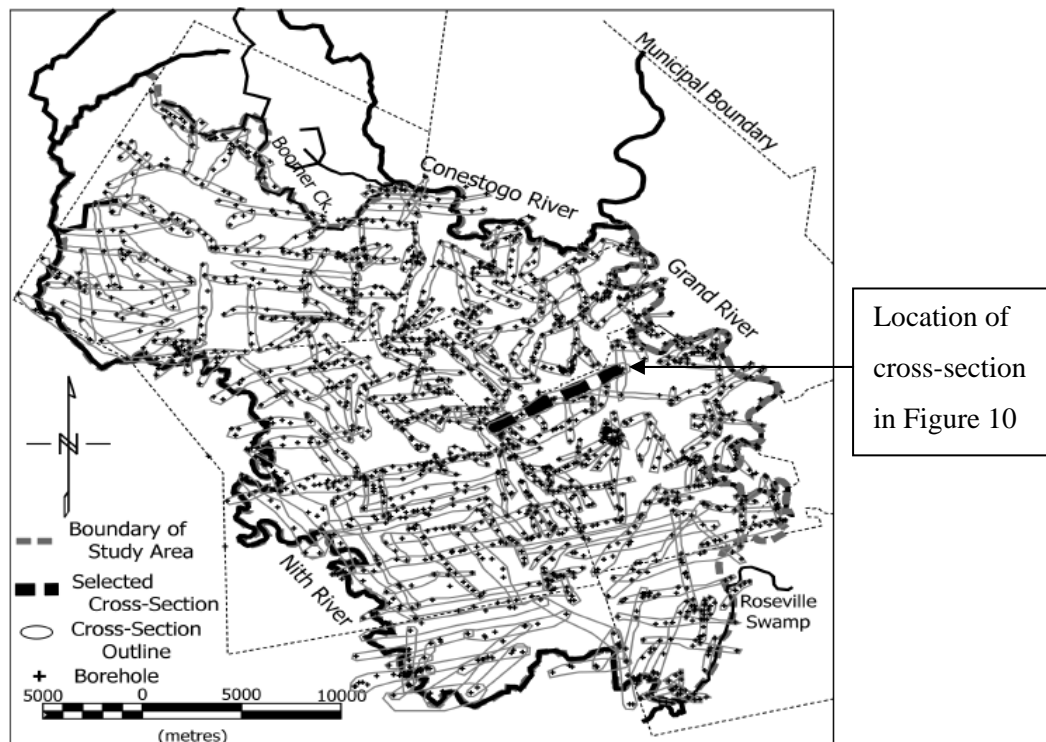


Figure 9: Location of Selected Boreholes and Hydrostratigraphic Cross-Sections (from Martin and Frind, 1998)

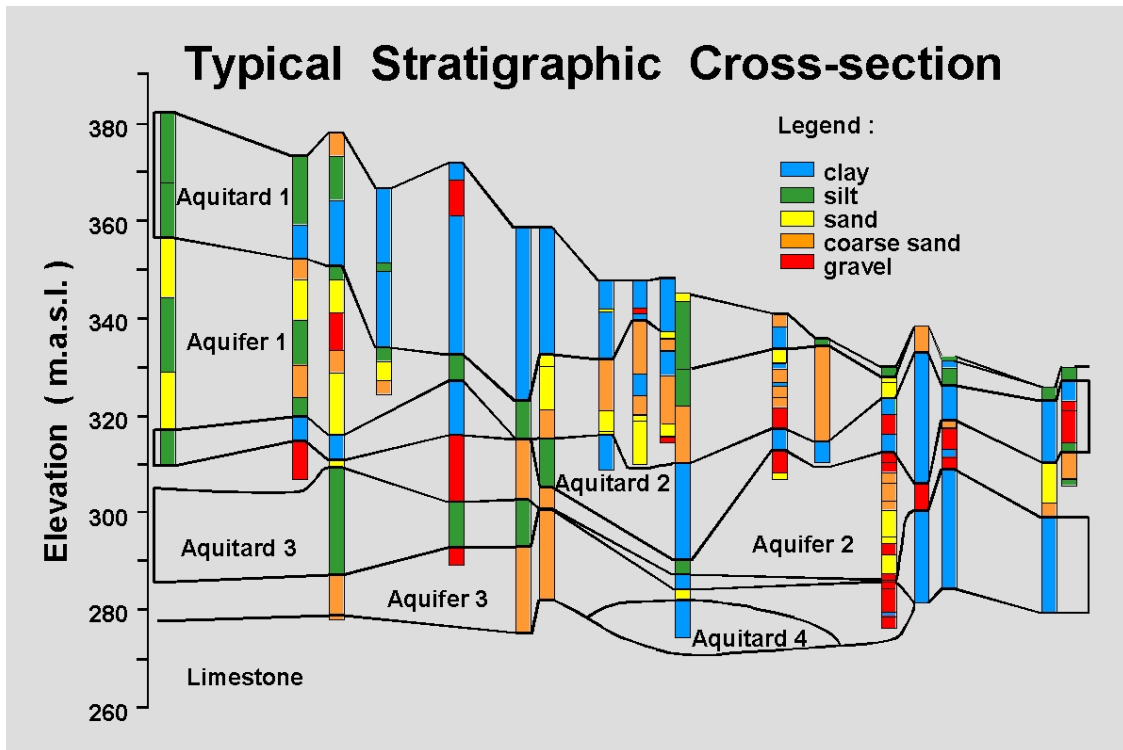


Figure 10: Typical Waterloo Moraine Hydrostratigraphic Cross-Section (from Martin and Frind, 1998)

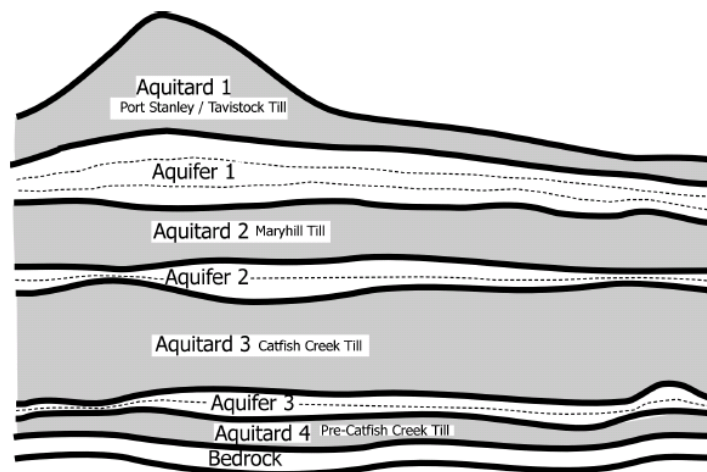


Figure 11: Conceptual Hydrostratigraphic Model of Waterloo Moraine (from Martin and Frind, 1998)

4.3 Pumping and Observation Wells

There are 10 pumping wells and 28 observation wells located in the Alder Creek Watershed.

Table 3 contains the coordinates of each pumping well, the well screen elevation and the average pumping rates from 1991 to 2000. Table 4 contains the coordinates, well screen elevation and average head level of the observation wells from 1991 to 2000. Figure 12 depicts the locations of the pumping and observation wells, only the pumping wells have been labeled to avoid overcrowding. The following wells are found in pairs and are represented by only one point on Figure 12: K91 and K92, ND2 and ND4, SA3 and SA4, and W7 and W8. Some wells (eg. K91 and K92) are located close to the watershed boundary and would likely cause a shift in the groundwater divide due to pumping.

Table 3: Coordinates, well screen elevation and pumping rates for pumping wells

Name	World Coordinates		Well Screen Elevation		Pumping Rate (m ³ /day)
	X (m)	Y (m)	Top Screen (m)	Bottom Screen (m)	
K22A	536538.2	4805045.9	313.05	313	-3010.85
K23	536770.3	4804781.7	312.85	312.8	-3765.41
K24	537054.7	4803860.8	314.4	307.4	-2733.62
K26	537733	4803203.8	315	308.6	-6755.77
K91	537687.6	4806010.5	313.94	312.94	-212.35
K92	537714.2	4806040	315.95	314.95	-212.35
ND2 and ND4	537938.1	4800208	307.7	306.9	-216.25
SA3 and SA4	530548.8	4809271.5	346	345.9	-10.47
W7	533126.6	4809135.9	335.1	327.1	-5004.63
W8	533130	4809148.9	336.2	314.6	-3910.14

(CH2MHILL and S.S. Papadopoulos & Associates, Inc., 2003)

Table 4: Coordinates, well screen elevation and head levels for observation wells

Name	X [m]	Y [m]	Mid-Point of Screen Elev. [m amsl]	HEAD [m amsl]
AC1A-01A	536156	4803610	316.695	330.1
AC1B-01B	536156	4803610	329.035	332.05
AC2B-01B	534625.7	4800798	320.78	336.98
AC3A-01A	537487	4801079	306.885	317.97
AC3B-01B	537487	4801079	316.025	317.95
AC4B-01B	537741	4800160	297.975	317.52
AC5B-01B	538748	4797797	298.395	299.95
OW10-67A	532387.5	4803920	307.815	353.25
OW2-61A	536299.6	4805356	316.135	332.58
OW2-77A	537924.3	4800200	309.18	313.49
OW2-85A	537189.3	4805605	322.425	330.4
OW3-61A	537095.5	4803858	309.48	325.27
OW8-61A	536545.3	4805108	314.655	328.37
TW11-69A	537758.4	4803201	307.035	326.69
TW1-70A	538192	4802541	312.385	327.52
TW3-69A	537565.6	4803941	312.925	327
WM17-93A	532895	4805752	314.619	351.98
WM17-93B	532895	4805752	333.819	352.08
WM17-93C	532895	4805752	352.369	353.08
WM18-93B	534070	4804188	334.094	349.22
WM20-93A	535523	4804855	316.592	334.54
WM22-93B	536072	4802225	314.99	326.3
WM23-93A	539310	4802680	307.685	327.89
WM23-93B	539310	4802680	328.935	327.78
WM2-93B	531481	4809394	341.647	356.13
WM2-94C	535430	4806050	323.275	338.01
WM9-93C	532940	4807705.99	339.5541	353.48
WM-OW3AC-92B	534887.1	4803341	335.895	341.59

Notes: m amsl= Metres above mean sea level

(CH2M HILL and S.S. Papadopoulos & Associates, Inc., 2003)

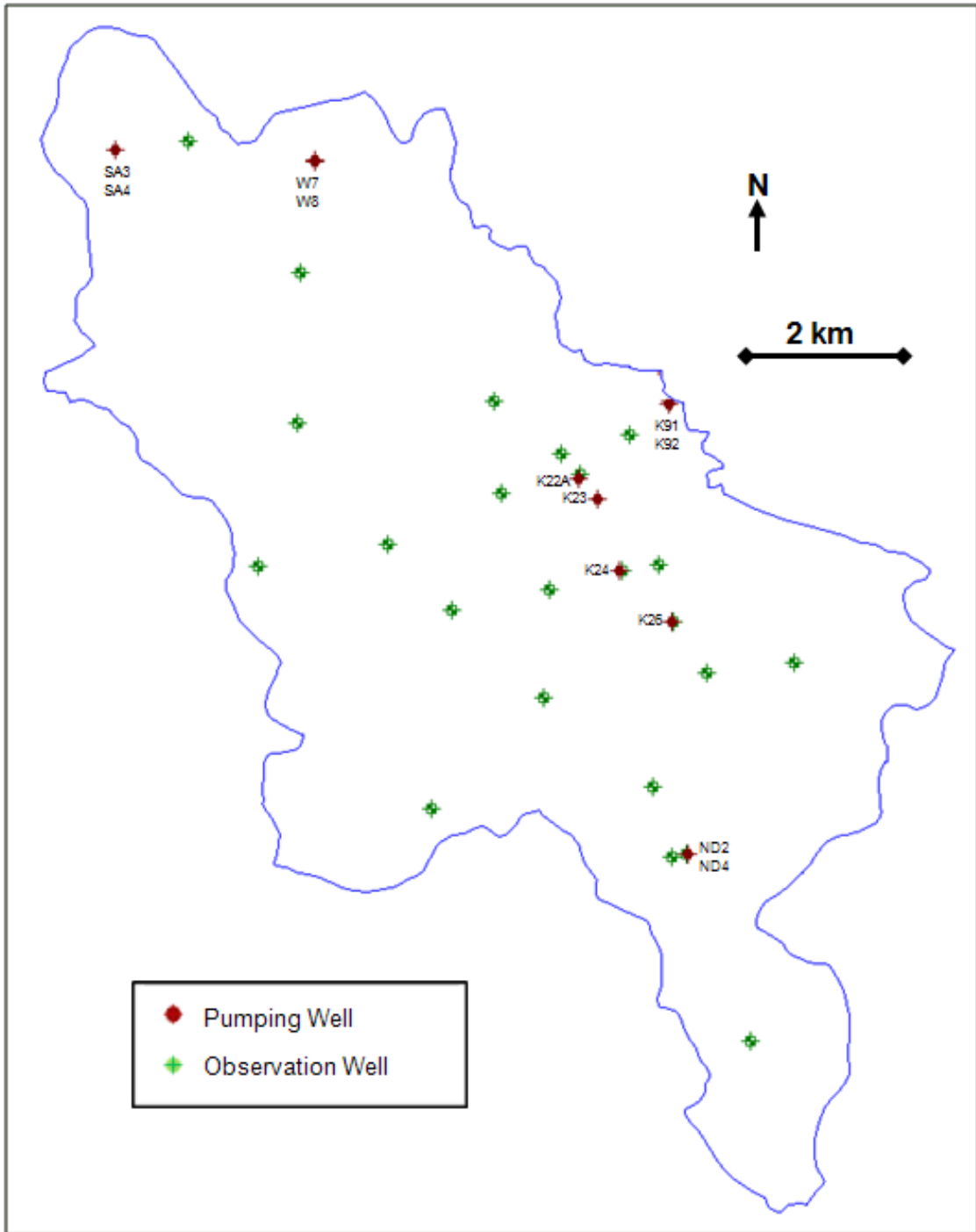


Figure 12: Alder Creek Watershed with Well Locations

4.4 Groundwater Flow

Figure 13 shows the average water table elevation contours from 1991 to 2000 in the Alder Creek watershed. These values were derived from the available water level data in the Regional Municipality of Waterloo's database and contoured by CH2MHILL and S.S. Papadopoulos & Associates, Inc. (2003). The regional groundwater flow direction within the Alder Creek watershed is from northwest to southeast. The groundwater flow generally occurs from an elevation high, located to the northwest of St. Agatha and the northern boundary of the Alder Creek Watershed, to the southeast, towards Alder Creek and to the southwest towards the Nith River. Within the Alder Creek Watershed, groundwater flows from the topographic highs along the watershed boundaries to Alder Creek and Alder Lake, where it discharges. There is also a distinct pattern of convergence at the southern tip of the watershed indicating that groundwater is discharging towards the creek.

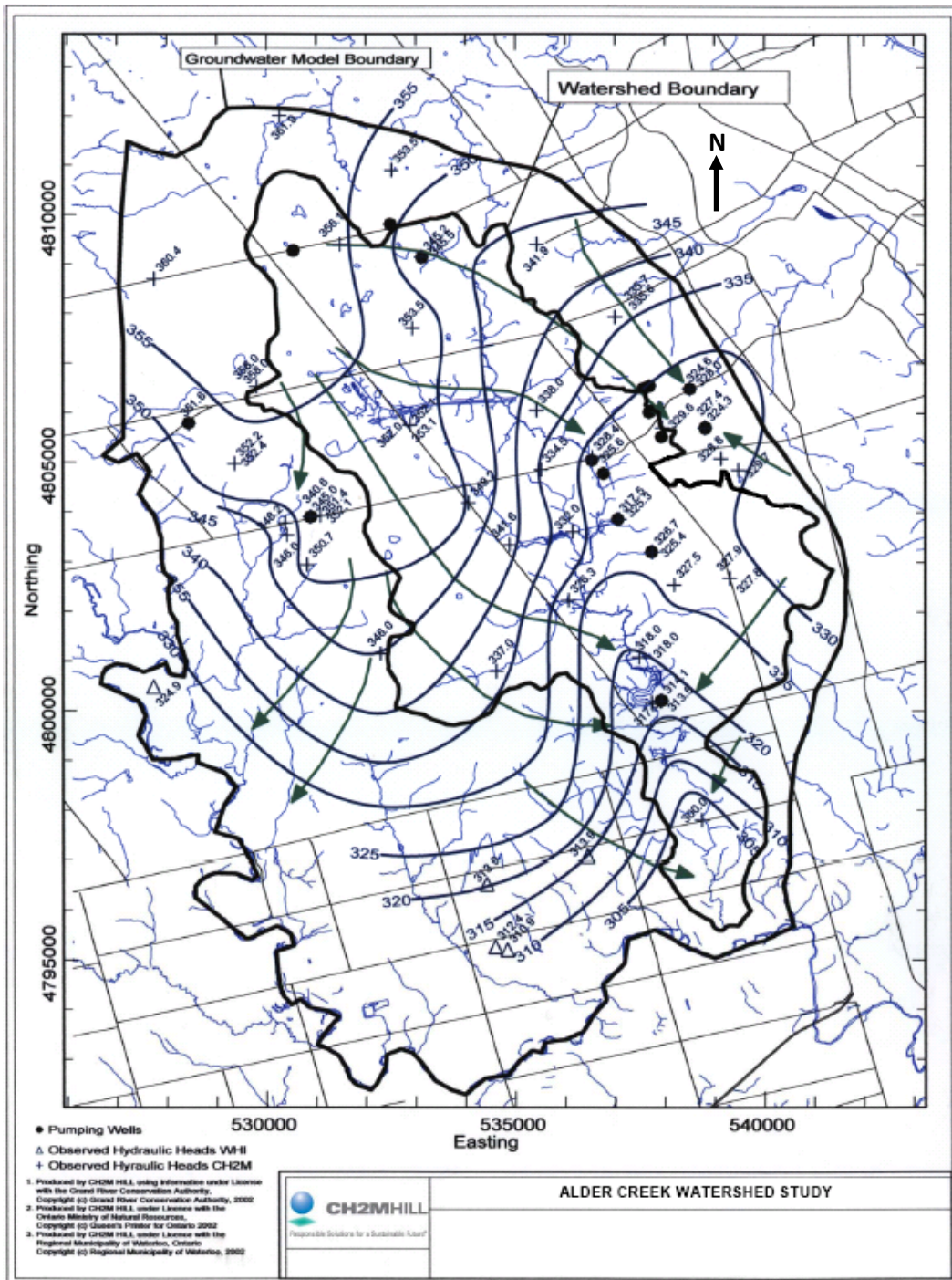


Figure 13: Observed Groundwater Elevations and Interpreted Groundwater Flow Directions
 (from CH2MHILL and S.S. Papadopoulos & Associates, Inc., 2003)

Chapter 5

Alder Creek Model

5.1 Conceptual Model

The Alder Creek model is based on a conceptual model created by Professor Jon Paul Jones at the University of Waterloo (Jones et al., 2009). In this model the bottom of the model domain is assumed impermeable, while the saturated headwater (northern edge) and discharge (southern edge) regions of the subsurface mesh are assigned type 1 - constant head values of 372.3 and 296.5 meters respectively [Figure 14a]. The sides of the model domain are thought to be a groundwater divide and are left to the default setting which was a type 2 - no flow boundary. For the top boundary a uniform net rainfall rate of 200 mm/year is applied. The model is run until steady-state conditions are reached.

It is important to note that in this model only 6 of the 10 pumping wells within the Alder Creek modelling domain are active. The active pumping wells within the modelling domain are: K22A, K23, K23, K26, ND2ANDND4 and SA3ANDSA4. Pumping wells K91, K92, W7, and W8 are located very close to the model domain boundaries, because of this the wells would run dry and cause convergence issues. For this reason these wells are inactivated.

The conceptual model of the Alder Creek Watershed by Jones et al. (2009) does not allow for regional flow along the western and eastern sides of the model, since it is a type 2 – no flow boundary. This could be problematic when delineating capture zones because reverse particles that encounter this no flow boundary will travel along the boundary until they exit through a type 1 boundary or until they reach the ground surface.

Therefore, a modified conceptual model was established that takes into account regional flow all around the model domain through a layer at the bottom of the model along its lateral boundaries.

The boundary conditions were altered by applying a type 1 - constant head boundary around the perimeter of the model domain [Figure 14b] in the lowest hydrostratigraphic layer [

Figure 15]. This will allow reverse particles that travel into the lowest hydrostratigraphic layer a way to exit the domain through the regional flow regime.

The head values used for the type 1 – constant head boundary were obtained from the regional scale Waterloo Moraine model (Sousa et al., 2010). The boundary nodes from the Alder Creek model did not coincide exactly with the nodes from the Waterloo Moraine model, therefore interpolation of head values was required. To obtain the constant hydraulic head values, each perimeter node in the Alder Creek model was matched with the six closest Waterloo Moraine nodes. At that point the head value for that perimeter node was linearly interpolated based on the distance from each of those nodes.

The perimeter of the remaining hydrostratigraphic layers were left to the default setting which was a type 2 – no flow boundary. This acts as a symmetry boundary/groundwater divide for the local and intermediate groundwater flow regime. With the modified boundary conditions set, the model was run until steady-state conditions were reached with a few minor adjustments to the unsaturated zone material properties settings which are discussed in greater detail in Section 5.6.

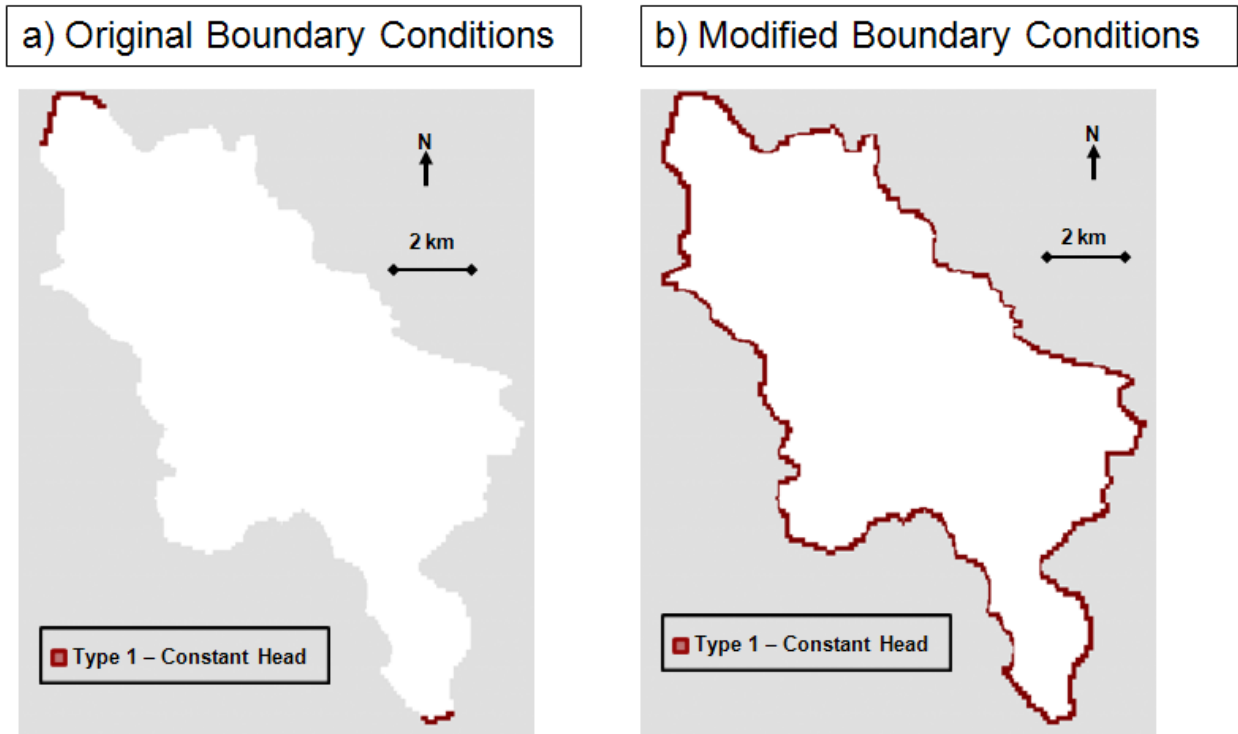


Figure 14: Boundary Conditions: (a) Original vs. (b) Modified Conceptual Model

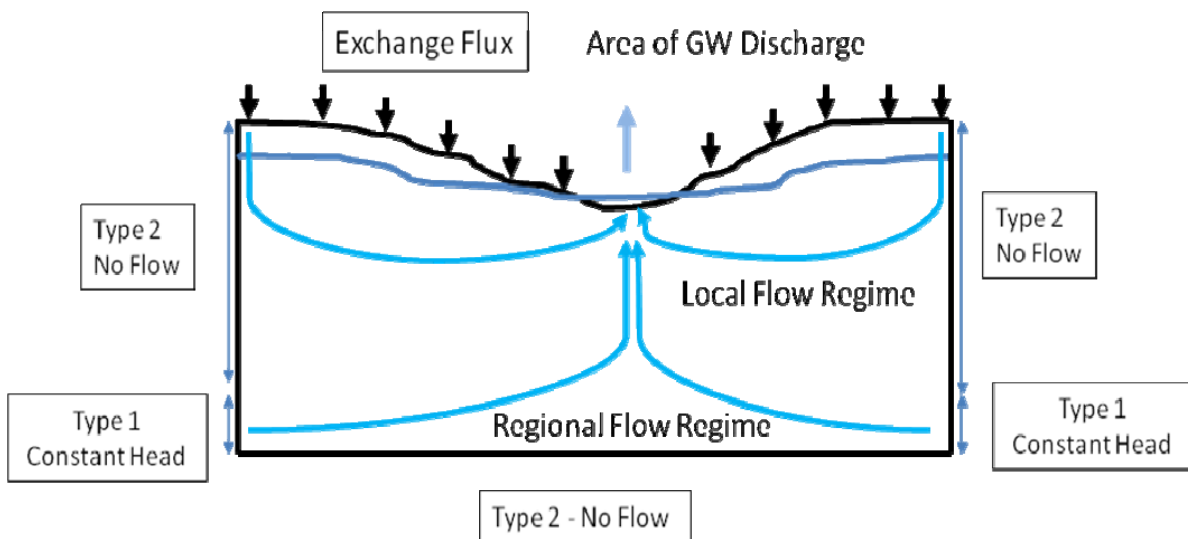


Figure 15: Boundary Conditions for Modified Conceptual Model

5.2 Finite Difference Discretization

The finite difference domain for Modflow was discretized horizontally with 26 083 active cells per layer [Figure 16]. The grid was refined horizontally in the location of pumping wells. Initially, a 25 layer Visual Modflow model from the University of Waterloo groundwater modelling research group with heterogeneous isotropic hydraulic conductivities was tested, revealing some instabilities.

Therefore, it was decided to simplify the grid by assigning one cell layer per hydrostratigraphic layer, thus converting the 25 layer model into a 7 layer model [Figure 16]. The layers were merged by grouping layers with similar hydraulic conductivities to form hydrostratigraphic layers. After the hydrostratigraphic layers were identified, the horizontal hydraulic conductivities were merged by using the arithmetic mean and vertical hydraulic conductivities were merged using the harmonic mean. This led to a heterogeneous anisotropic hydraulic conductivity distribution and produced a total of 182,581 cells in the whole model domain.

It is important to note that the cross-section depicted in Figure 16 is only one snapshot of the layer thicknesses and that the layers vary in thickness throughout the domain. The thickness in the layers depends on the hydrostratigraphic divides between the aquifer and aquitard units which were interpreted from the Waterloo Moraine conceptual model, as discussed in Section 4.2. In some areas the layers can be very thin while in other areas the layers are thicker.

In Visual Modflow, the perimeter cells for the bottom layer (Layer 7) were set to Type 1 constant head values to represent the regional flow regime. The rest of the perimeter cells from layers 1 to 6 were not set with any specific boundary condition and were therefore by default Type 2 – no flow boundary conditions.

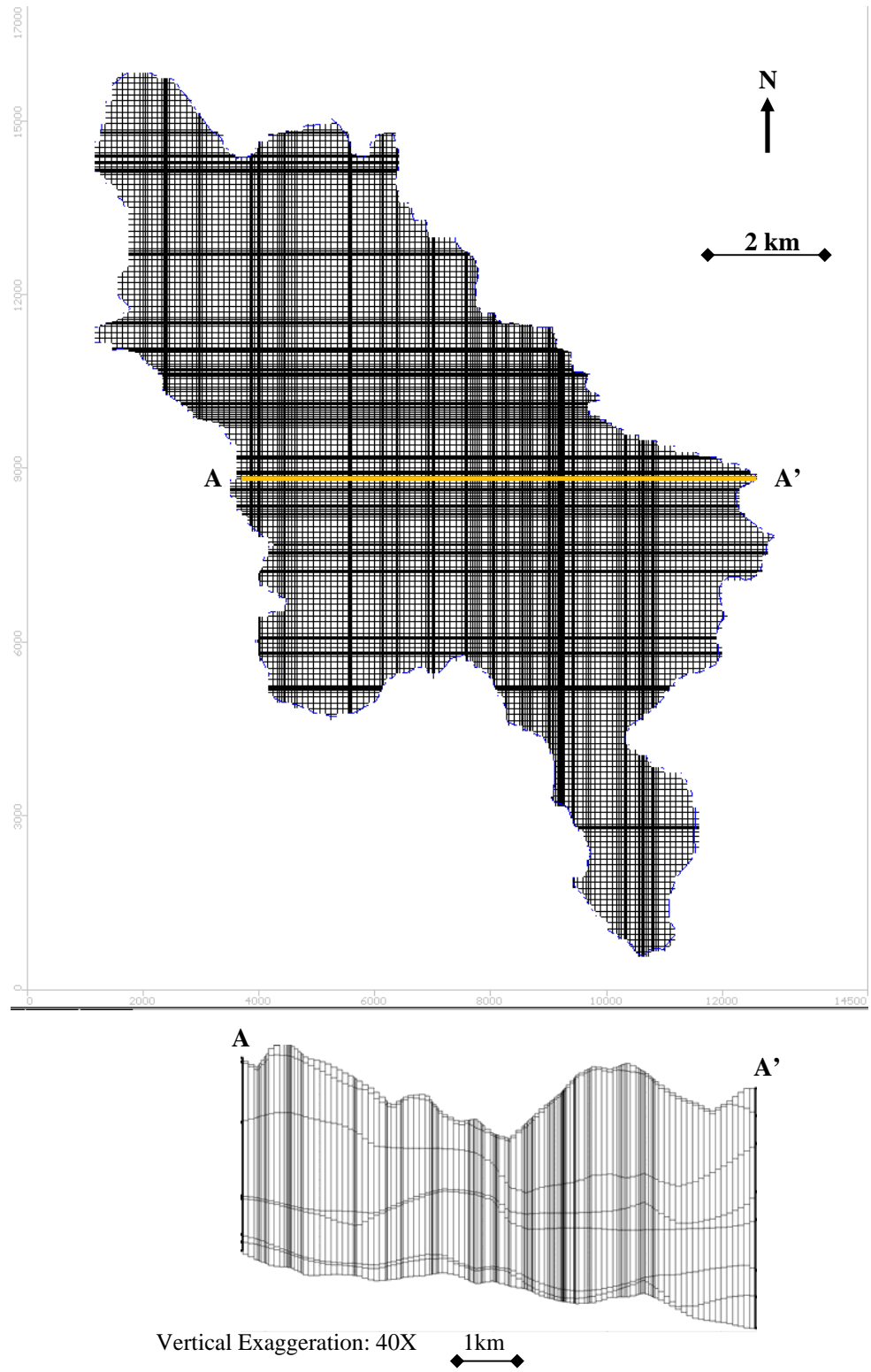


Figure 16: Alder Creek Watershed Visual Modflow Discretization

5.3 Finite Element Discretization

Both Watflow and HGS use triangular prismatic finite elements for their discretization of modelling domains, so the finite element grids for the Alder Creek watershed used for Watflow and HGS are the same. Each nodal layer contains 7216 nodes and 13844 elements [Figure 17]. The finite element grid was refined at well locations (pumping and observation wells) and along Alder Creek.

The model domain is vertically discretized into 87 elemental layers and 88 nodal layers. The first meter below ground surface is discretized with ten 10 cm layers, the next 19 meters with fifty-seven 33 cm layers and the final 20 meters to bedrock with 20 evenly distributed layers. Thus the model domain contains a total of 635008 nodes and a total of 1204428 elements. The high resolution discretization in the top part of the model domain was designed to investigate surface water and unsaturated zone processes in a study published by Jones et al. (2009).

To compare the results of the models it was necessary to be consistent with the boundary conditions for each model. The vertical discretization for the finite element mesh is much finer than for the Visual Modflow grid. For this reason the bottom 2 layers, which is the thickness of the bottom hydrostratigraphic layer, are assigned a Type 1 - constant head boundary. The remaining layers were not assigned specific boundary conditions, leaving the boundary to the default setting in Watflow and HGS which is a Type 2 – No Flow boundary.

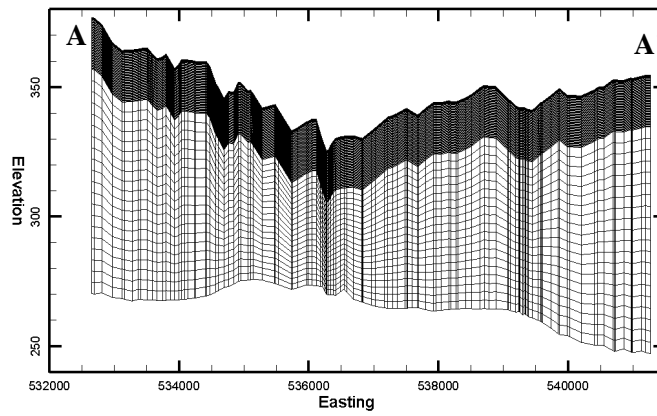
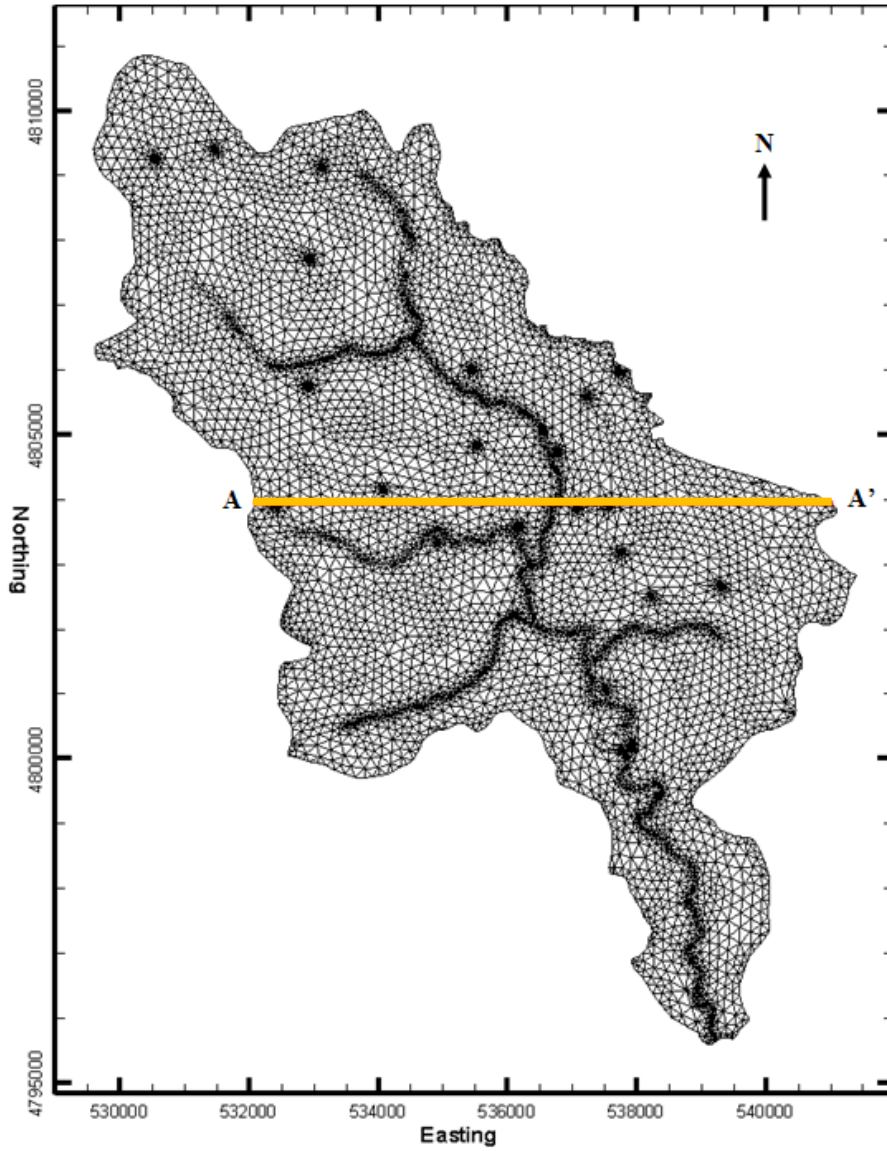


Figure 17: Alder Creek Watershed Watflow and HGS Discretization

5.4 Differences in Discretization

To make a fair comparison between the models it was necessary to keep the model discretization as similar as possible. Inherently there are big differences when comparing a finite difference model (Visual Modflow) with a finite element model (Watflow or HGS). Also, the Modflow model covers only the saturated zone below the water table, while the finite element models include the unsaturated zone. Another major difference between the two grids is that the Visual Modflow grid is significantly coarser in the vertical direction compared to the Watflow and HGS grid for the Alder Creek Watershed. The Visual Modflow grid has only 7 layers (one layer for each hydrostratigraphic layer) while the Watflow/HGS grid is comprised of 87 layers (very fine discretization in the unsaturated zone). Initially an attempt was made to have the same number of layers in the Visual Modflow model as the finite element models, however the model encountered problems converging to a solution. Visual Modflow has been notorious for having convergence problems when faced with too many layers.

Visual Modflow's main problem when it comes to having too many layers is that cells that are close to the ground surface that are variably saturated are seen either as wet (activated) or dry (inactivated). During simulations dry cells can be rewetted with a rewetting module contained in Visual Modflow, but this can still cause convergence issues. Brunner et al. (2010) notes that:

in principle, an aquifer can be modeled as one single layer. In many cases, this is a convenient setup because no or few cells dry out as a consequence of a dropping water table during the simulation. Dry cells cause convergence problems and once a cell has fallen dry it remains dry unless actively reactivated for example, by the rewetting package in Visual Modflow.

This is a typical example of how the model dictates the physics. In other words, the conceptual model has to be modified in order to function within the limits of the model's capability.

This explains the coarsening of the layering in the Visual Modflow model close to the ground surface. Although the model would be capable of handling more layering lower in the model domain, all layers were coarsened based on the logic that each layer in the model would be representing a hydrostratigraphic layer.

5.5 Exchange Flux Distribution

The exchange flux is the amount of water that flows through the ground surface; it is possible for the exchange flux to be positive for water that exfiltrates to the surface and negative for water that enters the subsurface. The exchange flux is different from groundwater recharge because it takes into account travel through the unsaturated zone. Thus, how the different groundwater models represent the unsaturated zone is important when applying the exchange flux to ground surface.

HydroGeoSphere computes the exchange flux values over the entire modelling domain. This exchange flux was applied to Modflow and Watflow. No other surface water models were tested since this study approaches capture zone delineation from the groundwater perspective. It should be noted however, that surface water modules are now available for Modflow, but were not used in this study.

Visual Modflow applies the exchange flux to the upper-most active layer; therefore exchange flux and groundwater recharge are equivalent in Visual Modflow. In Watflow the unsaturated zone is approximated using a linearized approximation, therefore the exchange flux must travel through the unsaturated zone before reaching the water table as groundwater recharge. In HGS the exchange flux travels through unsaturated zone before it becomes groundwater recharge. The unsaturated zone parameters such as saturation and hydraulic conductivity are approximated as function of pressure head using van Genuchten parameterization (van Genuchten, 1980). Figure 18 depicts how the unsaturated zones are depicted in HydroGeoSphere, Watflow and Visual Modflow.

Exchange flux is a critical boundary condition that can be difficult to quantify. Fortunately in our model comparison we used the exchange flux distribution produced by a steady-state HydroGeoSphere model of the Alder Creek watershed. HydroGeoSphere is able to quantify areas within the Alder Creek modelling domain where streams are gaining (groundwater discharge) and where streams are losing (groundwater recharge) at steady-state. This information is crucial for the capture zone delineation of streams. In order to delineate a capture zone, there must be a groundwater sink involved. Therefore areas where groundwater discharges into streams (gaining streams) must be identified.

In Visual Modflow, recharge is applied to each individual cell in the uppermost active layer (at the water table). Therefore the variability of the recharge distribution depends on the horizontal discretization of the model domain. Since the horizontal discretization differs considerably between HGS and Modflow, some file conversion was required in applying the HGS exchange flux in Modflow. Visual Modflow is only capable of reading a specific file format for recharge known as a polygon shapefile. Polygon shapefiles can be created in GIS software known as ARC Map.

To convert HGS exchange flux values into a file format that Visual Modflow could read required a few steps. First the centroid of each HGS element was found by taking the average of the three xy-coordinates that make up an element. The centroid was then assigned the exchange flux for the element. These point exchange flux values were then converted into a point shapefile in ARC Map. This file was then converted into a polygon shapefile using the Thiessen Polygons Tool in ARC Map. Figure 19 depicts the process of turning HGS point recharge values into recharge polygons that can be read by Visual Modflow. Visual Modflow would then take the polygon value closest to the centre of the rectangular cell as the value for the exchange flux.

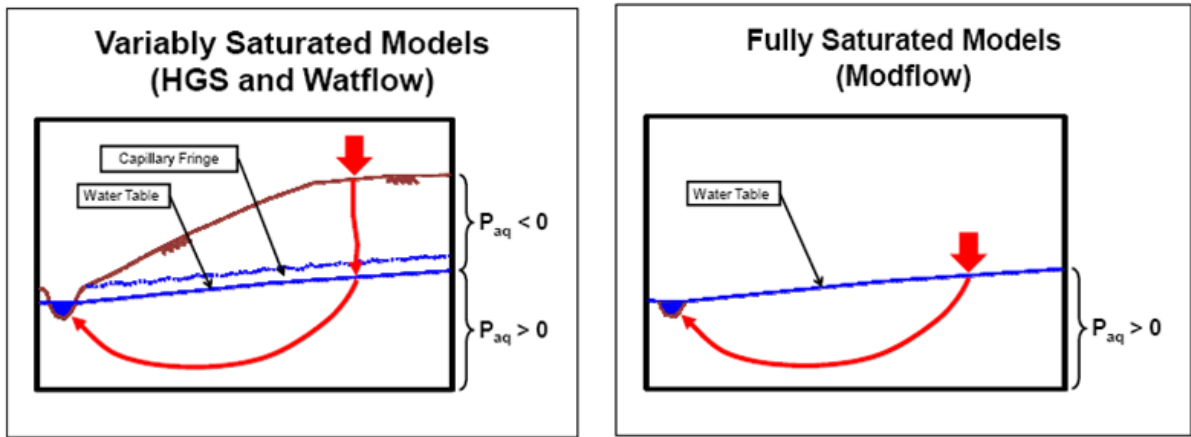


Figure 18: Depiction of Unsaturated Zone Representation in Different Models (from Sousa et al., 2010)

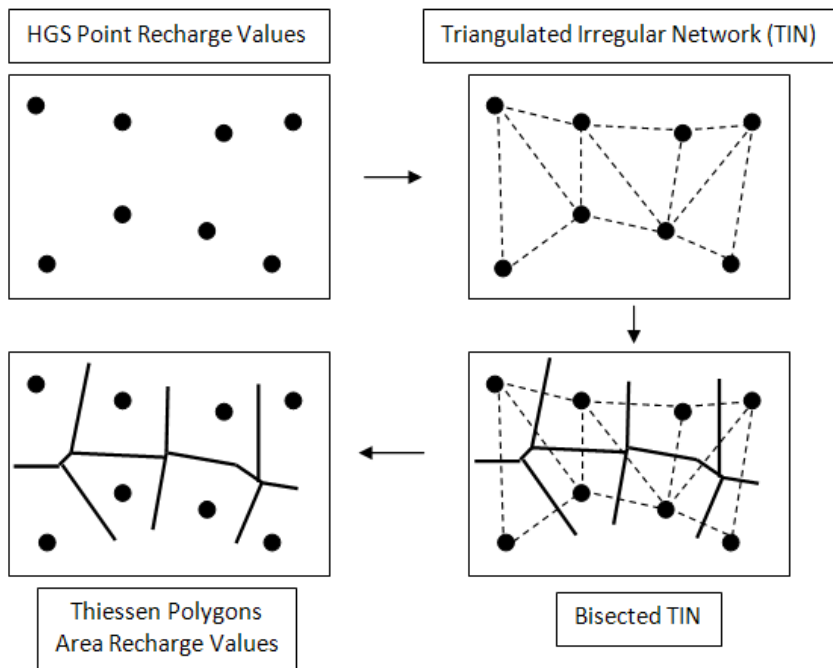


Figure 19: Changing HGS Point Recharge Values to Area Recharge Values for Modflow

5.6 Boundary Conditions

Both conceptual models discussed in Section 5.1 account for regional flow, but in different ways. They represent two scenarios interpreting the same physical flow system. Because the boundary conditions differ, it can be expected that the exchange fluxes generated from HydroGeoSphere would differ also.

Figure 20 depicts the exchange fluxes corresponding to the two scenarios.

Because HydroGeoSphere accounts for unsaturated flow in a rigorous way, convergence problems can occur with coarse-grained materials having a steep saturation-pressure curve. This type of problem was encountered with the modified boundary conditions; it was solved by replacing the unsaturated material properties for coarse sand and gravel with those of a medium sand.

Some stream reaches that were gaining according to the original boundary conditions became losing under the modified boundary conditions. The areas in red and orange are gaining stream segments and the areas in blue and green are where the exchange flux is entering the subsurface. The most noticeable change occurred in the northern stream reaches of the Alder Creek where a segment of stream dries up. This highlights the fact that the exchange fluxes calculated in HydroGeoSphere for rivers and streams, which is critical information for stream capture zone delineation, is highly sensitive to boundary conditions chosen in the model.

Both boundary conditions based on the differing conceptual models produce acceptable results, therefore it requires judgment to decide which conceptual model to choose. The stream levels in the Alder Creek watershed are known to fluctuate seasonally, some of which dry up in the summer. Therefore, the exchange flux generated by the modified boundary conditions was deemed reasonable and is the one used in the model comparison.

After the exchange flux was determined in HydroGeoSphere, this flux was applied to the surfaces of the Modflow and Watflow models. By applying the same boundary conditions and exchange fluxes to all three models, we should expect to generate similar flow fields in the three models. All three models have high head levels (approximately 360-370 meters) at the northwest edge of the model domain and both have low head levels (approximately 300-310 meters) at the southeast edge of the model domain. All three models show a general groundwater flow from northwest to southeast [Figure 21] which corresponds well with Section 4.3 which discussed groundwater flow direction. The hydraulic head contours for Modflow and Watflow are very similar. Hydrogeosphere shows more variability in the head levels, representing the topographic relief more accurately compared to the other two models, this is because it includes more physical processes.

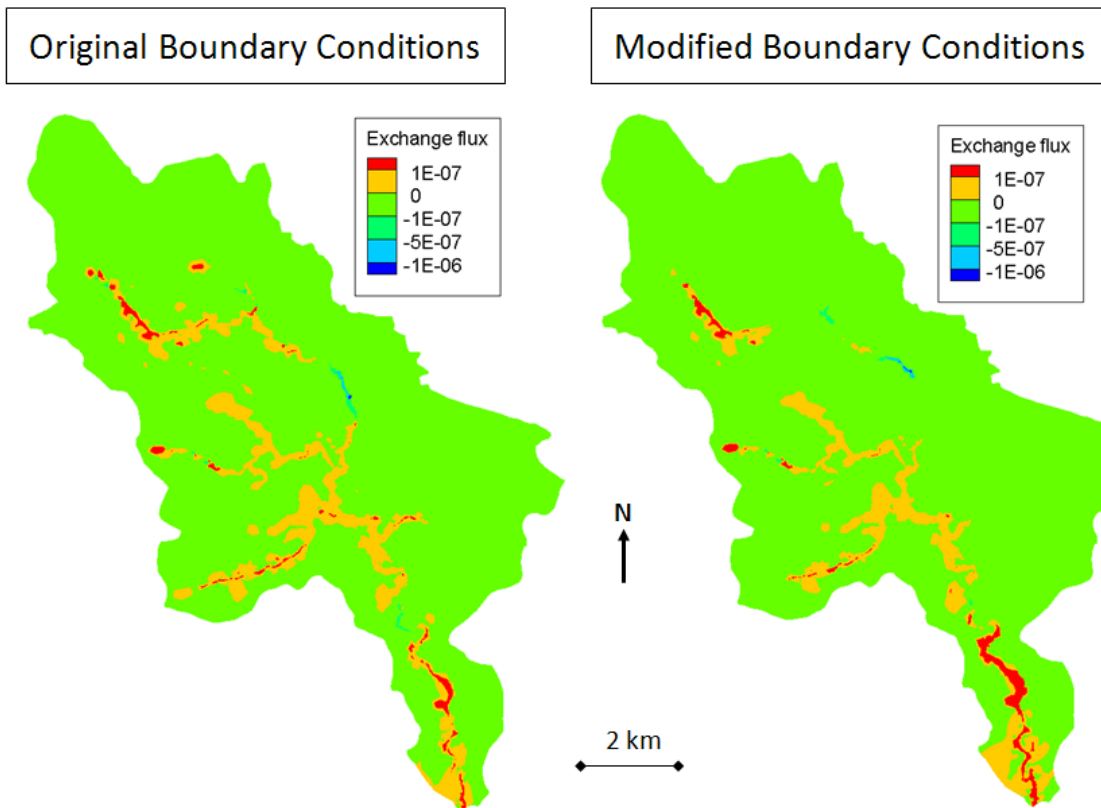


Figure 20: HydroGeoSphere Exchange Flux

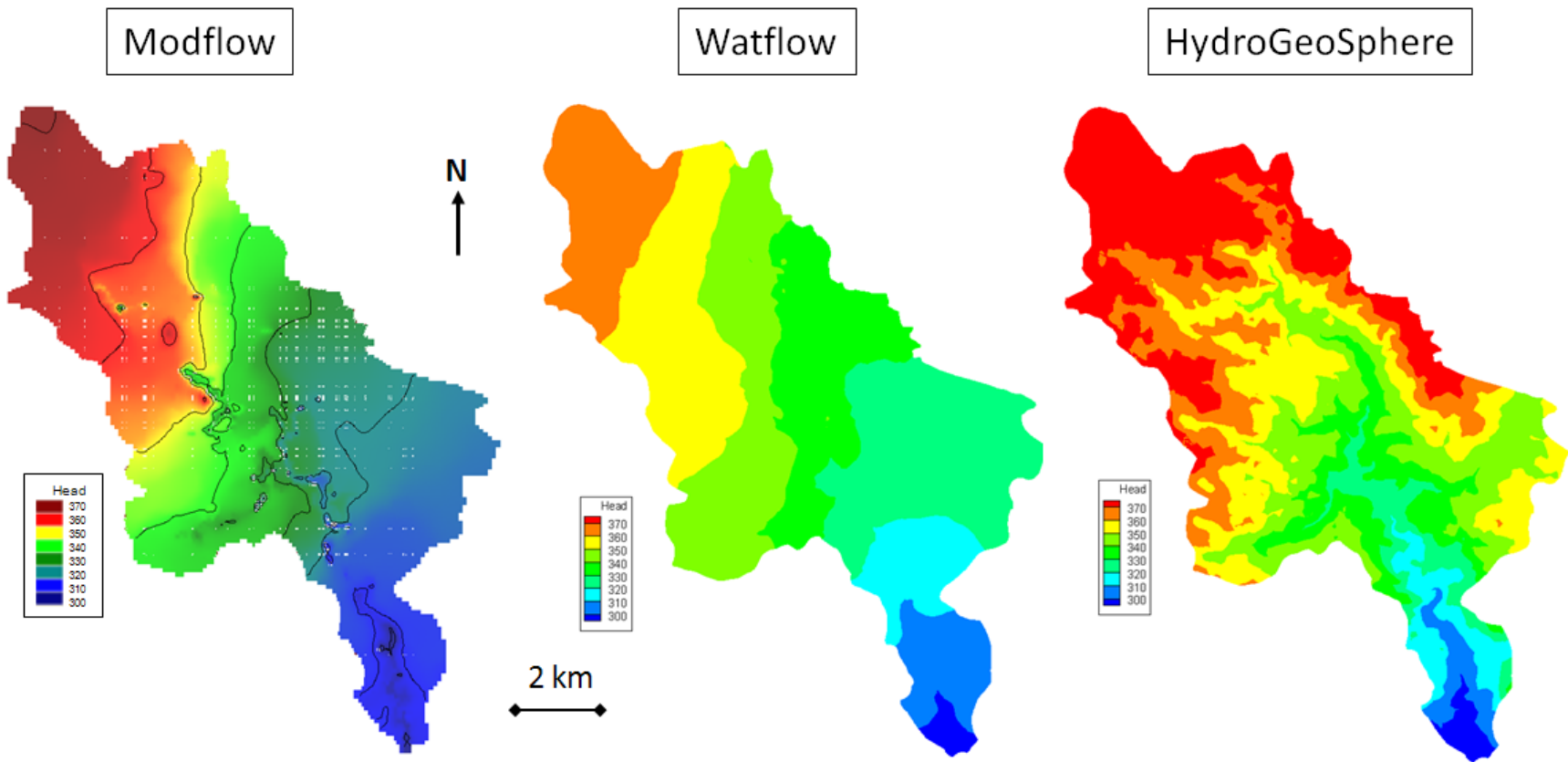


Figure 21: Hydraulic Head in Aquifer 1 with Original Calibration

5.7 Model Calibration

The original Alder Creek model was calibrated by Jones et al. (2009), who made a number of manual adjustments to the hydraulic conductivity distribution until a satisfactory fit between the calculated and observed heads was achieved. For the present study, the boundary conditions and exchange fluxes were modified to be compatible with the modified conceptual model. Although the original calibration appeared acceptable with the new boundary conditions, recalibration was considered.

With both Modflow and Watflow, calibration is straightforward since each has its own autocalibration routine. Modflow is linked to a calibration program called WinPEST (Schlumberger Water Services, 2007), while Watflow has its own auto-calibration routine (Beckers, 2001), which is built into the Watflow program. Therefore these models were recalibrated. HydroGeoSphere does not have a calibration routine and therefore could not be calibrated any further. The resulting calibration plots and the corresponding calibration statistics are shown in Figure 22.

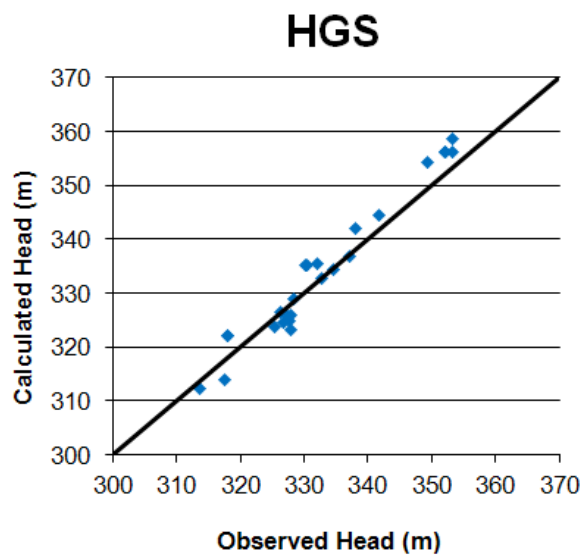
It is important to note that what is acceptable is subject to professional judgment and in no way is calibration sufficient proof of validity. Modflow and Watflow models were calibrated by adjusting the hydraulic conductivity fields within an order of magnitude in an attempt to match calculated head values to observed head values.

The difference between the calculated head and observed head is known as the residual. The calibration process seeks to minimize the residuals within the modelling domain. The mean error represents the mean of all the residuals and provides an indication of whether residuals are biased positive or negative. This parameter can be misleading because large negative residuals can be masked by large positive residuals and vice versa. The mean absolute error represents the magnitude of the residuals, which better represents mean error within the modelling domain. This parameter does not have the problem of opposing residuals cancelling each other out, conversely it does not

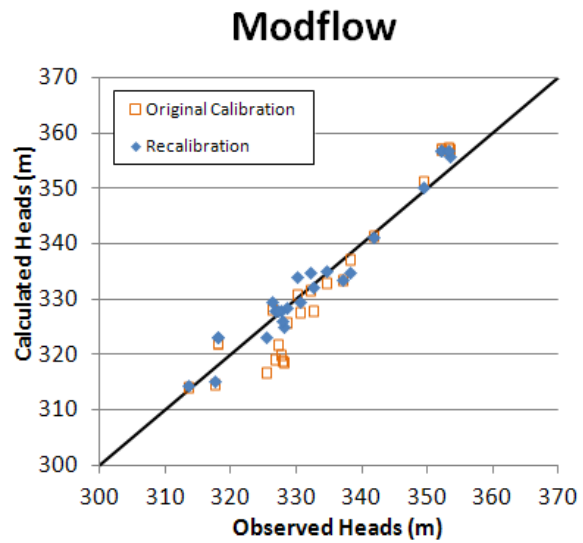
provide information on the overall trend of under-calculated or over-calculated heads. Therefore, it is important to analyze both statistics to gain better insight of the model precision.

After recalibrating the Modflow model with WinPEST, the absolute residual mean decreased from 3.9m to 2.3m, the average residual mean went from being -1.4m to 0.9m and the standard deviation decreased from 4.6 to 2.8. After using Watflow's autocalibration routine to recalibrate the model, the absolute residual mean decreased from 2.2m to 1.5m, the average residual mean went from being 1.7m to 0.2m and the standard deviation decreased from 2.6 to 1.8.

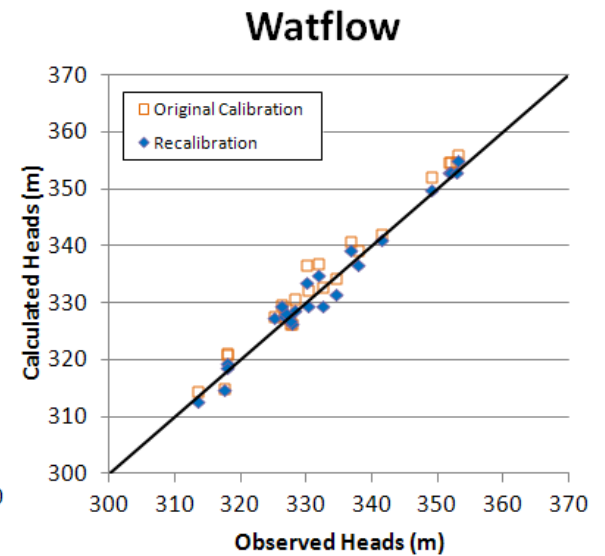
Figure 22 displays the original calibration and recalibration plots for Modflow and Watflow. Three observation wells (WM2-93B/1, AC5B-01B/1, and WM9-93C/1) were removed as objective functions for the recalibration of these models, because they were close to inactive extraction wells and boundaries. The middle of the modelling domain had the most observed head values to recalibrate the model to; therefore this part is taken to be better calibrated than the northern and southern parts.



Calibration Statistics	
Mean Error	1.56m
Absolute Error	2.85m
Standard Dev.	3.07



Calibration Statistics		
	Original	Recalib.
Mean Error	-1.40m	0.89m
Absolute Error	3.93m	2.33m
Standard Dev.	4.64	2.75



Calibration Statistics		
	Original	Recalib.
Mean Error	1.7m	0.2m
Absolute Error	2.2m	1.5m
Standard Dev.	2.6	1.8

Figure 22: Model Calibration Plots

After recalibrating Modflow and Watflow, the flow fields were compared again [Figure 23]. The hydraulic head elevation in Modflow seemed reasonable after calibration. However, the hydraulic head elevation in Watflow did not seem reasonable. The recalibration in Watflow caused the hydraulic head elevation to drop by approximately 10 meters in the northern end of the domain, which would cause a considerable change in the groundwater velocities throughout this region. Because of this noticeable head drop it was decided that the flow field in Watflow before recalibration would be a more reasonable approximation of reality. The calibration statistics before using the auto calibration routine were also deemed acceptable.

Problems with calibration show that retrieving head values from a larger model to be used as boundary conditions on a smaller model within it can be problematic. This should not be done if significant changes in flow conditions occur. Changing the exchange flux represents a change in flow conditions and in this case a drop in head in the Watflow model. Ideally, the Waterloo Moraine model would be revisited; however, this was impractical. Hence, the capture zones in Watflow were delineated using the flow field that existed before running the autocalibration routine. The much greater detail in the head distribution for the HydroGeoSphere simulation are thought to be due to the integrated form of the surface water flow mechanics, as well as the exact representation of unsaturated flow processes. The effects of the calibration on the capture zones are investigated in Section 6.4. This will illustrate the sensitivity of capture zones delineation with respect to calibration.

Table 5 shows the water budgets for the three models in terms of inflows and outflows at the constant head boundaries, the wells, and the recharge flux at the top boundary (exchange flux). Watflow does not provide separate in/out values for the recharge, but it does show the net recharge (in-out). The table shows that the net water balance is zero for each model, as required for a steady-state flow model. If the net exchange flux for Watflow is corrected by the difference in the pumping rates between Watflow and HGS ($-0.14E-01 \text{ m}^3/\text{s}$), then the corrected value agrees with the net exchange flux for HGS, which it should, as both have been generated by HGS. The exchange fluxes

for Modflow have also been generated by HGS, but they are slightly different due to the remapping required to match the different grid type.

Table 5: Model Water Budgets

	Modflow			Watflow			HGS		
	In (m ³ /s)	Out (m ³ /s)	Net (m ³ /s)	In (m ³ /s)	Out (m ³ /s)	Net (m ³ /s)	In (m ³ /s)	Out (m ³ /s)	Net (m ³ /s)
Constant Head	1.24E+00	-1.18E+00	5.59E-02	2.94E-01	-2.31E-01	6.31E-02	2.69E-01	-2.07E-01	6.17E-02
Wells	0	-1.91E-01	-1.91E-01	0	-1.91E-01	-1.91E-01	0	-2.05E-01	-2.05E-01
Recharge	5.18E-01	-3.83E-01	1.35E-01	N/A	N/A	1.28E-01	5.13E-01	-3.69E-01	1.43E-01
Total	1.76E+00	-1.76E+00	0	N/A	N/A	0	7.82E-01	-7.82E-01	0

At the constant head boundaries, the in/out values differ slightly between Watflow and HGS, which is explained by the different solution approaches for the finite element equations for these two models. The main difference in the mass balances occurs in the constant head boundaries for Modflow, which has about five times as much water flowing in/out at these boundaries than either HGS or Watflow. Since the hydraulic conductivity fields are approximately the same for all three models, this means that the velocity in the Modflow model must be significantly higher than in the other models in the parts of the model affected by the constant head boundaries. This applies mainly to the bottom layer in Modflow, which has a constant head boundary all around. The large volumes of water passing through the constant head boundaries in the Modflow model will require further investigation.

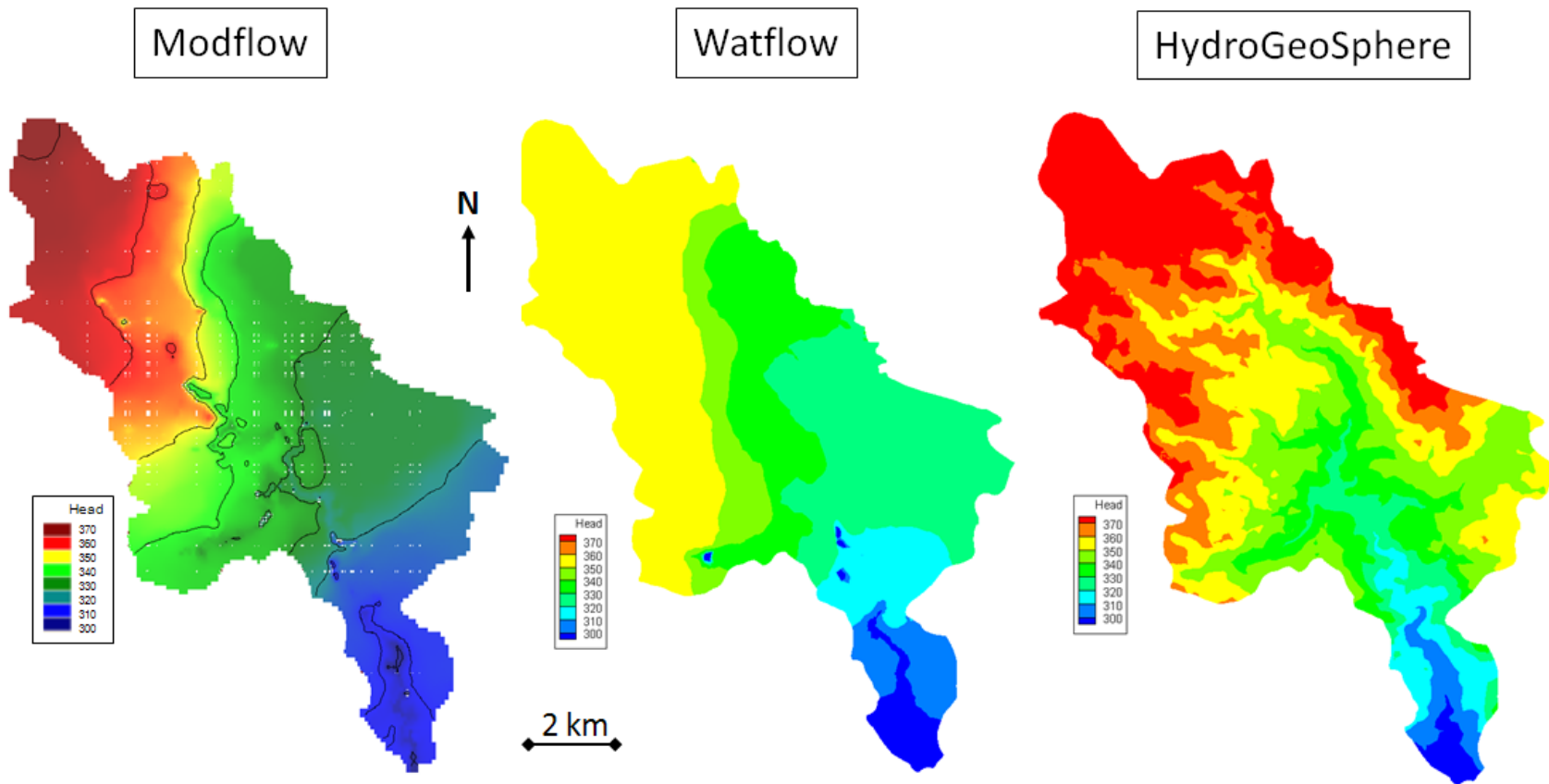


Figure 23: Hydraulic Head in Aquifer 1 After Recalibration

Chapter 6

Capture Zone Delineation for Alder Creek

6.1 Selecting Stream Segments for Capture Zone Delineation

Two main criteria must be satisfied when choosing an appropriate segment of stream within a watershed to perform capture zone analyses. Firstly, the stream needs to be a gaining stream on average (for a steady-state model). In other words, the stream has to be a groundwater sink. Secondly, the stream needs to be a sufficient distance away from any model boundaries, so that the boundary conditions would not overly influence the capture zone results.

Three stream segments were chosen for capture zone delineation. Two are in the center of the model domain located approximately 7.4 km upstream from the discharge outlet. This area is thought to be well calibrated as discussed in Section 5.7. Furthermore, this area is farthest from the modelling domain boundaries. Because of these reasons it would be prudent to choose two stream reaches in this area to see if similar results are obtained. Figure 24 depicts the two segments which are defined as mid-stream segments #1 and #2. The third reach is located at the northern end of the modelling domain and is defined as the upper stream segment #3. Two subsections of the Alder Creek watershed were selected around the chosen stream sections to help improve the efficiency and runtimes for reverse transport simulations. The two subsections are referred to as Reverse Transport Area #1 and #2 in Figure 24. Flow information within the selected subsections were generated by using a pre-processing program called *ptrans*, which is a FORTRAN program developed by Professor John Molson from Laval University in Quebec City, Quebec.

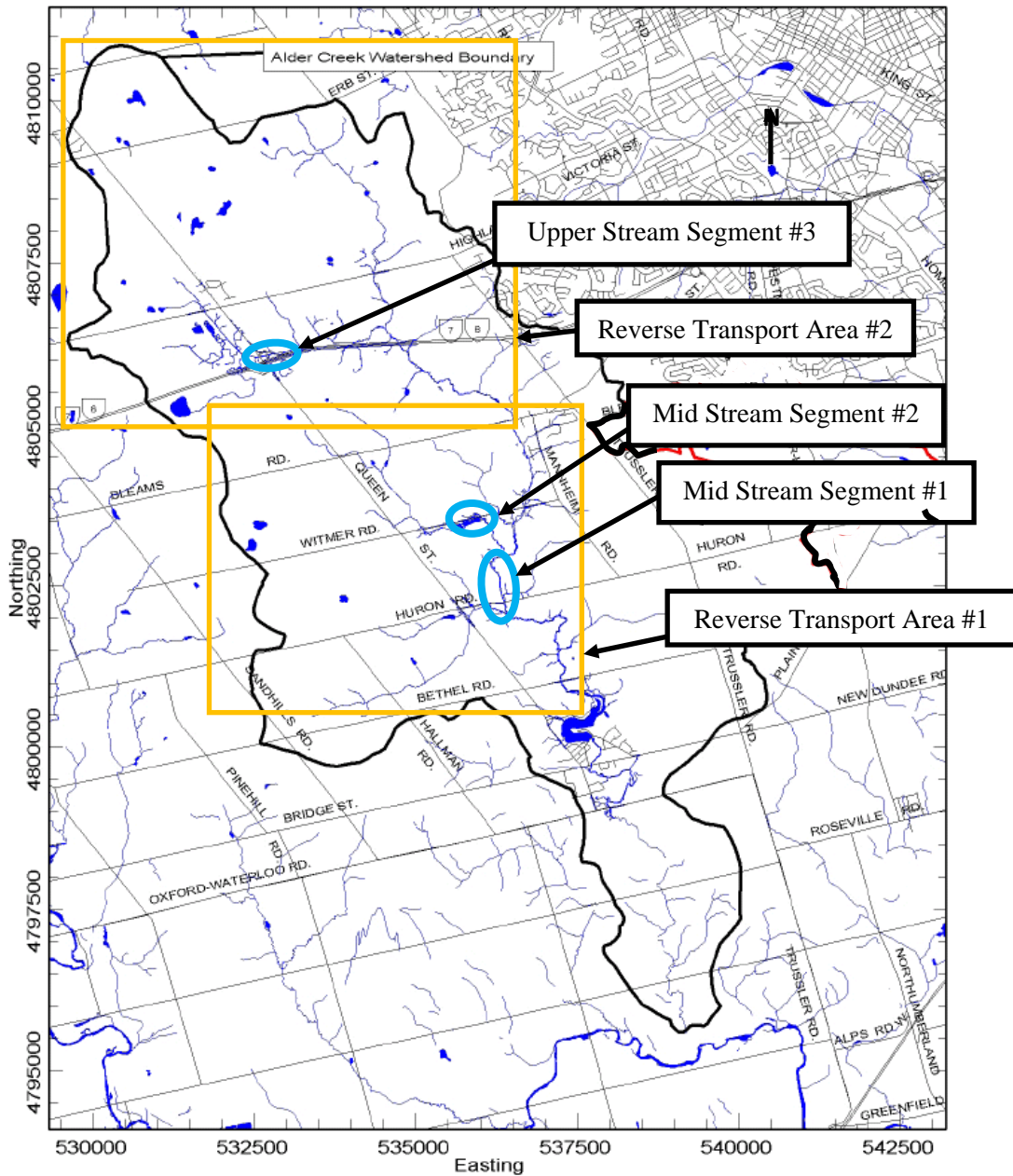


Figure 24: Alder Creek Watershed Depicting Stream Segments for Capture Zone Delineation and Subsections for Reverse Transport (from CH2MHILL and North-South Environmental Inc., 2008)

6.2 Capture Zones from Particle Tracking

Figure 25 shows an example of the initial particle placement for Mid-Stream Segment #1 in Visual Modflow and the finite element models. The number of particles placed within a particular stream reach was based on the number that could fit within the stream reach. The particles in Visual Modflow, Watflow and HydroGeoSphere are within the first layer of the model. Vertical particle placement can cause slight changes to the capture zone delineated. Due to differences in the vertical discretization the initial particle positions for Visual Modflow and the finite element models will be slightly different. Tests showed that the differences between the initial particle positions from Visual Modflow to the finite element models will not cause a significant difference in the capture zones delineated.

Although the modelling of the Alder Creek watershed was completed in three dimensions, the following capture zones are plan view representations of the particle tracks projected in the horizontal plane and run until steady-state [Figure 26, 27 and 28].

Figure 26 depicts the capture zones delineated for mid-stream segment #1. 150 particles were released from the initial position, taking approximately 700 years for the particles to reach steady state. The particles reach steady state when there is no longer any change in their position over time. However, for mid-stream segment #1 less than 4% of the particles continued to move after 300 years. The similarities in the capture zones for all three models are that they extend to the west. HydroGeoSphere and Watflow capture zones appear to be similar, both extend straight west, with the Watflow capture zone extending the farthest west and deviating northwards. Comparing Modflow and Watflow, both capture zones have the same general shape, however the Modflow capture zone extends more to the northwest than the other two models. With all three models, the westerly migration of the particles takes place mostly in the bottom layer.

For mid-stream segment #2, 200 particles were released from the initial position, taking approximately 400 years for the particles to reach steady-state [Figure 27]. The capture zones delineated from mid-stream segment #2, which is just north of the first stream reach, shows a significant difference across the three models. The only similarity between the three capture zones is that they all extend in the same general direction. All three differ in shape and size. In Modflow the capture zone extends to the northwest and has one stray particle that travels along the western edge of the model. In Watflow the capture zone is significantly smaller and extends to the west of the stream segment. HydroGeoSphere creates a capture zone somewhere in between the two models. The HydroGeoSphere capture zone extends farther west than the Watflow capture zone, but does not extend as far north as the Modflow capture zone.

From choosing two stream reaches in close proximity from one another we can see drastically different results. In mid-stream segment #1 [Figure 26] we can see that the capture zones are comparable. All three extend in the same general direction. In particular, the sizes of the capture zones in Modflow and Watflow are very similar, however the capture zone tip in Modflow extends approximately 1 km farther to the north. In this case one may conclude that the choice between groundwater models for stream capture zone delineation is not important since they produce similar results. By going a step further and choosing another stream reach in close proximity to the first we can see that the capture zones can differ greatly from one model to another. In mid-stream segment #2 we can see that differences in the capture zones are more pronounced and that there is little predictability in how the capture zones will form depending on the model chosen.

Finally, capture zones were delineated in upper stream segment #3 by releasing 180 particles from the initial position, taking approximately 100 years for the particles to reach steady state [Figure 28]. This area that did not have many calibration points and is considered to be a poorly calibrated area. There are a few similarities between the capture zones. They all extend in the same direction,

encompassing the same southwest area that HydroGeoSphere delineated. Also, the sizes of the capture zones are similar in Watflow and HydroGeoSphere. The Watflow capture zone extends a bit further to the north than the HydroGeoSphere capture zone.

The Modflow capture zone extends farther to the north than the Watflow capture zone and also has a number of particles that extend directly northwest from the particle source area, splitting the particle tracks into two parts. If the area enclosed is considered as the capture zone, then it makes for a very big capture zone with considerable uncertainty. The particles that extend to the west from the source end up travelling north along the boundary. This is due to the Type 2 no flow boundary that represents the intermediate and local groundwater divide. In reality the particles would likely travel further west beyond the boundary of the modelling domain.

In all three models the cross-sections show that the particles travel deep into the model domain, passing through several hydrostratigraphic layers. The cross-section for upper-stream segment #3 in Watflow and HydroGeoSphere showed fewer particles penetrating deeper into the lower hydrostratigraphic layers. There is no clear pattern for particles travelling through any specific hydrostratigraphic layers when comparing the cross sections from the models.

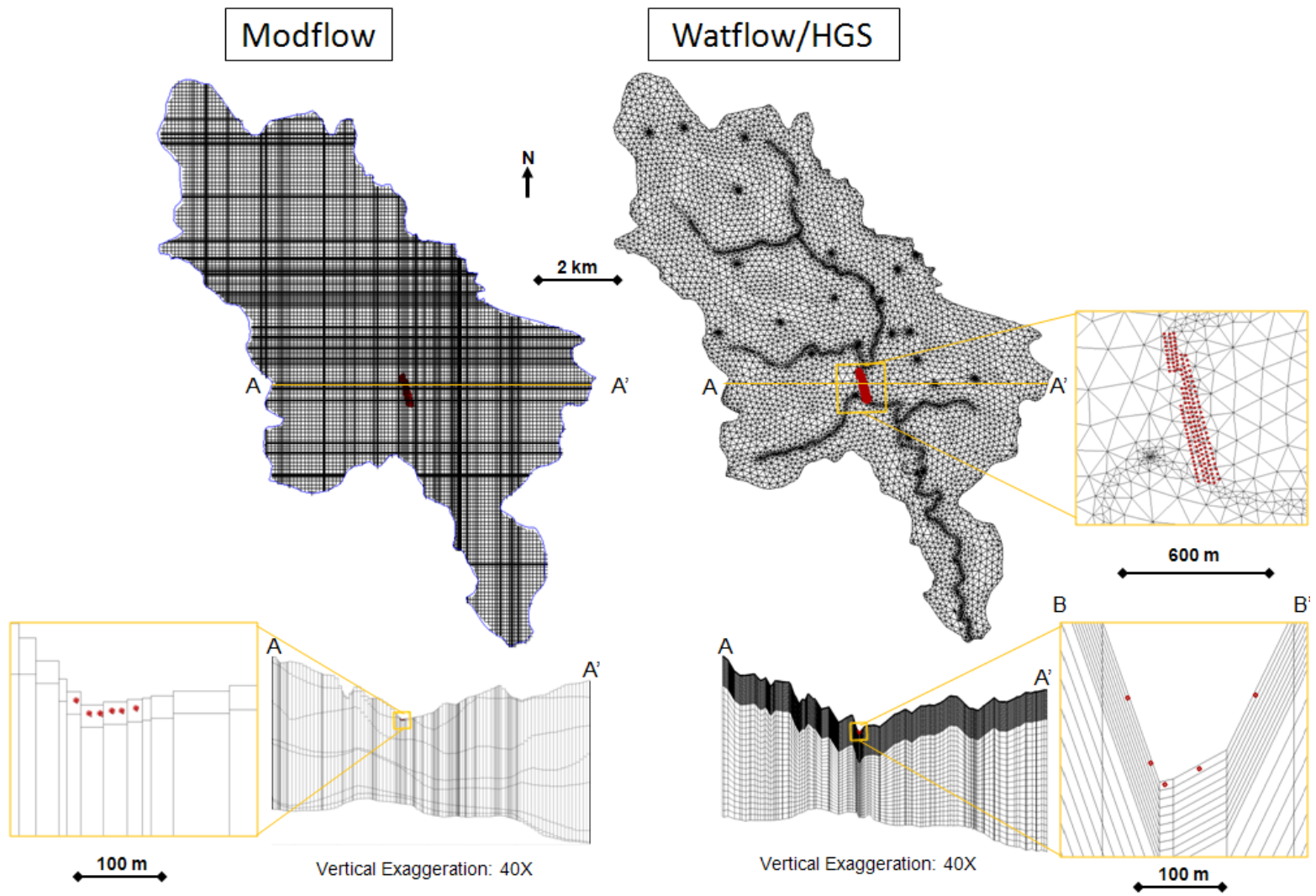


Figure 25: Initial Particle Placement for Mid-Stream Segment #1

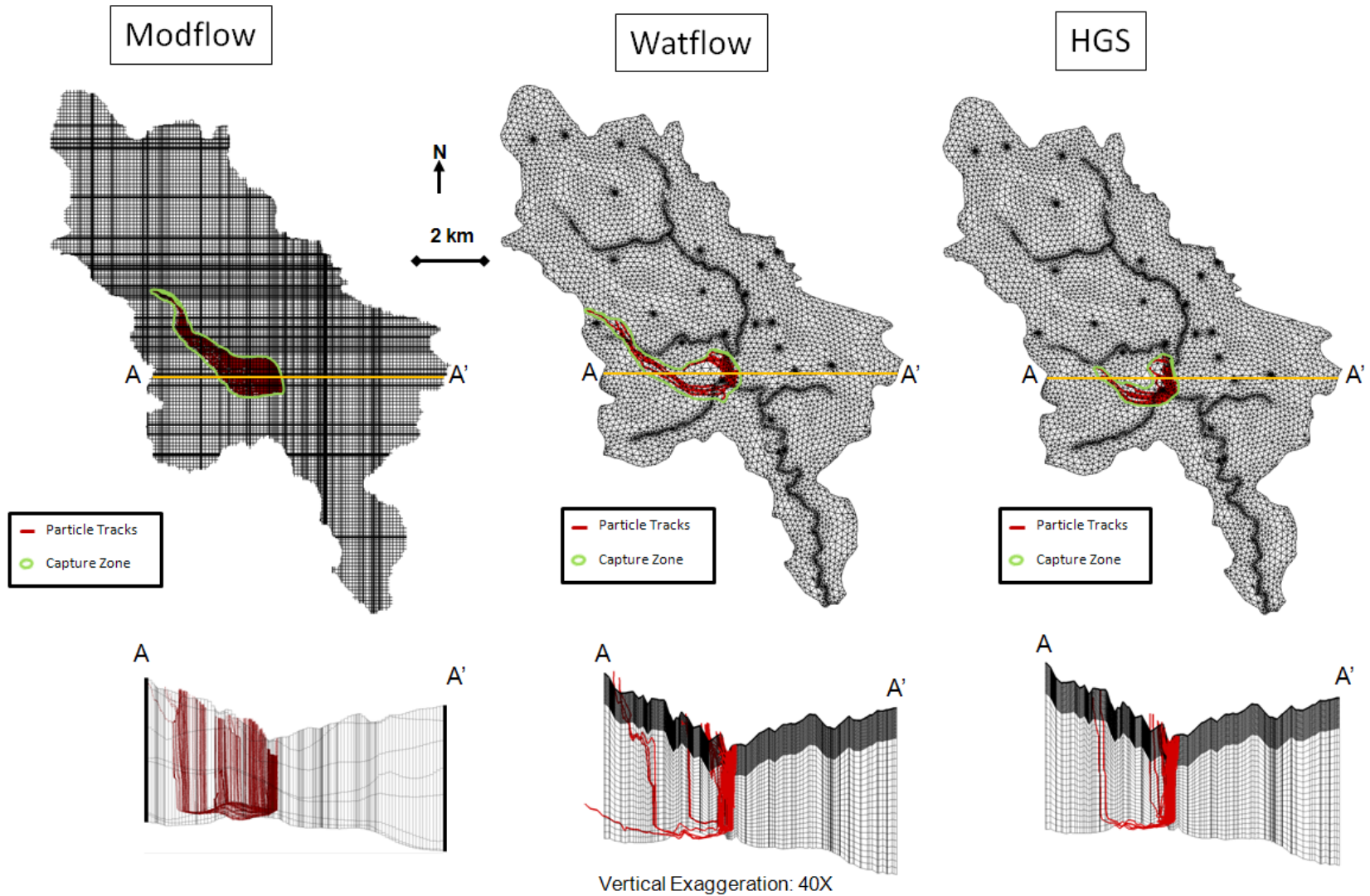


Figure 26: Reverse Particle Track Capture Zones for Mid-Stream Segment #1

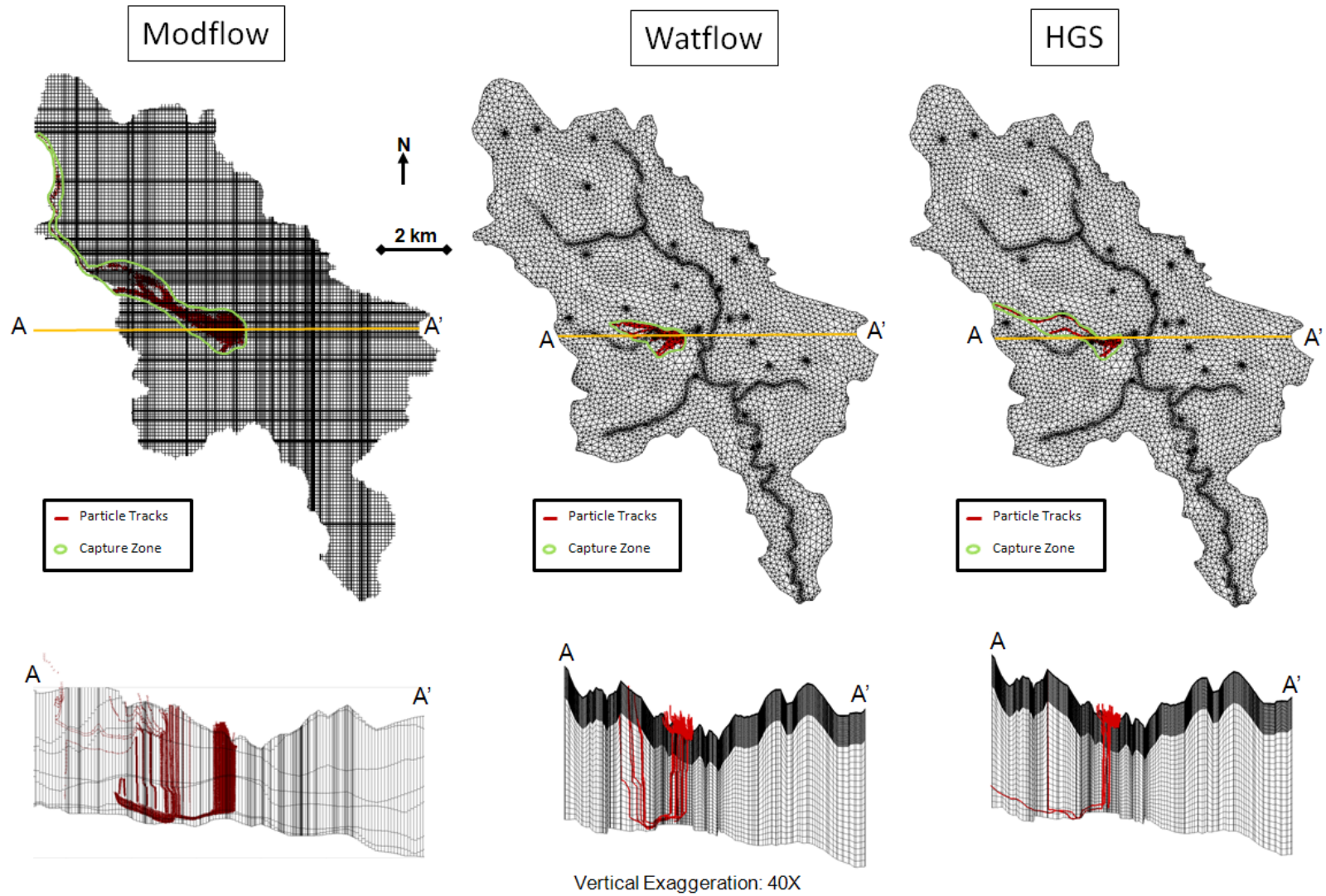


Figure 27: Reverse Particle Track Capture Zones for Mid-Stream Segment #2

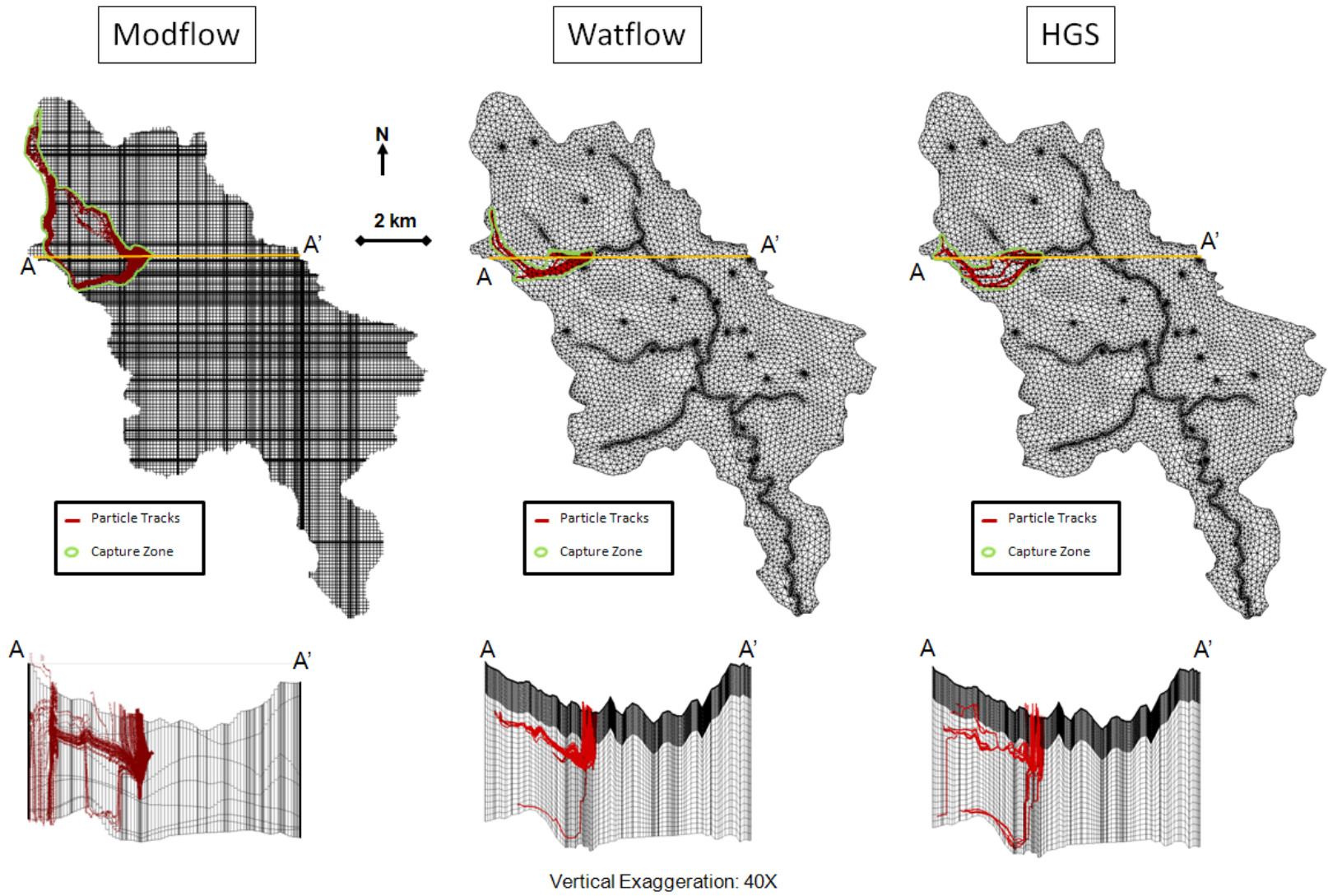


Figure 28: Reverse Particle Track Capture Zones for Upper-Stream Segment #3

6.3 Implications from Reverse Particle Tracking

In all three models the capture zones extend in the same general direction, however they differ significantly in size and shape. For stream segments #2 and #3, the Modflow capture zone extends farther than with either of the other models. The main reason that the Modflow capture zones are different from the HGS and Watflow capture zones are due to differences in discretization, hydraulic conductivity distribution and the way the unsaturated zone is represented in the models. In the Visual Modflow model there is significantly less resolution in terms of vertical discretization (7 layers) compared to the Watflow and HydroGeoSphere model (87 layers). A possible reason for the greater length of the Modflow capture zones for stream segments #2 and #3, could be the proximity to the constant head boundary. As shown in Table 5, the constant head boundary in the Modflow seems to generate large rates of inflow/outflow resulting in locally high velocities.

An important concept to note is that the finite difference and finite element models should converge to the same answer as the discretization becomes finer horizontally and vertically. With a finer grid comes greater accuracy in the numerical solution (Pinder and Frind, 1972). The HydroGeoSphere and Watflow results should be more accurate than the Modflow results, because the flexible discretization scheme in finite elements allows for a more efficient refinement of the discretization in critical areas.

Another significant factor that contributes to the differences in the capture zones is that Modflow is calibrated with a different hydraulic conductivity distribution which in turn would lead to differences in the hydraulic head distribution. To compare different models it is important to use the model the same way it would be used in practice.

The differences in hydraulic conductivity shed light on an important aspect of groundwater modelling and the inherent problem of non-uniqueness. There are an infinite number of possible combinations in hydraulic conductivity that could produce acceptable calibration results; each one of

these solutions could in theory produce different capture zones. It is difficult to know which one is the most valid. In this case further refinement in the understanding of the hydrogeological setting is required to constrain the possible calibration parameters. This means more boreholes and more monitoring wells need to be installed in the study area, as well as the hydrogeological testing (i.e. permeameter, slug and pumping test) necessary to better characterize the study area. Filling in these information gaps could help produce a more physically based model that is more representative of the natural system.

From comparing the capture zones created by Watflow and HydroGeoSphere we can see that there are differences in shape and size of the capture zones. They both generally extend in the same direction. In this case the discretization, hydraulic conductivities and boundary conditions are the same. The only differences lie in the ways the models treat the unsaturated zone and that HydroGeoSphere takes into account surface water processes while Watflow does not. HydroGeoSphere has a rigorous formulation of the unsaturated zone, while Watflow has a simplified linearized representation of the unsaturated zone.

When comparing Modflow to the finite element models it becomes less obvious what factors are contributing to the differences we see in the capture zones. Therefore, it becomes clear that the capture zones are quite sensitive to unsaturated zone representation and surface water processes. By adding Modflow to the comparison we can see that capture zones are also sensitive to differences in discretization and hydraulic conductivity distributions. The comparison also shows that capture zones can be sensitive to differences in the boundary conditions and to the way the various boundary conditions are handled in each model. It would be interesting in future studies to quantify the sensitivity of capture zones to these differences.

Another important thing to note is that the impact of numerical errors in capture zone calculations will also depend on the magnitude of the hydraulic gradient. This is a factor that is not

model specific, but would be encountered by any groundwater model in general. In the case of an extraction well, the induced gradients near the well are normally larger than the natural gradients, meaning that numerical errors may be less consequential. On the other hand, natural hydraulic gradients occurring within and next to streams are much more gradual, sometimes changing only a metre over a kilometre. Hence, numerical and calibration errors may be the same order of magnitude as the hydraulic gradient being calculated. Therefore, capture zone delineation for stream base flow contribution areas are expected to be more sensitive to numerical errors and uncertainty than well capture zone delineation. In addition, because natural gradients may decline with distance, uncertainty in the stream capture zone may increase with distance from the stream.

6.4 Comparison of Watflow Capture Zones: Before and After Calibration

Calibration of groundwater models by varying hydraulic conductivity to match calculated head values to observed head values is standard practice when producing a defensible groundwater model. For this reason it takes professional judgment to determine whether the flow field reasonably represents the conceptual model.

Watflow was calibrated with its own calibration routine, however after recalibration it was found that the new flow field seemed unreasonable when compared with the flow fields from Modflow and HGS. Also, when comparing it with historical groundwater flow data, as discussed in Section 5.4, the flow field before calibration was more comparable. It could be argued that Watflow was over-calibrated to match observed values mainly concentrated in the central area, and as a consequence the flow field in the northern section of the domain was no longer representative. The observation points in the northern section of the domain were removed as objective functions. This is because the extraction wells in that area were inactivated due to their proximity to the boundary, as discussed in Section 5.1.

In Figure 29 and Figure 30 we can see for Mid-Stream Reach #1 and #2 respectively, that after recalibration the capture zone does not extend as far north, reducing the size of the capture zone. Also, the cross-sections show that fewer particles penetrate through the hydrostratigraphic layers after calibration. In Figure 31 for Upper-Stream Reach #3 the opposite is true. After recalibration the capture zone extends further north, reaching the northern edge of the model domain. This causes a dramatic increase in the capture zone size. These results show that the capture zones can be highly sensitive to differences due to calibration. In this case, the flow field after recalibration in the northern section is not considered representative; therefore, the capture zones after recalibration are not reliable.

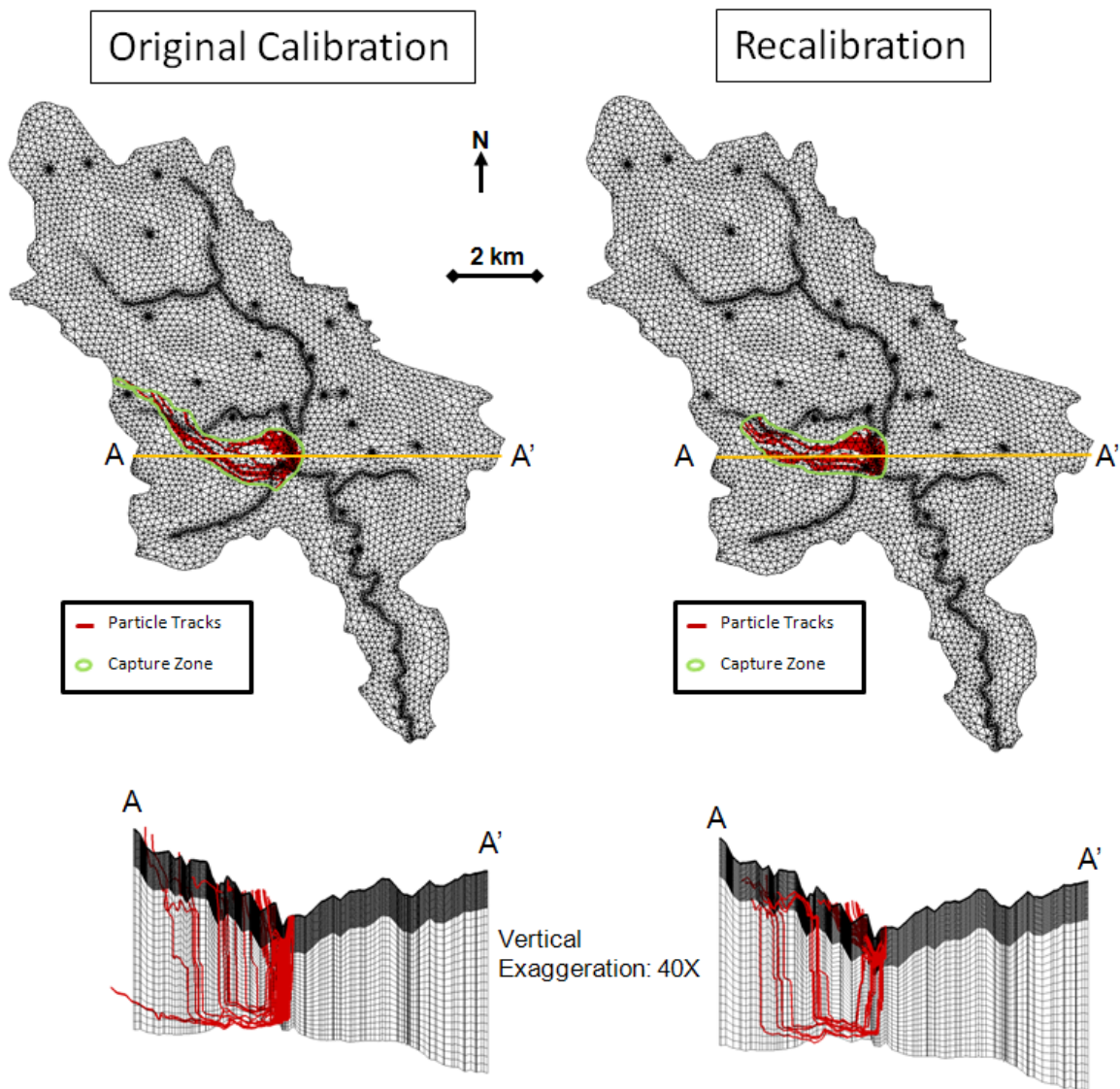


Figure 29: Watflow Capture Zones for Mid-Stream Segment #1: Original Calibration and Recalibration

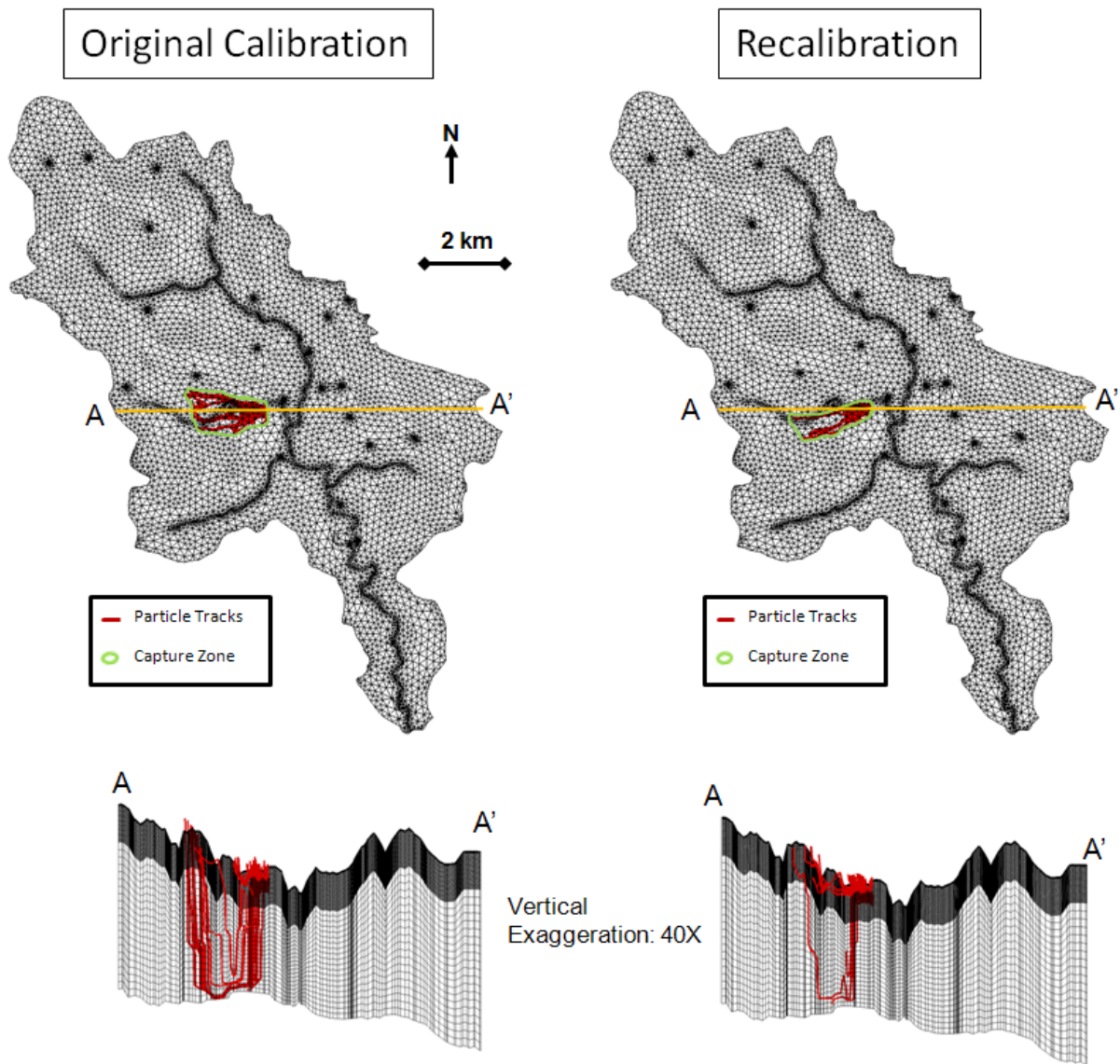


Figure 30: Watflow Capture Zones for Mid-Stream Segment #2: Original Calibration and Recalibration

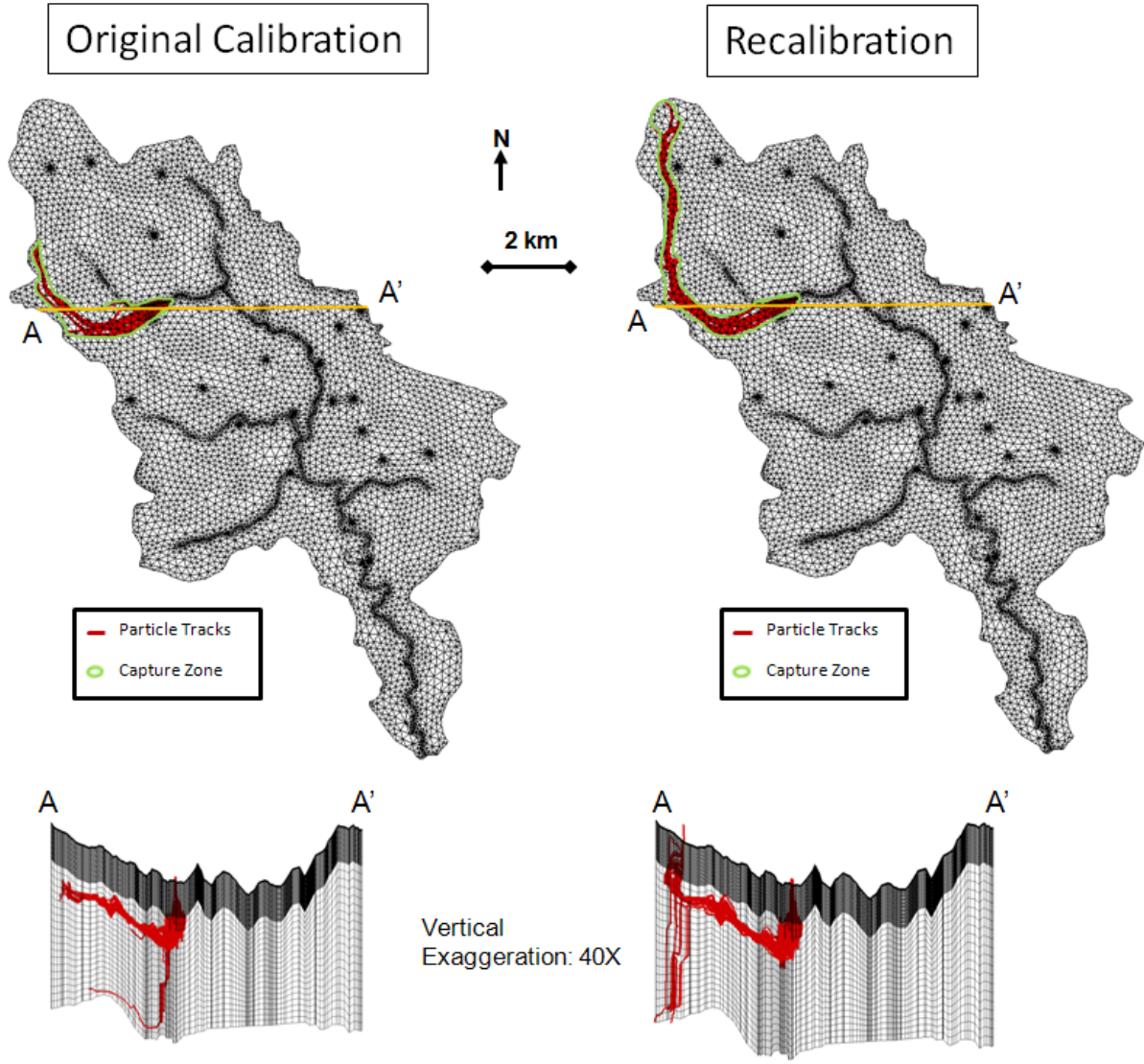


Figure 31: Watflow Capture Zones for Upper-Stream Segment #3: Original Calibration and Recalibration

6.5 Capture Zones from Reverse Transport

The model WTC has been applied to generate the capture probability plumes for the three stream segments. The model uses the hydraulic head distribution from Watflow (original calibration). For the reverse transport runs, the finite element nodes under the streambed are set to a specified probability of $P=1.0$. Figure 32 shows the position of these boundary nodes for Mid-Stream Segment #1 (See enlargement to the right of grid and cross-section). Longitudinal dispersivity was set to 20 m, transverse dispersivity was set to 5 m and transverse vertical dispersivity was set to 0.02 m. Diffusion was set to $1.0E-10 \text{ m}^2/\text{s}$.

Reverse transport was run to 300 years for all three stream segments, since changes beyond a few 100 years would not be relevant for practical purposes. Figure 33 shows the growth of the capture probability plume for the mid-stream segment #1 from 1 year up to 250 years, while Figure 34 shows the pseudo steady-state 300 year capture probability plume with the 300 year particle tracks superimposed in magenta. The peak concentration in 3D is projected to the surface with the 0.5 contour highlighted by a dark black line. The capture probability plume grows with the advance in time in the opposite direction of groundwater flow. At 50 years the 0.01 probability contour begins extending towards the west. At 100 years the 0.01 probability contour extends further west and slightly to the north. From 100 to 300 years the probability plume continues to extend to the west. At 300 years the 0.01 contour is approximately half a km from the boundary and the 0.5 contour has moved about half a km to the west.

The capture probability plume extends in the same direction as the reverse particle tracks [Figure 34], however we can see that the capture zone delineated by the particle tracks extends into the low probability contours depicted in light blue and blue (0.01 to 0.3). Only 5 of 150 particle tracks (less than 4% of the particles) extend to the west beyond 0.1 capture probability contour, the vast majority of the particles can be found within the 0.5 probability contour.

Figure 35 shows the growth of the capture probability plume that originates from mid-stream segment #2 from 1 year up to 250 years. Figure 36 superimposes the pseudo steady-state 300 year capture probability plume with the 300 year particle tracks superimposed in magenta. At 50 years the 0.5 to 0.9 probability contours extend southward, while the 0.01 probability contour starts to extend to the northwest. From 100 to 300 years we can see that the 0.5 to 0.9 probability contours extend approximately 0.75 km to the south and staying relatively close to the source area. The 0.01 to 0.5 probability contours extend further northwest until encountering the boundary of the model domain.

From examining Figure 36 we can see that the probability capture zone and the reverse particle tracks coincide with each other very well. Only 2 of the 200 particle tracks (1% of the particles) extend past the 0.5 probability contour. For this plume there is a dense network of particles that seem to agree well with the 0.5 contour which was a trend noticed by Frind et al. (2002) after delineating capture zones by particle tracking and reverse transport for an extraction well.

Figure 37 shows the growth of the capture probability plume that originates from upper-stream segment #3 from year 1 up to 250 years. The particle tracking results in Section 6.2 showed that steady state was being reached at approximately 100 years, for this reason the 100 year particle tracks will be superimposed in magenta, on the 100 year capture probability plume shown in Figure 38. At 50 years the 0.01 probability contour depicted in light blue, extends to the west until it encounters the boundary where it starts to travel northwards along it. From 100 to 250 years the 0.01 probability contour does not change much in size or shape indicating that the probability plume has reached steady state and that it is likely exiting through the deeper regional flow system in the north. The 0.5 probability contour extends to the southwest by approximately 0.25 km, while the 0.9 probability contour never extends from the source.

In Figure 38 we can see that the capture probability plume and the reverse particle tracks coincide with each other well. The particles extend in a narrow path that never expands wider than the

0.3 probability contour. Approximately 60 particles out of the 180 (33% of the particles) extend beyond the 0.5 probability contour. This is significantly more particles extending beyond the 0.5 probability contour than the previous two stream segments. The particle tracks extend all the way into the 0.01 probability contour following the same northwest path.

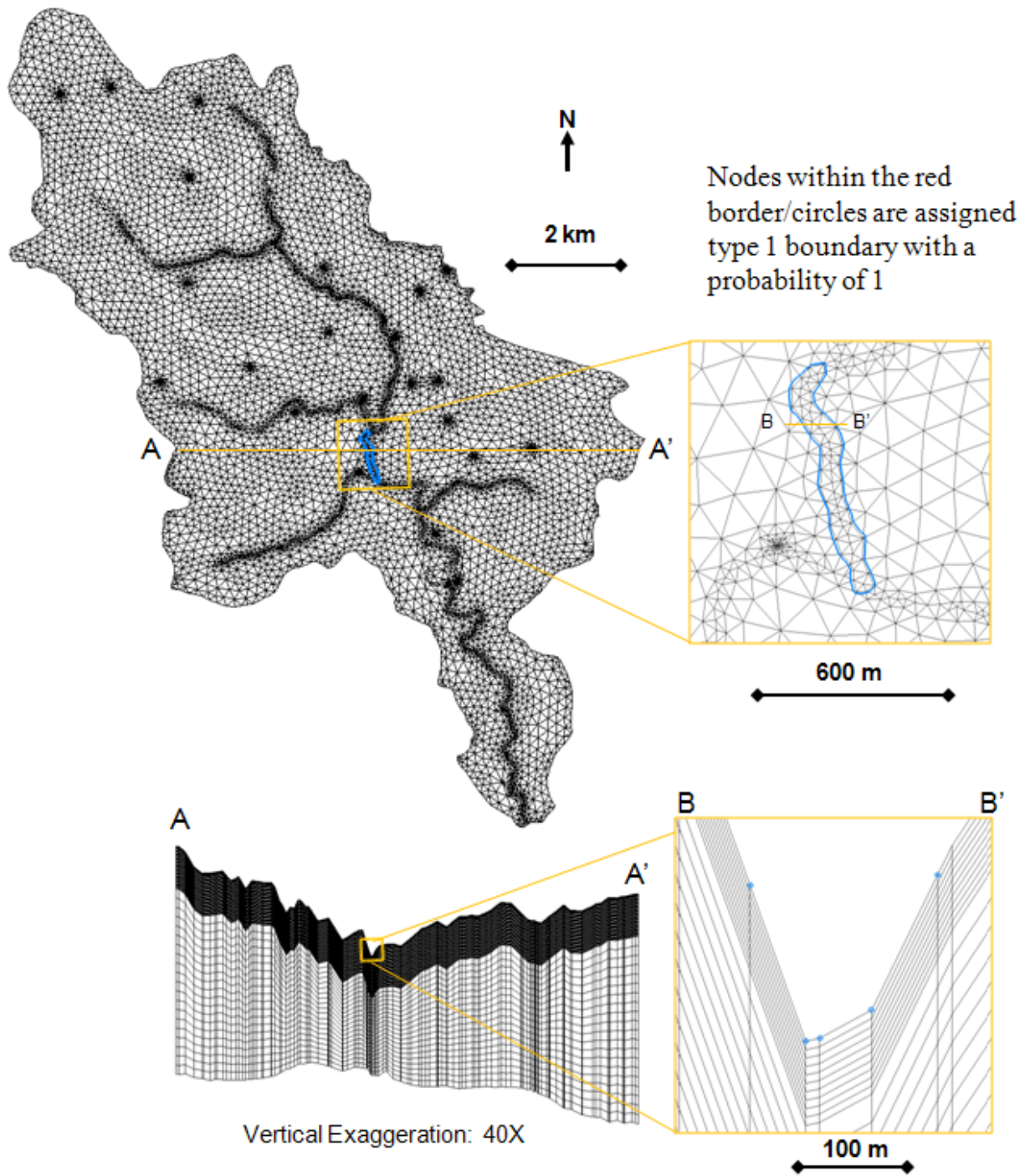


Figure 32: Initial Probability Placement for Mid-Stream Segment #1

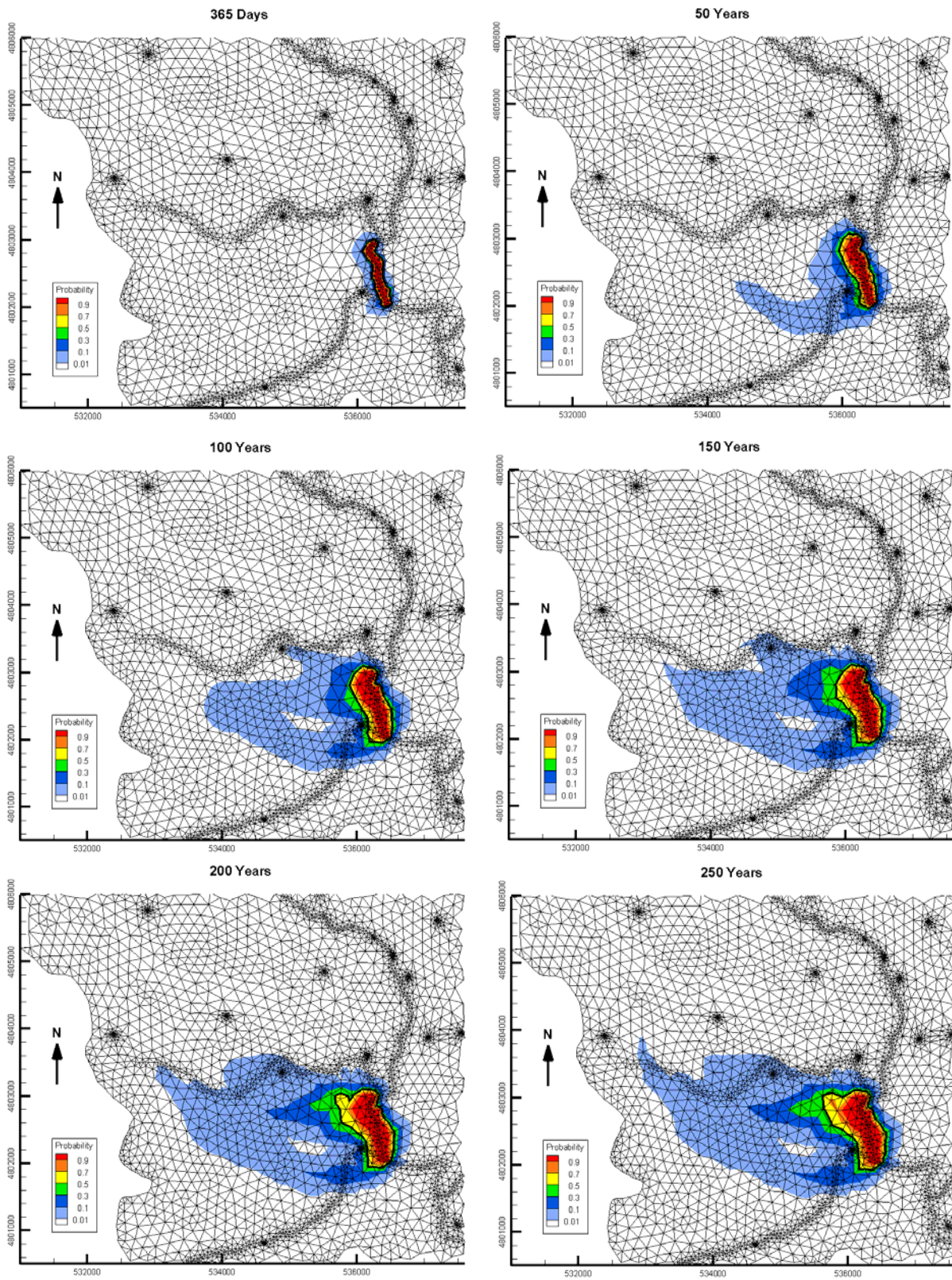


Figure 33: Growth of Capture Probability Plume for Mid-Stream Segment #1

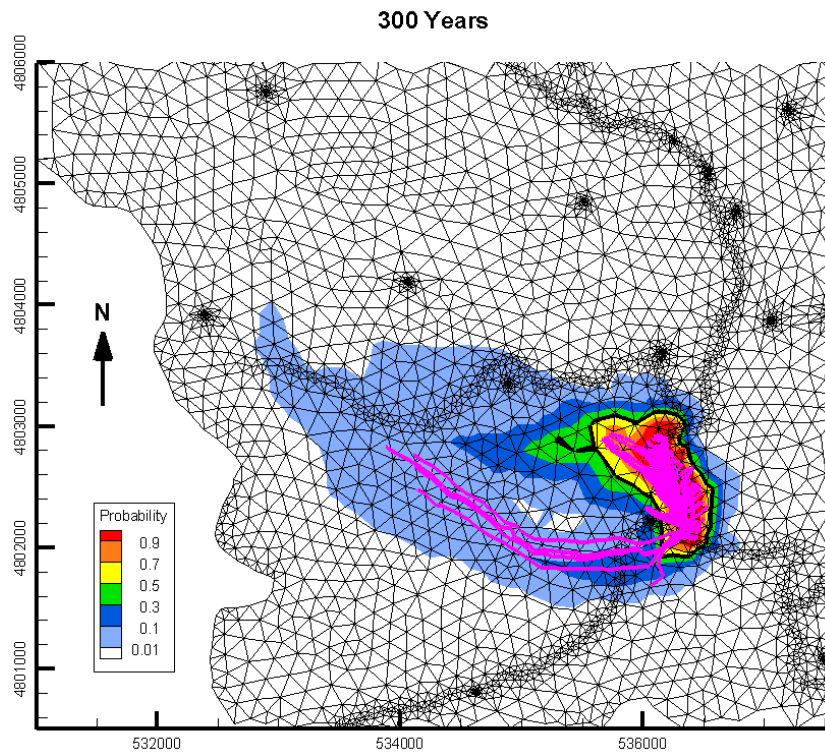
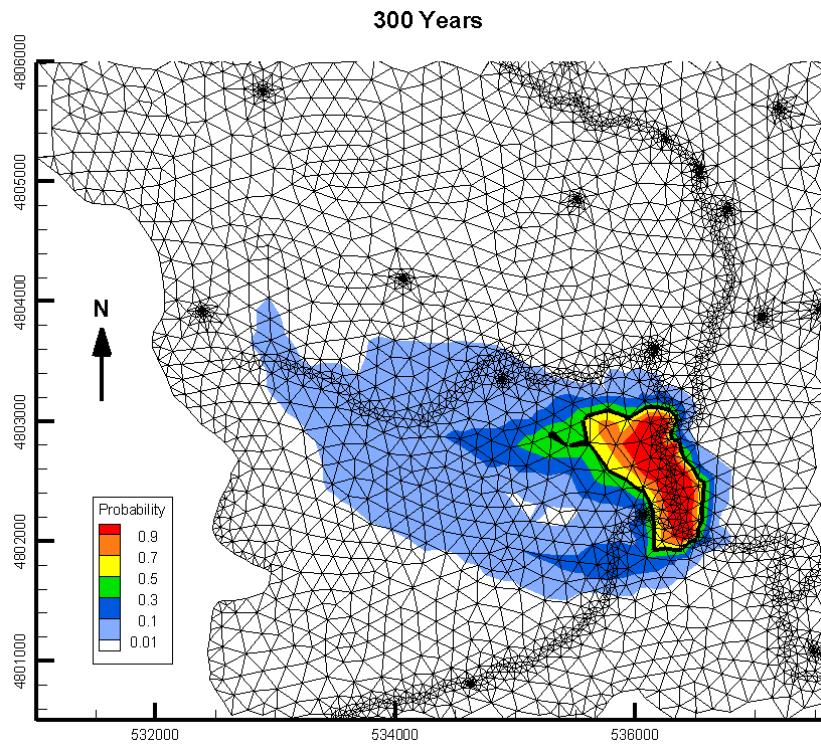


Figure 34: Capture Probability Plume with Reverse Particle Tracks at 300 Years, for Mid-Stream Segment #1

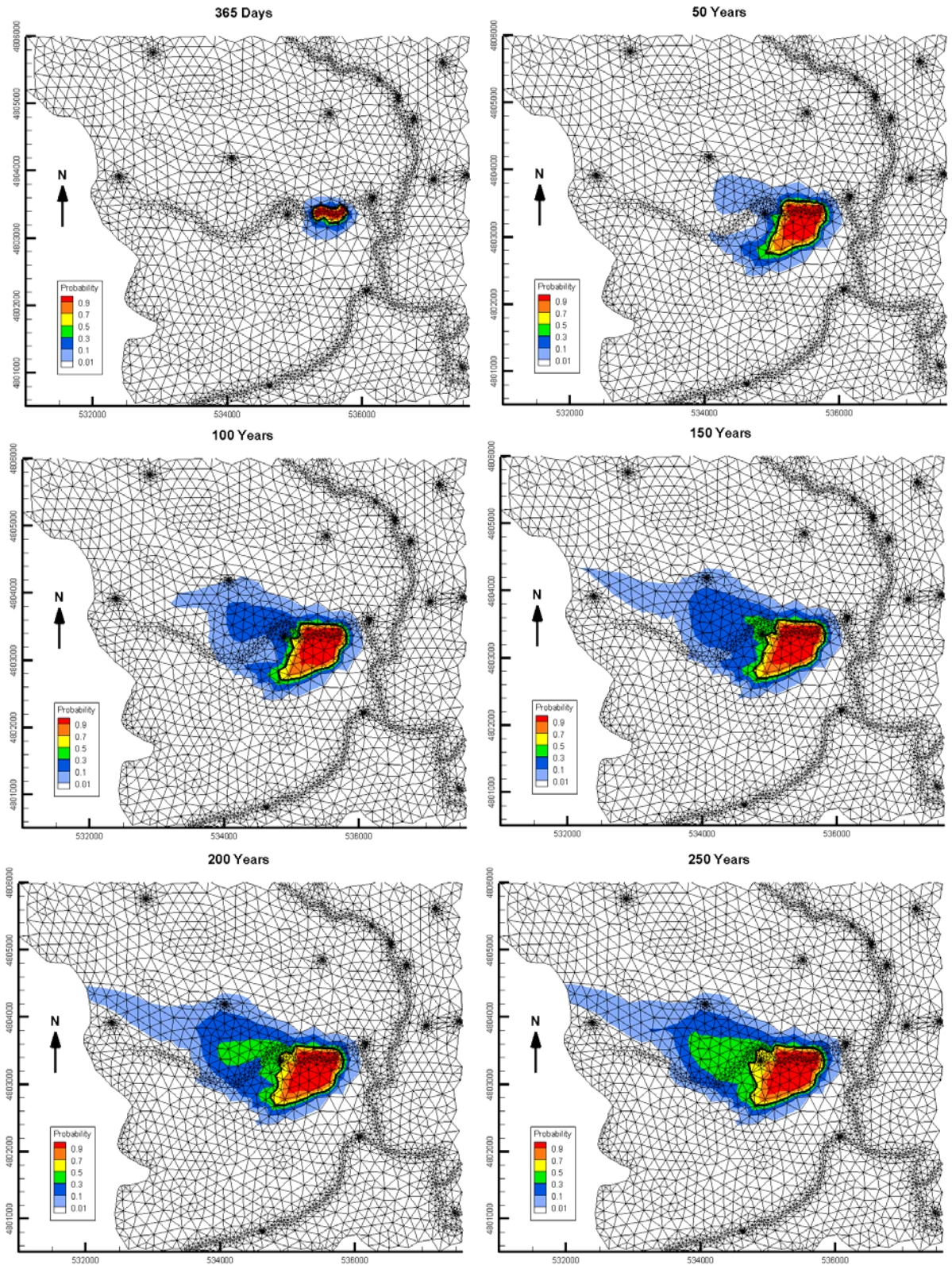
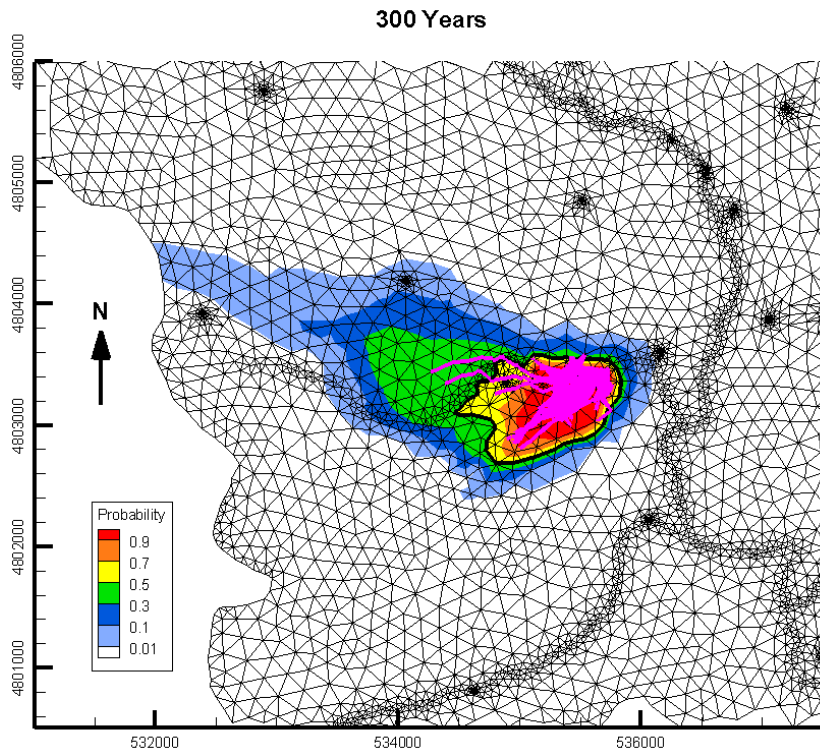
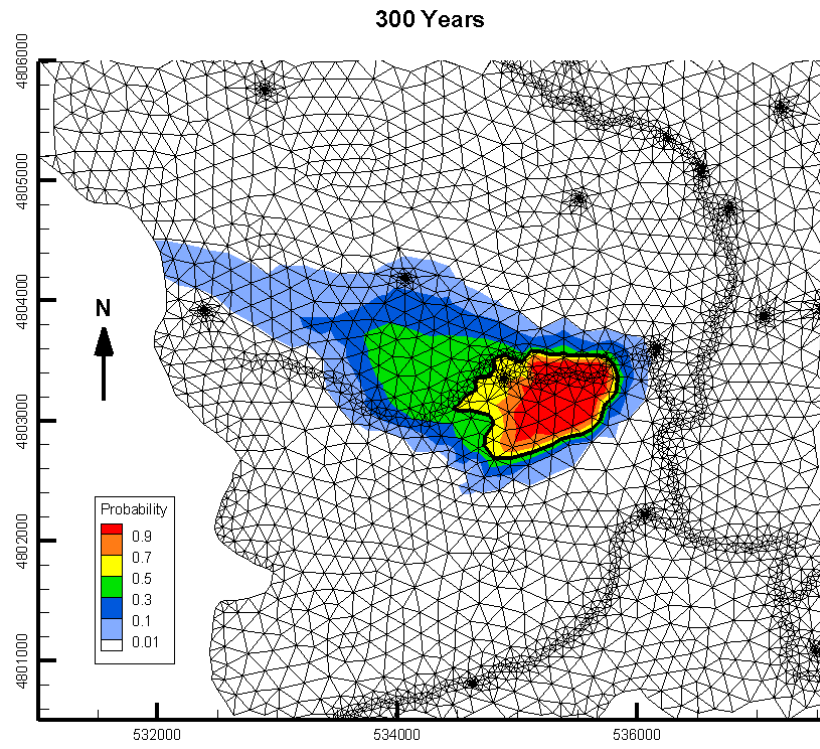


Figure 35: Growth of Capture Probability Plume for Mid-Stream Segment #2



**Figure 36: Capture Probability Plume with Reverse Particle Tracks at 300 Years,
for Mid-Stream Segment #2**

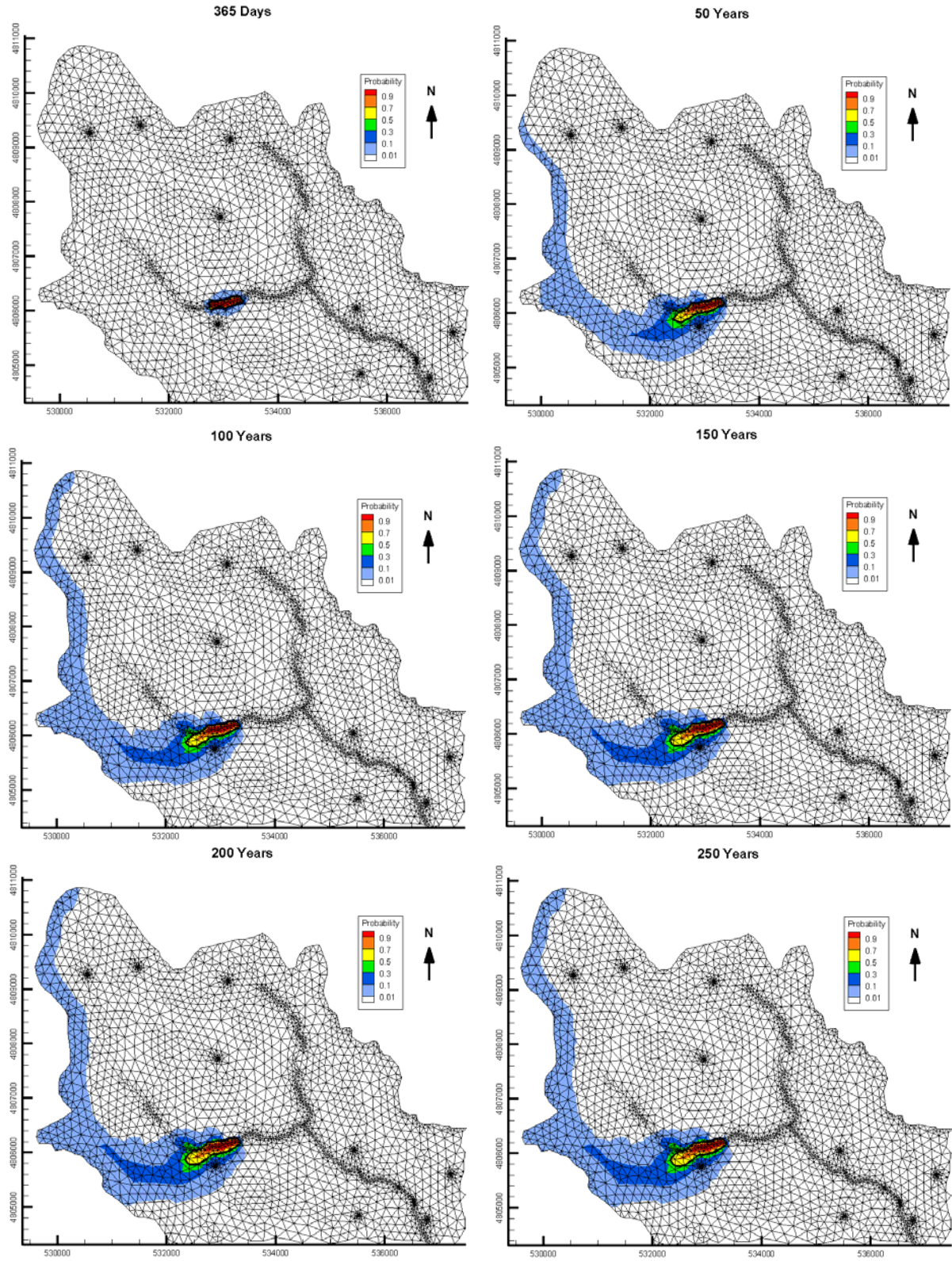
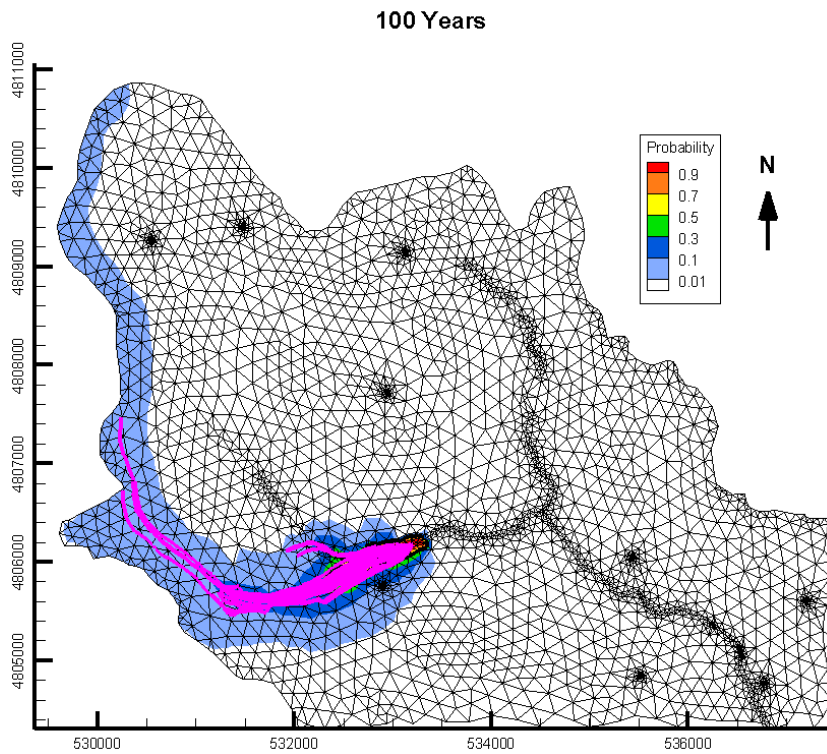
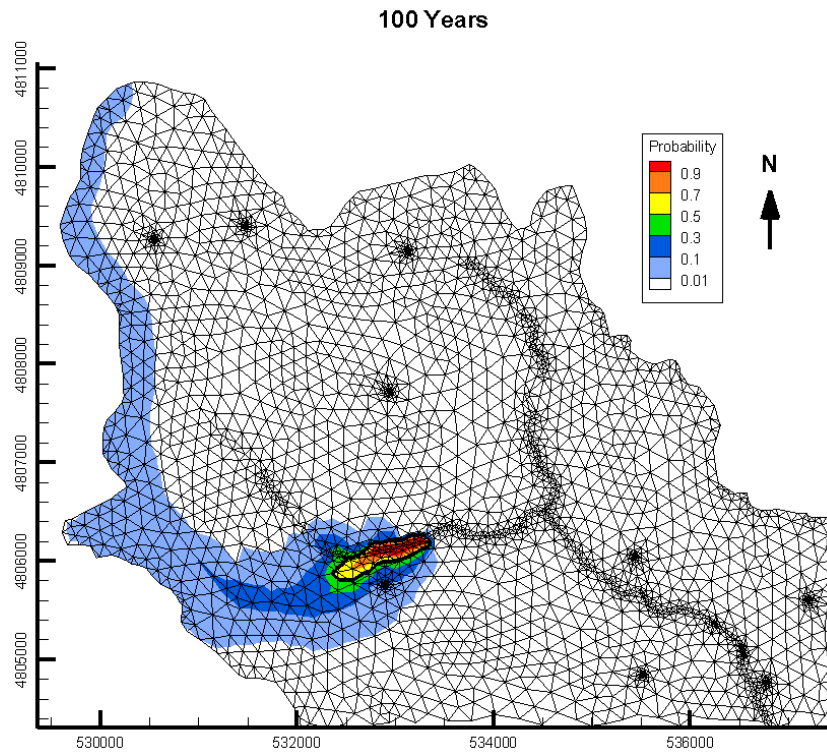


Figure 37: Growth of Capture Probability Plume for Upper-Stream Segment #3



**Figure 38: Capture Probability Plume with Reverse Particle Tracks at 100 Years,
for Upper-Stream Segment #3**

6.6 Implications from Reverse Transport

From the three stream segments that were tested, it is clear that the capture zone can vary in size depending on the delineation method. If the capture probability plume were to be used to extract a capture zone, it would not be clear which probability contour to choose. For extraction wells, Frind et al. (2002) suggested that the 0.25 probability contour would be an appropriate well capture zone on the basis of mass balance between the recharge and the pumping. On the other hand, the capture zone delineated within the 0.5 contour is suggested by Molson and Frind (2011) to be a significant capture zone based on life expectancy considerations. For extraction wells, it was found that the majority of steady-state particle tracks tend to fall within the 0.5 probability contour. In the case of streams, the hydraulic gradient is small compared to the gradient induced by extraction wells, which adds to the uncertainty and could be a factor causing the particle tracks to travel further than the 0.5 probability contour. We can see that only a few (less than 4%) of the particle tracks travel beyond the 0.5 probability contour for stream segments #1 and #2. However, for stream reach #3 approximately 33% of the particles extend beyond the 0.5 probability contour. We should keep in mind that stream reach #3 is located in an area of the domain where the flow field is more uncertain due to the inactivation of pumping wells.

Traditionally, reverse particle tracking is seen more as a screening tool because results can be generated quickly. It helps give a first approximation of the capture zone size delineated by reverse transport. Reverse particle tracking can give insight into which areas to crop in the model so that more efficient reverse transport simulations can be run. Reverse transport, on the other hand, can take hours to run depending on the domain size. However, in the case of extraction wells, reverse transport produces more credible capture zones taking into account local-scale uncertainty, with less need for subjective judgment. We can now see from our study that delineating capture zones for streams is much more uncertain since there is no clear trend in determining how far the steady-state particle

tracks will travel in comparison to the reverse probability plumes, leaving the choice of a proper contour in doubt. Therefore, it is important to use all the tools available to help determine which contour level is an appropriate choice for the final capture zone.

The probability contour that is chosen as the appropriate capture zone should encompass a majority of the steady-state particles. For stream segments #1 and #2 that probability contour should be the 0.5 probability contour, since the majority (greater than 96%) of particles are contained within this contour. For stream segment #3, approximately 33% of the particles extend beyond the 0.5 contour, which is far too many to make it an appropriate capture zone. Approximately 27 out of 180 particles (15%) extend beyond the 0.1 probability contour. Thus most particles are contained within the 0.1 probability contour making it a more acceptable choice as a capture zone.

It was found that in some of the reverse transport scenarios that were tested, instabilities would occur if the Courant criterion $\left(Cr = \frac{v\Delta t}{R\Delta x} \leq 1 \right)$ was exceeded. Exceedance of the Courant criterion causes the dependant variable (concentration, probability) to travel farther than one element during one time step. The remedy is to shorten the time step.

To ensure that the capture probability plumes were created properly it is crucial to not have these instabilities contact the capture zone. In some cases it was necessary to apply Type 1 zero concentration to some elements in the domain. This ensured that mass would not be created by the instabilities. As long as these boundaries were set at a sufficient distance away from the capture probability plume and that the capture probability plume was not moving in the direction of these manually set boundaries, the transport results would be unaffected.

Chapter 7

Conclusions

There are four main conclusions that can be drawn from this research. Firstly, the capture zones delineated by using different modelling software can vary dramatically from one another. The first stream reach showed good agreement between the three models when comparing the size, shape and direction of the capture zone. With those results one could conclude that choosing between the different models is arbitrary. However, after testing another two stream segments, it was clearly shown that the results can be drastically different from model to model. Therefore, different stream reaches can give different degrees of agreement and because of this it is difficult to know which model to use and which capture zone to trust.

It is impossible to predict the size, shape and direction of the capture zones delineated by the different models. Careful analysis and professional judgment will always be necessary in scrutinizing the capture zones before they are used in the decision making process. This is a concern, because most capture zone delineations today are done by running only one model with only one scenario. By relying on only one model/scenario, a practitioner may not realize that different solutions may exist.

The modified conceptual model for this study involved the extraction of head values from a larger scale model to be used as type 1 constant head boundaries for the perimeter of a smaller scale inset model. This technique is only valid if there are no changes in the flow conditions going from a larger scale model to smaller scale. If flow conditions change, boundary conditions should be updated.

Through this research it was made clear that finite element modelling allows for greater flexibility in terms of grid refinement, especially for stream reaches. This would not be possible in finite difference modelling with a quadrilateral grid. In addition, Visual Modflow tends to have

stability issues when there are too many layers near the ground surface and because this study involves groundwater - surface water interactions it is a poor model choice for the capture zone delineation of streams. Finite element based integrated groundwater - surface water models such as HydroGeoSphere prove to be advantageous for the delineation of capture zones for streams and can be applied to other surface water features.

Secondly, non-uniqueness or differences in hydraulic conductivity of the models due to calibration can cause dramatic differences in the capture zones created. The act of model calibration, where calculated values are matched with observed values by altering variables, is an essential part of creating a useful model but is not sufficient proof of model validity. In practice, once a model is calibrated, it is thought to be a valid representation of reality, forgetting there may be other realizations that will give equally valid results. Differences in calibration can lead to slight variations in hydraulic head distributions and as already noted, capture zones are extremely sensitive to slight variations in hydraulic head distributions.

Thirdly, capture zones for base flow are subject to greater uncertainty than capture zones for extraction wells. The reason being is that the hydraulic gradients for natural features are small, frequently changing less than a metre over a kilometre. Therefore, numerical and calibration errors can be the same order of magnitude as the gradient that is being modelled, which leads to greater uncertainty of the capture zones delineated. It is also more challenging because it involves both groundwater and surface water flow processes, whereas extraction wells involve mostly groundwater processes.

Finally, it is evident from this study that both particle tracking and reverse transport should be considered as necessary tools in choosing the appropriate probability contour as the capture zone for a stream reach. In practice, capture zones are usually delineated by particle tracking alone. Reverse transport provides insight into local uncertainties of the study area, but at a greater computational

cost. However, using reverse transport alone to delineate capture zones for streams, the results may be subject to greater uncertainty than for extraction wells. The choice of an appropriate probability contour as a representative capture zone for a stream reach remains unclear.

For extraction wells, 0.25 (on the basis of mass balance) and 0.5 (on the basis of life expectancy) contours have been proposed. For stream reaches, on the other hand the 0.1 contour may be a viable choice since a majority of particle tracks are contained within this contour. Again, the choice may vary for different stream reaches since there is no clear way of predicting how far the particle tracks will extend when compared with the reverse probability plume. This may be due to the fact that the hydraulic gradients for streams are much smaller than those of an extraction well, adding to the ambiguity.

Combining both techniques can help set areas of high protection priority where the probability contours overlap with the largest number of particles. Particle tracking also gives a good first estimate to the size, shape, direction and time taken for the capture zone to reach steady-state. This provides guidance on how to set up the reverse transport simulation. In any case, both particle tracking and reverse transport should be used together when delineating capture zones for streams.

Modelling of groundwater has progressively taken steps in adding additional layers of complexity to take into account more processes (i.e. saturated groundwater flow, unsaturated groundwater flow, surface water flow, atmospheric processes). The development of governing equations for natural systems has allowed the creation of these sophisticated models and has opened up many research avenues. This study would not have been possible without the existence of an integrated groundwater - surface water model such as HydroGeoSphere. However, with each additional layer of complexity come greater data requirements and more uncertainty. Addressing the uncertainty surrounding the use of these models will be a growing area of research.

In addition, a capture zone is not a static line on a map but evolves and changes as more site information is uncovered and as groundwater models improve. It is important for decision-makers to note that capture zones are not delineated in stone and that over time they are likely to change since hydrogeologists are still wrestling with the fact that capture zones are very sensitive to changes due to model selection, boundary conditions, recharge distribution, and non-uniqueness in calibration. Therefore, future policies for land use planning should be flexible and allow capture zones to be revisited periodically as new hydrologic information is uncovered and better models are developed.

References

- Bear, J. (1972). *Dynamics of Fluids in Porous Media*. American Elsevier, New York, NY.
- Beckers, J., and E.O. Frind (2001). Simulating Groundwater Flow and Runoff for the Oro Moraine Aquifer System. Part II. Automated Calibration and Mass Balance Calculations. *Journal of Hydrology*, Vol. 243, pp. 73-90.
- Barry, F., D. Ophori, J. Hoffman, and R. Canace (2008). Groundwater flow and capture zone analysis of the Central Passaic River Basin, New Jersey. *Environmental Geology*, Volume 56, Issue 8, pp. 1593-1603.
- Brunner, P., C. T. Simmons, P. G. Cook, and R. Therrien (2010). Modeling Surface Water-Groundwater Interactions with MODFLOW: Some Considerations. *Ground Water*, Vol. 48, No. 2, pp. 174-180.
- Cameron, D. (1995). The Making of a Polluter: A Social History of Uniroyal Chemical in Elmira. *Environmental Sociology: Theory and Practice*, Captus Press Inc., York University Campus, pp. 297-320.
- CH2MHILL and S.S. Papadopoulos & Associates, Inc. (2003). Alder Creek Groundwater Study: Final Report. *Prepared for The Regional Municipality of Waterloo*.
- CH2MHILL and North-South Environmental Inc. (2008). Alder Creek Watershed Study and Upper Strasburg Creek Subwatershed: Plan Update, Final Report. *Prepared for the Grand River Conservation Authority*.
- Chow, R., E.O. Frind, M. Sousa, J.P. Jones, D.L. Rudolph, and J.W. Molson (2011). Delineating Capture Zones for Environmentally Sensitive Features – A Model Comparison. *Geohydro Conference, Quebec City, Quebec Canada*.

- Cleary, T.C.B.F., and R.W. Cleary (1991). Delineation of Wellhead Protection Areas: Theory and Practice. *Water Science and Technology*, Vol. 24, No. 11, pp. 239-250.
- Correll, M.R., J.H. Lillydahl, and L. D. Singell (1978). The Effects of Greenbelts on Residential Property Values: Some Findings on the Political Economy of Open Space. *Land Economics*, Vol. 54, No. 2, pp. 207-217.
- Doherty, J. (2005). PEST: Model Independent Parameter Estimation. *Fifth edition of user manual. Watermark Numerical Computing, Brisbane, Australia.*
- Evers S., and D.N. Lerner (1998). How Uncertain is Our Estimate of a Wellhead Protection Zone? *Ground Water* 36, pp. 49–57.
- Franke, O.L., T.E. Reilly, D.W. Pollock, and J.W. LaBaugh (1998). Estimating Areas Contributing Recharge to Wells: Lessons from Previous Studies. *U.S. Geological Survey Circular 1174.*
- Frind, E.O., E.A. Sudicky, and S.L. Schellenberg (1987). Micro-Scale Modelling in the Study of Plume Evolution in Heterogeneous Media. *Stochastic Hydrology and Hydraulics*, 1(4), pp. 263-279.
- Frind, E.O., D.S. Muhammad, and J.W. Molson (2002). Delineation of Three-Dimensional Capture Zones in Complex Multi-Aquifer Systems. *Ground Water*, Vo. 40, No. 6, pp. 586-589.
- Frind, E.O., and J.W. Molson (2004). A New Particle Tracking Algorithm for Finite Element Grids. *FEM-MODFLOW Conference, Carlsbad, Czech Republic.*
- Frind, E.O., J.W. Molson, and D.L. Rudolph (2006). Well Vulnerability: A Quantitative Approach for Source Water Protection. *Ground Water*, Vol. 44, No. 5, pp. 732-742.
- Frind, E.O., M. Sousa, J.P. Jones, and D.L. Rudolph (2009). Well Vulnerability: A Model Comparison – Issues and Pitfalls. 2nd International FEFLOW User Conference, Potsdam/Berlin, Germany.

- Gelhar, L.W., and C.L. Axness (1983). Three-Dimensional Stochastic Analysis of Macrodispersion in Aquifers. *Water Resources Research*, 19(1), pp.161–180.
- Grand River Conservation Authority (2001). Alder Creek Watershed Study. Phase 1 –Discussion Paper. Draft Report prepared by the Regional Municipality of Waterloo.
- Harbaugh, A.W., E. R. Banta, M.C. Hill, and M.G. McDonald (2000). MODFLOW -2000, The U.S. Geological Survey Modular Ground-Water Model-User Guide to Modularization Concepts and the Ground-Water Flow Process. U.S. Geological Survey. Open File Report 00-92. Reston, Virginia.
- Huyakorn, P.S., and G.F. Pinder (1983). Computational Methods in Subsurface Flow. *Academic Press, Orlando, Florida*.
- Jones, J.P., M.R. Sousa, E.O. Frind, and D.L. Rudolph (2009). Determining the Influence of Surface, Unsaturated and Saturated Processes on Source Water Protection Strategies: A Multi-Model Study. *GeoHalifax. Halifax, Nova Scotia, Canada*.
- Karrow, P.F. (1993). Quaternary Geology of the Stratford-Conestogo Area, Ontario. Ontario Geological Survey – Open File Report 283.
- Leismann, H.M., and E. O. Frind (1989). A Symmetric-Matrix Time Integration Scheme for the Efficient Solution of Advection-Dispersion Problems. *Water Resources Res.*, 25(6), pp. 1133-1139.
- Martin, P.J. (1994). Modelling of the North Waterloo Multi-Aquifer System. MSc Thesis, University of Waterloo.
- Martin, P.J., and E.O. Frind (1998). Modeling a Complex Multi-Aquifer System: The Waterloo Moraine. *Ground Water. Vol. 36, No. 4*, pp. 679-690.
- McDonald, M.G., and A.W. Harbaugh (1988). A Modular Three-Dimensional Finite-Difference Ground-Water Flow Model: U.S. Geological Survey Techniques of Water-Resource Investigations, book 6, Chapter A1, pp. 586.

- McLaren, R. G. (1997). Gridbuilder 5.0 user's guide. A Pre-Processor for 2D Triangular Finite Element Programs. *Waterloo, Centre for Groundwater Research, University of Waterloo, Waterloo, Ontario, Canada.*
- Molson, J.W., J. Beckers, E. O. Frind, and P.J. Martin (2002). WATFLOW/3D: A Three-Dimensional Numerical Model for Coupled Groundwater Surface Water Flow, Version 4.0. Department of Earth Sciences, University of Waterloo.
- Molson, J.W., and E. O. Frind (2004). WTC: Waterloo Transport Code, Version 3.0, Advective-Dispersive Mass Transport Model in Three Dimensions, User Guide. Department of Earth Sciences, University of Waterloo.
- Molson, J.W., and E.O. Frind (2011). On the Use of Mean Groundwater Age, Life Expectancy and Capture Probability for Defining Aquifer Vulnerability and Time-Of-Travel Zones for Source Water Protection. *J. Contam. Hydrol.*, doi:10.1016/j.jconhyd.2011.06.001.
- Muhammad, S.D. (2000). Methodologies for Capture Zone Delineation for the Waterloo Moraine Well Fields. M.Sc. thesis, University of Waterloo.
- Neuman, S.P. (1980). A Statistical Approach to the Inverse Problem of Aquifer Hydrology 3. Improved Solution Method and Added Perspective. *Water Resource*, 16(2), pp. 331-346.
- Neupauer, R.M., and J.L. Wilson (1999). Adjoint Method For Obtaining Backward-In-Time Location and Travel Time Probabilities of a Conservative Groundwater Contaminant. *Water Resources Research*, Vol. 35, No. 11, pp. 3389-3398.
- O'Connor, D. (2002). Report of the Walkerton Inquiry: The Events of May 2000 and Related Issues, Part One: A Summary. Ontario Ministry of the Attorney General.
- O'Connor, D. (2002). Report of the Walkerton Inquiry: A Strategy for Safe Drinking Water, Part Two. Ontario Ministry of the Attorney General.

- Ontario Ministry of the Environment (2006). Clean Water Act, S.O. 2006, Chapter 22 (Bill 43).
Legislative Assembly of Ontario, Canada.
- Pinder, G.F., and E.O. Frind (1972). Application of Galerkin's Procedure to Aquifer Analysis. *Water Resources Research. Vol. 8, No. 1*, pp. 108-120.
- Pollock, D.W. (1988). Semianalytical Computation of Pathlines for Finite-Difference Models. *Ground Water, Vol. 26, No. 6*, pp.743-750.
- Rahman, R. (2008). On the Implications of Various Approaches to Groundwater Source Protection.
PhD Thesis, University of Waterloo.
- Refsgaard, J.C., H.J. Henriksen, W.G. Harrar, H. Scholten, and A. Kassahun (2005). Quality Assurance in Model Based Water Management - Review of Existing Practice and Outline of New Approaches. *Environ. Modell. Softw., 20(10)*, pp. 1201-1215.
- Regional Municipality of Waterloo (1994). Water Resources Protection Strategy Implementation Plan.
- Schleyer R., G. Milde, and K. Milde (1992). Wellhead Protection Zones in Germany: Delineation, Research and Management. *Journal of the Institute of Water & Environmental Management 6, no. 3*, pp. 303-311.
- Schlumberger Water Services (2009). Visual MODFLOW, Version 2009.1 Pro, Build: 4.4.0.156. 460 Phillip St. – Suite 101, Waterloo, Ontario, Canada.
- Schlumberger Water Services (2007). WinPEST: Non-linear Parameter Estimation and Predictive Analysis Program, 460 Phillip St. – Suite 101, Waterloo, Ontario, Canada.
- Sophocleous, M. (2002). Interactions Between Groundwater and Surface Water: The State of the Science. *Hydrogeology Journal, Volume 10, Number 1*, pp.52-67.

- Sousa, M.R., E.O. Frind, and D.L. Rudolph (2010). Capture Probability Maps Addressing Uncertainty: Protection vs. Mitigation. *Q10: Groundwater Quality Management in a rapidly Changing World. Proc. 7th International Groundwater Quality Conference*. 13-18 June 2010, Zurich, Switzerland.
- Sousa, M.R., E.O. Frind, and D.L. Rudolph (2012). An Integrated Approach for Addressing Uncertainty in the Delineation of Groundwater Management Areas. *In submission*.
- Sudicky, E.A. (1986). A natural gradient experiment on solute transport in a sand aquifer: Spatial variability of hydraulic conductivity and its role in the dispersion process. *Water Resour. Res.* 22, pp. 2069-2082.
- Sudicky, E.A., A.J.A. Unger, and S. Lacombe (1995). A Noniterative Technique For The Direct Implementation of Well Bore Boundary Conditions in Three-Dimensional Heterogeneous Formations. *Water Resources Research*, Vol. 31, No. 2, pp. 411-415.
- Tarbut, E.J., F.K. Lutgens, and C.J. Tsujita (2005). *Earth: An Introduction to Physical Geology*, Canadian Edition. Pearson Education Canada Inc., Toronto.
- Therrien, R., R.G. McLaren, E.A. Sudicky, and S.M. Panday (2006). *HydroGeoSphere: A Three-Dimensional Numerical Model Describing Fully-Integrated Subsurface and Surface Flow and Solute Transport*. Groundwater Solutions Group, University of Waterloo.
- U.S. Environmental Protection Agency (1988). *Wellhead Protection Area Delineation, A "Hands On" Training Course*, Fairfax.
- United States National Park Service (1991). *Economic Impacts of Protecting Rivers, Trails and Greenway Corridors: A Resource Book 2nd Edition*. Rivers, Trails and Conservation Assistance, National Park Service.
- van Genuchten, M.Th. (1980). A Closed-Form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils. *Soil Sci. Soc. Am. J.*, Volume 44, pp. 892-898.

Waterloo Hydrogeologic Inc. (2006). Visual MODFLOW v.4.2 User's Manual: A Professional Application for 3D Groundwater Flow and Contaminant Transport Modeling. Waterloo Hydrogeologic Inc.

Winter, T.C., J.W. Harvey, O.L. Franke, and W.M. Alley (1998). Ground Water and Surface Water: A Single Resource. *U.S. Geological Survey Circular 1139. Denver, Colorado.*