ADVANCES IN MODELING, SAMPLING, AND ASSESSING THE ANTHROPOGENIC CONTAMINATION POTENTIAL OF FRACTURED BEDROCK AQUIFERS

by

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This thesis is dedicated to Ellena Marlène Kozuskanich.
Abstract

Groundwater is an important resource that is relied on by approximately half of the world’s population for drinking water supply. Source water protection efforts rely on an understanding of flow and contaminant transport processes in aquifers. Bedrock aquifers are considered to be particularly vulnerable to contamination if the overburden cover is thin or inadequate. The objective of this study is to further the understanding of modeling, sampling, and the potential for anthropogenic contamination in fractured bedrock aquifers. Two numerical modeling studies were conducted to examine geochemical groundwater sampling using multi-level piezometers and the role of discretization in a discrete fracture radial transport scenario. Additionally, two field investigations were performed to study the variability of bacterial counts in pumped groundwater samples and the potential for anthropogenic contamination in a bedrock aquifer having variable overburden cover in a semi-urban setting. Results from the numerical modeling showed that choosing sand pack and screen materials similar in hydraulic conductivity to each other and the fractures intersecting the borehole can significantly reduce the required purge volume. Spatiotemporal discretization was found to be a crucial component of the numerical modeling of solute transport and verification of the solution domain using an analytical or semi-analytical solution is needed. Results from the field investigations showed fecal indicator bacterial concentrations typically decrease on the order of one to two orders of magnitude from the onset of pumping. A multi-sample approach that includes collection at early-time during the purging is recommended when sampling fecal indicator bacteria for the purpose of assessing drinking water quality. Surface contaminants in areas with thin or inadequate overburden cover can migrate quickly and deeply into the bedrock aquifer via complex fracture networks that act as preferential pathways. While the presence of fecal indicator bacteria in groundwater samples
signifies a possible health risk through human consumption, it was the suite of pharmaceuticals and personal care products that allowed the identification of septic systems and agriculture as the dominant sources of contamination. Land-use planning and source water protection initiatives need to recognize the sensitivity of fractured bedrock aquifers to contamination.
Co-Authorship

John Kozuskanich is the primary author on this thesis. Chapters 2 to 5 were written as independent manuscripts. Drs. Kent Novakowski and Bruce Anderson provided intellectual supervision and editorial comment for all chapters, and are co-authors on all the manuscripts. Chapter 2 is submitted to the journal *Ground Water*. Chapter 3 is submitted to the journal *Water Resources Research*. Chapter 4 is published in the journal *Ground Water*. Allan Crowe and Vimal Balakrishnan (both from Environment Canada) were additional co-authors on Chapter 5 which is submitted to the journal *Water Research*. 
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Chapter 1

Introduction

Recent estimates indicate approximately 30% of Canadians rely on groundwater for potable water supply, two-thirds of whom live in rural areas and use private water wells (Government of Canada 2006; Novakowski et al. 2006). According to UNESCO (2004), approximately half of the world’s population depends on groundwater in part because surface water is not always available and aquifers are generally better protected from contamination. However, some hydrogeological settings, such as fractured bedrock aquifers with minimal overburden, are considered to be especially vulnerable to contamination (Malard et al. 1994; Pronk et al. 2006). This particular setting is present in eastern and northern Ontario, Quebec, the northeastern United States, and northern Europe. The degradation of groundwater quality is often attributed to anthropogenic contaminant sources, including agriculture and septic systems (Fetter 2001). The potential for human consumption of contaminated groundwater in most rural settings is compounded by the co-presence of private wells and septic systems and close proximity to agricultural activity. Particular concern is given to the health risks associated with nitrate and pathogenic microorganisms in the effluent from these sources.

In the last decade, municipal water management in Ontario has shifted away from a reliance on present and future water treatment technologies to a source water protection approach through the Clean Water Act (MOE 2006). Developing source water protection plans for groundwater resources requires an understanding of flow and contaminant transport processes in aquifers. In practice, hydrogeologists can use a variety of tools to help understand these processes, both conceptually and physically, over many orders of magnitude in spatial scale. Laboratory studies, aquifer tests, tracer tests, monitoring well networks, groundwater sampling, and mathematically-
based models are examples of methods that are commonly used for this purpose. The number of studies that have employed these methods in porous media aquifers far outweighs those conducted in fractured bedrock. The need for research in the field of fractured rock hydrogeology and its importance in water management for both municipal systems and private wells is substantiated by the recent establishment of technical information forums like the “Fractured Bedrock Working Group” by Conservation Ontario.

The objective of this research is to further the understanding of modeling, sampling, and the potential for anthropogenic contamination in fractured bedrock aquifers. This was accomplished through two numerical modeling studies (Chapters 2 and 3), and two field-based investigations conducted at a research site in a semi-rural setting (Chapters 4 and 5). The following provides a brief overview of the scope and objectives of each chapter, which are stand-alone manuscripts (each includes an introduction with the review of pertinent literature, methodology, results, discussion, conclusion, and reference list):

- Chapter 2 focuses on well dynamics and the influence of the screen and sand pack materials used in multi-level piezometer construction on obtaining representative geochemical groundwater samples from a discretely fractured bedrock aquifer. Part of the objective is to determine if the choice of screen and sand pack can be optimized to reduce the required purge time and volume. The study also provides a better understanding of how to simulate convergent pumping scenarios using numerical models.
- Chapter 3 examines the role of discretization in a discrete fracture model in the context of radial transport in a steady flow field. Appropriate spatiotemporal discretization and other implementation considerations in the numerical model necessary for matching point-to-point and borehole-to-point simulations with the semi-analytical solutions by Novakowski (1992) are discussed. A new borehole mixing model, based on Palmer
(1988), is developed for the case of a well-mixed, finite volume observation borehole intersected by multiple fractures in a steady radial flow field. The results are useful for developing numerical modeling approaches in radial transport scenarios involving continuous or pulse source injection or pumping conditions in fractured rock, such as tracer experiments, wastewater injection, and domestic well pumping near a source of contamination.

- Chapter 4 investigates the variability of fecal indicator bacteria (E. coli, total coliform, fecal coliform, fecal streptococci) and heterotrophic plate counts in groundwater samples in a variety of pumping regimes. Two bedrock monitoring wells located in a semi-urban setting were constructed as multi-level piezometers and bacterial enumeration was conducted using standard membrane filtration methods. A conceptual model is developed to better understand the results in the context of the distribution of bacteria between the sand pack and well-aquifer system. The study highlights the need to consider the differences between bacterial and solute transport mechanisms and what a “representative sample” is intended to be representative of when designing sampling protocols and using fecal indicator bacteria to assess drinking water quality. This research has been published the journal Ground Water (Kozuskanich et al. 2010).

- Chapter 5 assesses how anthropogenic contaminant sources in a semi-rural setting, where both septic systems and agriculture are present, might be impacting groundwater quality in an underlying bedrock aquifer having variable overburden cover. A multiparameter sampling program involving nutrients, chloride, fecal indicator bacteria, stable isotopes, and 40 pharmaceuticals and personal care products (PPCPs) was used to track anthropogenic effects. To my knowledge, this is the first study to report on PPCPs in a bedrock aquifer. Eight monitoring wells were instrumented as multi-level piezometers in a lakeside village surrounded by rural housing and undeveloped and agricultural land.
Chemical, isotopic, and bacterial analyses were conducted using conventional methods. A conceptual model based on a balance of field data is developed and used to understand the observed contaminant concentrations. The results are useful for understanding the complexities of flow and contaminant transport in fractured bedrock aquifer systems and their vulnerability to contamination.

Lastly, Chapter 6 is a general discussion and Chapter 7 provides a summary of conclusions and recommendations pertinent to the research presented.
1.1 References


Chapter 2

The Influence of Sand Packs and Screens on Obtaining Representative Geochemical Groundwater Samples from Multi-level Monitoring Wells in Bedrock Aquifers – A Numerical Study

2.1 Introduction

The objective of groundwater sampling is to obtain samples that are representative of the in situ chemical or biological conditions in the underlying aquifer (Pohlmann and Alduino 1992; Nielsen 2007). Monitoring wells are routinely employed to act as sampling points. The presence of the monitoring well itself however may influence the quality and meaning of the sample because of issues relating to the installation of the well, the types of construction materials used, the presence of a free-water surface, the potential for intra-borehole flow and cross-contamination between otherwise hydraulically disconnected features, borehole dilution and mixing, and the stagnation of water in unscreened portions of the borehole (Barcelona and Helfrich 1986; Pohlmann and Alduino 1992; Church and Granato 1996; Shapiro 2002; Nielsen 2007). Sampling technique (pump type, flow rate, discharge tube materials, purge volume, etc.) has also been shown to influence the resultant samples and their representativeness of formation water, particularly for volatile organic compounds (Barcelona et al. 1984; Keely and Boateng 1987; Robin and Gillham 1987; Gibbs and Imbrigiotta 1990; Puls and Barcelona 1996; Herzog et al. 1998).

Multi-level piezometers (see Figure 2-1) are often constructed in boreholes to allow for multiple sampling points at specific hydrogeological features with depth in the aquifer (fractures or
granular media units of interest) and to reduce the problems of dilution and mixing associated with sampling open wells. An inexpensive method is to place a short well screen at the location of the feature with riser extending to surface. The annular space between the screen and borehole wall is filled with commercially available sand or gravel-sized inert silica grains (typically called the sand pack, gravel pack or filter pack) designed specifically for this usage. The “interval” (sand pack and screen) is hydraulically isolated within the borehole using bentonite (clay) “caps” on either end of the sand pack. The number of zones that can be constructed depends on the diameter of the borehole and screen and riser materials.

The selection of screen slot size and sand pack material depends on the nature of the aquifer materials. Their selection should be based on the retention of aquifer materials and sand pack material. The combination of appropriately selected sand pack material and screen slot size will prevent the mobilization of fines in the aquifer, screen slot clogging, and well sedimentation and will reduce turbidity in pumped samples (Nielsen 2007). Unlike in unconsolidated materials, the sand pack in a bedrock well installation is not typically needed to retain the formation. Sand pack material should be selected to prevent loss into the fractures (the largest fracture apertures typically encountered are approximately 1500 microns). The use of the sand pack as a filter of fines may depend on the rock type, the degree of cementation and weathering, and the natural turbidity levels under natural flow conditions in the fractures (due to groundwater-surface water connectivity, for example). The influence of the sand pack and screen, however, on the nature of flow and transport between a fracture and the pump intake is poorly understood.
Current geochemical sampling protocols call for the purging of the well prior to sample collection to eliminate the fractional contribution of the original borehole contents to the pump discharge (Puls and Barcelona 1996; Nielsen 2007). A fixed well-volume approach whereby three to five or four to six well volumes of water are purged prior to sampling has been traditionally used in practice mainly out of administrative convenience (Nielsen and Nielsen 2007). This method is misleading as there is no set number of well volumes (or standard definition of what constitutes a “well volume”) that when purged results in representative samples for all sites and hydrogeological conditions (Barcelona et al. 1994; Nielsen 2007). Also, the time-dependent contribution from drawdown and the formation to pump discharge is the same regardless of the volume of water stored in the riser, which is typically part of the well volume calculation – thus, the required purge time remains unchanged. The stabilization of field parameters (pH, conductivity, temperature, dissolved oxygen and oxidation-reduction potential) in the pump discharge is also thought to be a good indicator of when a representative sample can be obtained (Nielsen and Nielsen 2007). However, as indicated by Gibs and Imbrigiotta (1990), the stabilization of field parameters does not imply the stabilization of the solute of interest.

Several open borehole mixing models have been developed in the past for porous media to estimate the purge time or purge volume required for obtaining a representative ground water geochemical sample using a mass balance approach (Barber and Davis 1987; Robbins and Martin-Hayden 1991). The formulations utilize a variety of assumptions on the location of the pump intake, the nature of mixing in the borehole, the initial concentrations in the borehole and formation, and the target concentration in the pump discharge. A mixing model has also been developed that incorporates the varying properties of multi-level completion materials (Palmer
1988), but it is only intended for the case of a passive monitoring well (no pumping) in a uniform flow field. While most of the models do consider flow and the transient nature of the water level in the borehole during pumping, none of them account for the transport properties of the aquifer or borehole, or the chemical properties of the solute. These models are intended for application to confined homogenous granular aquifers, but can be converted to the case of a confined single fracture (Shapiro 2002). Consideration of transient flow, transport properties, multiple fractures, and aquifer heterogeneity requires the use of a numerical model.

HydroGeoSphere (HGS) is a three-dimensional (3-D) numerical model describing fully-integrated subsurface and surface flow and transport (Therrien et al. 2006). Simulations can be conducted using porous or discretely-fractured media or combination of both. Wells are implemented as a one-dimensional (1-D) string of nodes in the 3-D domain using a common node approach. The pump intake can be placed at any of the nodes defining the borehole. Flow and transport in the well is treated as analogous to a finite diameter pipe using the equations derived in Sudicky et al. (1995), Therrien and Sudicky (2000), and Therrien et al. (2006). Dispersion along the axis of the borehole is accounted for using the formulation by Lacombe et al. (1995). Borehole concentration (i.e. concentration in the pump discharge) is calculated using a flux-averaged approach. Borehole mixing is dictated by the flow and transport solution, and is not based on an assumption on the nature of the mixing process (no-mixing, complete mixing, etc.) as is used in the analytical models discussed previously. HGS is capable of solving complex scenarios involving simultaneous transient flow and transport, complex fracture networks, and heterogeneous flow and transport properties in the modeling domain.
The objective of this study is to examine the influence of the screen and sand pack on the collection of a representative groundwater sample from a discretely fractured bedrock aquifer. HGS and visualization software are employed to simulate and visualize transient flow and transport during pumping open wells and in the sand pack for a variety of screen and sand pack combinations and aquifer scenarios (single and multiple fractures in bedrock). The optimization of screen-sand pack combinations is explored for the potential of reducing purging times and volumes in practice. The influence of the location of the fractures along the well screen, fracture aperture, screen length, and pumping rate on the required purging time is also considered. The results are best used to explore the relative difference each tested scenario has on the required purging time, not for determining absolute purging times. This study provides a better understanding of well dynamics and the use of numerical models like HGS in simulating convergent pumping scenarios.

2.2 Modeling Methods

The following sections outline the methods and parameters used in the numerical modeling. A conceptual model is presented to establish a base case for the modeling scenarios. Implementation of the boundary conditions, variations in the flow and transport properties of the aquifer, variation of the screen and sand pack materials, and the manipulation of the spatiotemporal discretization are also described. A brief overview of the solute transport governing equations used in HGS and an example set of HGS input files are provided in Appendix A.

2.2.1 Conceptual Model

A depiction of the general conceptual model for a multi-level interval constructed in a confined aquifer is provided in Figure 2-2A. For simplicity, only the case of a 0.0254 m (2 inches)
diameter screen in a 0.1524 m (6 inches) borehole was considered (similar to the bottom interval in Figure 2-1). The presence of risers from deeper intervals (as shown in the mid- and upper-intervals in Figure 2-1) and asymmetry in the placement of the screen in the sand pack (i.e. not down the z-axis of the well) were not considered. Potential turbulence and inertial effects at the well screen (Elsworth and Doe 1986) are ignored.

The pump is placed in the screened interval of the well and pumping is maintained at a constant rate under transient flow conditions. The top and bottom of the domain are no-flow boundaries. The outer boundary in the radial domain is constant-head. The matrix and bentonite are considered impermeable, and the fracture (or fractures) that intersect the interval is horizontal. The choice of screen and sand pack material depends on the aperture of the largest fracture, as previously discussed.

The borehole (sand pack and screen/riser) have an initial concentration of zero (arbitrary units) for a conservative solute. The rest of the domain (fractures and matrix) has specified concentration of one (arbitrary units). The pump discharge is considered to be representative of the formation water when its concentration is equal to 0.99 (i.e. 99% of the pump discharge is new water from the formation). The time at which this occurs is denoted as \( t_{99} \) in this chapter.

2.2.2 Implementation of the Numerical Model

The geometry of the screen and sand pack (cylinders) and radial flow in the domain was accommodated for by using axisymmetric coordinates in the numerical model. Axisymmetric coordinates allow for the simulation of 3-D radial flow in a two-dimensional (2-D) domain which can substantially reduce the number of nodes required and the simulation runtime (Langevin
2008). HGS employs a 2-D domain of unit thickness (in the y-direction) when axisymmetric coordinates are specified (Therrien et al. 2006). Figure 2-2B provides a schematic of the implementation of the conceptual model from Figure 2-2A in the 2-D unit-thickness domain. The numerical model requires the placement of two equivalent injection/withdrawal wells at $x = 0$, $y = 0$ and $x = 0$, $y = 1$ m ($x$ is used to denote the radial direction, $r$, since the grid is still being constructed using Cartesian coordinates).

The actual dimensions of the modeling domain (in $x$ and $z$) are outlined in the section on discretization. The screen and sand pack are implemented as porous media layers of 1 mm and 49.8 mm, respectively, for a total thickness of 0.0508 m (2 inches). All flow boundaries are no-flow, except for the boundary at $x_{\text{max}}$, which is constant-head.

2.2.2.1 Spatiotemporal discretization

Interactive block generation was employed to grade block sizes (coarsen) away from physical boundaries in the domain, such as the screen-sand pack, sand pack-aquifer, and fracture-matrix interfaces (see Figure 2-3). The objective of refinement around these features is to reduce error associated with velocity changes, particularly for the transport solution. A variety of gridding schemes were tested, however, as there is no analytical solution (that accommodates for the presence of the screen, sand pack and fractured bedrock system in transient divergent or convergent injection/pumping conditions) for verification. Adaptive timestepping was employed in the form of concentration control (set to 0.05, meaning no more than a 5% change in concentration can occur at any node for a given timestep) to refine the temporal discretization in the flow and transport solutions. The final spatial discretization was selected for this study (Table 2-1) when further refinement in the grid or concentration control had minimal influence (<5%
difference) on the solute concentration at a particular point in time and space. The grading routine in z is maintained for both single and multiple fractures – grid blocks coarsen away from each fracture until the midpoint between. The same method was used for discretizing in x between the screen and the sand pack-aquifer interface (see example in Table 2-1). The maximum block size in z was set to 0.1 m to provide better resolution in the output files used for visualizations.

2.2.2.2 Model Parameters
A summary of the general model parameters is provided in Table 2-2. The screen, sand pack, and matrix/fracture are defined between x = 0 and 0.001 m, 0.001 and 0.0508 m, and 0.0508 m and 250 m, respectively. The hydraulic conductivity and porosity for the screens and sand packs examined in this study will be discussed in the proceeding section. The transport simulations were conducted under transient flow conditions using the flow and transport boundary conditions discussed earlier. Simulations were conducted using the finite element method under a variety of pumping rates, fracture apertures, and screen/sand pack combinations. Ranges in parameter values are provided in Table 2-2. Upstream transport time weighting and upstream weighting of velocities (default for finite element simulations because a control volume is employed) were used.

2.2.2.3 Screen and Sand Pack
Screen and sand pack materials modeled in this study are based on commercially available products. Table 2-3 provides detailed information on the different grades of sand pack material. Hydraulic conductivity for each grade reported in Table 2-3B was approximated using the Hazen Method from the grain size distributions from Table 2-3A. The midpoint in the calculated hydraulic conductivity range for each grade of sand pack (due to a range in the fitting coefficient,
C) was used in the modeling. The hydraulic conductivity of the sand pack was considered isotropic, and the specific storage was set to $2 \times 10^4 \text{ m}^3$ (storativity was set to $1 \times 10^{-5}$). Porosity was varied between 0.2 and 0.35 to reflect the range in grain size, grading, angularity, and possible variations in packing that might occur during installation. Longitudinal and traverse/vertical transverse dispersivity were set to low values of 0.0005 m and 0.0001 m, respectively.

Table 2-4 provides detailed information on screen properties. Calculations of hydraulic conductivity and porosity are based on three columns of slots on a 0.0508 m (2 inches) diameter pipe with standard slot penetration of 0.0254 m (one inch) minimum inside length and $6.35 \times 10^{-3}$ m (0.25 inch) slot spacing. Porosity is calculated as the ratio of open area of the slots divided by the surface area of the pipe without slots over the same length. The bulk hydraulic conductivity of the screen is calculated using an equivalent porous media approach by equating Darcy’s law (Equation 1) with the cubic law for uniform flow through a single slot (Equation 2), written as:

$$Q = -K_{\text{screen}}Ai$$

$$\frac{Q}{\Delta H} = -\frac{\rho g}{12\mu} (2b)^3 \frac{W}{L}$$

where $Q$ is the flow rate [$\text{L}^3 \text{T}^{-1}$], $K_{\text{screen}}$ is the hydraulic conductivity of the screen [$\text{L} \text{T}^{-1}$], $i$ is the hydraulic gradient [$\text{L} \text{L}^{-1}$], $\Delta H$ is the change in head along the length of the screen slot [$\text{L}$], $\rho$ is the density of water [$\text{M L}^{-3}$], $g$ is the gravitational acceleration constant [$\text{L T}^{-2}$], $\mu$ is the viscosity of water [$\text{M L}^{-1} \text{T}^{-1}$], $2b$ is the aperture of the slot [$\text{L}$], $W$ is the width of the slot [$\text{L}$], and $L$ is the length of the slot [$\text{L}$] (i.e. the wall thickness of the screen). The cross-sectional area of the screen, $A$, for a single slot is equal to the product of the slot spacing and one-third of the
circumference of the screen (for the case of three rows of slots). Equating $Q$ in Equations (1) and (2) and simplifying yields:

$$K_{\text{screen}} = \frac{\rho g (2b)^3 W}{12 \mu A_{\text{screen}}}$$  \hspace{1cm} (3)

Both the porosity and $K_{\text{screen}}$ are input parameters in the numerical model. The hydraulic conductivity is considered anisotropic with $K_x = K_y = K_{\text{screen}}$ and $K_z = 1 \times 10^{-10} \text{ m/s}$ (impermeable). Longitudinal and traverse/vertical transverse dispersivity were set to low values of 0.0005 m and 0.0001 m, respectively.

Table 2-3 indicates that certain sand pack grades are only compatible with some of the screen slot sizes (Table 2-4) to retain the material (99%, based on grain diameter). Table 2-5 shows all of the compatible combinations using the sand pack and screen materials presented.

### 2.3 Results

The following sections outline the results from modeling simulations examining the influence of different screen and sand pack combinations on obtaining a representative geochemical groundwater sample. The effect of the sand pack porosity, pumping rate, single fracture aperture and location, and multiple equally-spaced, equal-aperture fractures on the timing of 99% fractional contribution of formation water to the pump discharge ($t_{99}$) are also examined.

#### 2.3.1 Screen and Sand Pack Combinations

Two configurations are considered: 1) a 3 m-long screen and sand pack with a single fracture intersecting at $z = 1.5$ m, and 2) a 6 m-long screen and sand pack with a single fracture intersecting at $z = 3$ m. The pump is located at the same $z$ as the fracture in both cases and withdraws water at a constant rate of 1 L/min for the duration of the simulation. Fracture
apertures of 500 and 750 microns are considered. The compatible screen and sand pack combinations for these two different apertures are summarized in Table 2-5.

The resultant $t_{99}$ are plotted for each screen-sand pack combination and fracture in Figure 2-4. A visualization of the concentration and velocity vector profile in the screen and sand pack ($x = 0$ to 0.0508 m) is shown for each fracture-screen slot-sand pack combination in Appendix B, Figures B1-B4 (it should be noted that there is significant horizontal exaggeration of approximately 118 in all the concentration profiles shown in Appendix B). Two general trends are noted in the data: 1) $t_{99}$ increases in cases where the same screen is used in combination with coarsening grades of sand pack material (shown by the dashed line in Figure 2-4B), and 2) $t_{99}$ decreases for a particular sand pack grade in combination with increasing screen slot sizes (shown by the solid line in Figure 2-4B). There are cases where the opposite of these trends are observed, shown in bolder colours in Figure 2-4.

### 2.3.2 Sand Pack Porosity

The results of varying the sand pack porosity between 0.2 and 0.35 are shown in Figure 2-5 for the case of a 500 micron fracture intersecting a 3 m screen and sand pack at a pumping rate of 1 L/min. Both the pump intake and fracture are located at $z = 1.5$ m. The difference in $t_{99}$ for the two porosity cases ranges between 19 and 33%.

### 2.3.3 Pumping Rate

The influence of pumping rate on $t_{99}$ is tested at $Q = 0.1, 0.5, 1, 5,$ and $10$ L/min. The sand pack grade and screen slot size are grade F and 0.508 mm, respectively. The length of the screen and sand pack is 6 m, and the fracture (750 microns) and pump are both located at $z = 3$ m. The results are shown in Figure 2-6 and a visualization of the concentration and velocity vector profile
in the screen and sand pack is shown for each case in Appendix B, Figure B5. The $t_{99}$ varies between 640 min ($Q = 0.1$ L/min) and 7 min ($Q = 10$ L/min), and is scaled roughly in the same proportions as the pumping rate. For example, when $Q = 1$ L/min: $t_{99}$ is 62 min, and when $Q = 0.1$ L/min: $t_{99}$ is 690 min – the difference in $Q$ is a factor of 10 while the difference in $t_{99}$ is a factor of 11.1.

2.3.4 Single Fracture Location

This case was explored using the same configuration as in 2.3.3 except $Q$ is maintained at 1 L/min while the location of the 750 micron fracture is moved to $z = 0, 1, 2,$ and $3$ m. The influence of changing the location of the fracture on the concentration breakthrough curve for the pump discharge and $t_{99}$ is shown in Figure 2-7A. A visualization of the concentration and velocity vector profile in the screen and sand pack for each fracture location case is shown in Appendix B, Figure B6. The required purging time, $t_{99}$, ranges from 36 to 62 min with the shortest time and largest velocity vectors occurring when the fracture is located at the bottom of the screen, and the longest time and smallest velocity vectors occurring when the fracture is at the midpoint along the screen (coinciding with the location of the pump intake). The ratio of the maximum velocity vectors between these two fracture placements (top/bottom and middle of the screen) is approximately three.

2.3.5 Single Fracture Aperture

The influence of the aperture for a single fracture located at $z = 3$ m on $t_{99}$ is tested using the same domain configuration as in 2.3.3. The pump is located at $z = 3$ m and the pumping rate is 1 L/min. The single fracture apertures tested are 400, 600, 800 and 1000 microns. The fracture longitudinal and transverse longitudinal dispersivities are kept at 0.05 m and 0 m, respectively, for all cases. The influence of the different fracture apertures on $t_{99}$ is shown in Figure 2-7B. A
visualization of the solute concentration and velocity vector profiles in the screen and sand pack are shown in Appendix B, Figure B7. The required $t_{99}$ generally increases with increasing fracture aperture. It should be noted that the concentration profile in the sand pack at $t_{99}$ is very similar for all cases of fracture aperture (Appendix B, Figure B8).

### 2.3.6 Multiple Equivalent-Aperture Fractures

The same test configuration is used as in 2.3.3 except the transmissivity of the aquifer is divided into two, three, four, and five equally-spaced fractures. The equivalent aperture of a single 750 micron fracture is 595 microns (two fractures), 520 microns (three fractures), 472 microns (four fractures), and 439 microns (five fractures). The single fracture is located at $z = 3$ m. The locations of the multiple fractures are $z = 2$ and 4 m (two fractures), $z = 1.5, 3,$ and 4.5 m (three fractures), $z = 1.2, 2.4, 3.6,$ and 4.8 m (four fractures), and $z = 1, 2, 3, 4,$ and 5 m (five fractures). The pump location is maintained at $z = 3$ m in all cases. The fracture longitudinal and transverse longitudinal dispersivities are kept at 0.05 m and 0 m, respectively. The results of the breakthrough curves in the pump discharge are shown in Figure 2-8. A visualization of the solute concentration and velocity vector profile in the sand pack and screen at $t_{99}$ is shown in Appendix B, Figure B9. The $t_{99}$ varies between 62 and 138 minutes with the shortest purging time occurring for the case of a single fracture and the longest purging time for the case of three fractures. The $t_{99}$ decreases when there are more than three fractures in the cases shown.

### 2.4 Discussion

It is evident from Figure 2-4 to 2-8 that $t_{99}$ is inconsistent within the screen, sand pack and fracture configurations explored in this study using a numerical model. It should also be noted that the screen and sand pack concentration profiles in Appendix B (which also display velocity vectors) show substantial variability in the volume of sand pack that remains passive during
pumping conditions (shown by zero concentration of the solute). The following discussion provides an explanation for the variability in $t_{99}$ based on hydraulic conductivity ratios, flow field truncation, and time-dependent drawdown. The applicability of the findings in this study to optimizing multi-level construction in fractured bedrock aquifers, and the limitations of the modeling approach are also discussed.

2.4.1 The Role of Hydraulic Conductivity Ratios

Figure 2-4 shows that the screen-sand pack combination can have a sizeable impact on $t_{99}$. For example, a 500 micron fracture intersecting a 3 m interval constructed with grade D sand pack and 0.254 mm screen slots has a purge time of approximately 73.1 min, while the $t_{99}$ can be reduced to approximately 27.7 min using grade G sand pack and 1.626 mm screen slots. The cause for this disparity is the result of the amount of spreading that occurs in the sand pack (as shown in Appendix B) due to changes in hydraulic conductivity between the fracture, sand pack and screen. Table 2-6 provides a summary of the ratios of these hydraulic conductivities for the cases presented in Figure 2-4.

The results show that $t_{99}$ increases when the difference in hydraulic conductivity between the screen and sand pack becomes larger, which causes increased spreading in the sand pack (the same as the refraction in flow lines observed as water passes through one stratum to another with different hydraulic conductivity). This increase is the result of the development of larger “envelopes” of spreading. The enlargement acts to prolong $t_{99}$ by introducing lower concentration water at low velocities (i.e. low concentration flux) from the fringe of the envelope at late-time, effectively diluting the flux-averaged concentration in the borehole. There are cases where the envelope cannot expand to its normal size (noted in bold colours in Figure 2-4 and by
gray shading in Table 2-6), as dictated by the ratio of the hydraulic conductivities, due to boundary effects at the top and bottom of the sand pack. This is discussed further in the following section.

Spreading decreases when the same sand pack grade is used with increasing screen slot sizes as the screen becomes less of a flow-limiter. The concentration profiles in Appendix B, Figures B1-B4 show this the best. The shortest purging times occur when the ratio of hydraulic conductivities between the screen, sand pack, and intersecting fracture is close to 1:1:1 (Table 2-6) in cases not influenced by boundary effects. However, the role of the fracture hydraulic conductivity in the ratios is not as crucial to reducing $t_{99}$ as just designing the hydraulic conductivities of the screen and sand pack to be as close as possible.

2.4.2 Truncation of the Flow Field

A reversal in the general $t_{99}$ trend with respect to screen and sand pack combinations was noted in Figure 2-4 (bold colours), particularly in cases where the length of the screen was 3 m (also indicated by gray shading in Table 2-6). This is attributed to the truncation of the flow field by the upper and lower boundaries of the sand pack. For example, the spread of the flow field observed in the concentration profile for a 500 micron fracture intersecting a 6 m interval constructed using grade F sand pack and 0.254 m screen slots is approximately 4 m (see Appendix B, Figure B3) with a resultant $t_{99}$ of 148.7 min. However, a reduction of the screen length to 3 m confines this spreading, resulting in higher velocities along the screen and a reduction of $t_{99}$ to 43.6 min. This same truncation of the flow field due to the boundary of the sand pack occurs as the fracture location is moved along the axis of the screen (Figure 2-7A; Appendix B, Figure B6).
Flow field truncation also explains the changes observed in $t_{99}$ in the case of multiple equivalent-aperture fractures (Figure 2-8; Appendix B, Figure B9). As the number of fractures increases, so does the degree of flow field truncation both at the upper and lower sand pack boundary and between the fractures as well. This is much more evident as $t_{99}$ decreases from 138 min to 104 min between the three- and five-fracture cases.

2.4.3 Time-Dependent Drawdown and Capture Zone
The fractional, time-dependent contribution of original borehole water to pump discharge (from drawdown) has little impact on $t_{99}$ in the cases tested. Increases in pumping rate (Figure 2-6; Appendix B, Figure B5) would cause more drawdown in the borehole. However, the resulting increase in velocities through the sand pack and the higher velocities along the envelope of spreading outweigh the effects of drawdown. It should be noted that the envelope of spreading is more tapered towards the screen in the cases with pumping rates of 5 and 10 L/min (Appendix B, Figure B5). This suggests that the flow system is still transient at the time $t_{99}$ is reached compared to the other examples where the shape of the flow envelope is quite rectangular in the sand pack.

The effects of drawdown on the flux-averaged concentration in the borehole are also observed in the tests where the intersecting fracture aperture is reduced (Figure 2-7B; Appendix B, Figure B8). The fractional contribution of drawdown to pump discharge is most evident in the case of the 400 microns fracture where there is a delay in the early stages of the breakthrough curve. However, this early-time lag does not result in a longer $t_{99}$ compared to the other cases with larger fracture apertures because of the hydraulic conductivity ratios, for the reasons discussed in 2.4.1.
The capture zone is defined as the distance away from the well that current pump discharge is sourced from. The reach of the capture zone is influenced by time-dependent drawdown in the riser and the duration of pumping. The radius of the capture zone is variable since $t_{99}$ has such a broad range in the cases explored in this study, and $t_{99}$ is weakly influenced by the time-dependent drawdown. For example, Table 2-6 shows the $t_{99}$ for the case of F grade sand pack combined with a 0.254 and 1.016 mm screen slots as 148.7 and 28.6 min, respectively (6 m screen, 500 micron fracture). Drawdown (at $t_{99}$) in the riser is 0.259 and 0.244 m for each combination, respectively. However, the capture radius for the first example is 9.7 m and 4.2 m for the second. In comparison, the $t_{99}$ and the drawdown (at $t_{99}$) in the riser for the case of a 750 micron fracture in combination with F grade sand pack and 0.254 mm screen slots (6 m screen) is 151.2 min and 0.086 m, respectively. The resultant capture radius in this case is 8.0 m. The difference in the capture zone radii presented here is approximately a factor of two. However, the absolute radii calculated here are not large, meaning the capture zone remains relatively local to the well at $t_{99}$.

2.4.4 Optimizing Multi-level Construction and Field Implementation

As is evident from these results, shorter screen lengths do not make for shorter purging times unless there is a truncation in the flow field. The easiest way to reduce purging times is by increasing the pumping rate. However, this may not be favourable depending on the solute of interest, as previously discussed. Without the need to retain the bedrock itself in the borehole (unlike in porous media), the only restriction to what screen and sand pack materials can be used is the aperture of the largest fracture (assuming the rock is stable and there are not any turbidity issues). The modeling results show that $t_{99}$ is reduced when the ratio of the screen and sand pack hydraulic conductivities is 1:1. Conversely, $t_{99}$ increases as the hydraulic conductivity ratio
between the materials increases. The purge time is optimized (lowest $t_{99}$) when neither material acts as a flow limiter. However, the sand pack grain size required when large fractures are present might be problematic. For example, the hydraulic conductivity of a 1000 micron fracture is approximately equal to $7.3 \times 10^{-1}$ m/s. The equivalent sand pack material would likely be medium- to coarse-grained gravel (Freeze and Cherry 1979). There may be issues trying to get this size of material down into the annular space around the screen to make a proper pack, especially when there is a riser from a deeper interval also passing through the interval (see Figure 2-1). Creating a proper seal with bentonite on either side of a sand pack with such large grain diameters and pore throats might also be difficult. The bentonite chips would likely enter into the pore spaces at the top of the sand pack in this case before hydrating and expanding. The extent to which the bentonite might migrate into the sand pack during installation is not known, but it could seal off fractures of interest.

An optimal multi-level completion in bedrock wells requires a detailed hydraulic characterization of the borehole, including locations of the significant fracture features and approximations of fracture hydraulic conductivity and equivalent aperture. This can be done using a variety of techniques, including: straddle packer testing, borehole caliper, and making observations using a submersible video camera (Novakowski and Sudicky 2006). This allows for the proper placement of the interval within the borehole and selection of appropriate screen and sand pack materials. Trying to reduce purging times using flow field truncation by way of locating the top and/or bottom of the sand pack at a fracture (see 2.3.4 and 2.4.2) is not recommended since the subsequent velocities that might occur at or near the sand pack-bentonite seal interface may cause the scour, mobilization, and removal of the bentonite.
2.4.5 Limitations to the Modeling Approach

The assumption that the initial concentration of the solute is zero in the borehole and one in the aquifer has a few short-comings. Firstly, previous work has shown that the initial borehole water is typically not more than 25% different than the aquifer (Barber and Davis 1987). Thus, the estimations of \( t_{99} \) are likely very conservative. Secondly, the distribution of the solute concentration is assumed to be homogeneous in the aquifer. This is not a realistic estimate of how solutes are likely to be distributed in the subsurface at a given site. However, the capture zone estimates presented earlier show that the radii remain relatively small (<10 m). The heterogeneity of the solute distribution in the fracture on this scale may be low.

Purging a monitoring well is a fully-transient scenario and should be modeled as such. One issue with this approach is that the transient transport solution cannot be verified using an analytical model. Thus, it is difficult to determine what spatiotemporal discretization is correct. The spatiotemporal discretization used in this study was the result of a sensitivity analysis of the flow and transport solution at a specified point in space and time to changes in the grid generation parameters and concentration control. The final spatiotemporal discretization employed was a balance between how much the solution changed between different realizations of the model domain and computation runtime.

Another issue with the fully-transient scenario is dealing with dispersivity. It is quite clear from Gelhar et al. (1992) that dispersion is scale-dependent. As the capture zone radius continues to enlarge during pumping, so too should the dispersivity. This is not accommodated for in the numerical model as only a single value of dispersivity in each principal direction can be used.
However, the short lengths and narrow ranges of the capture zone radii calculated in 2.4.3 suggest this may not be a significant source of error. Also, a sensitivity analysis indicated that $t_{99}$ is not greatly influenced by changes in the fracture dispersivity (~1% difference in $t_{99}$ over 3.5 orders of magnitude). The required purging time is more sensitive to changes in dispersivity in the sand pack (ten percent difference in $t_{99}$ over 2.5 orders of magnitude). However, it is not expected that the sand pack dispersivity would be large or very variable since the commercially available grades are well-sorted and the grains are generally smooth and rounded.

### 2.5 Conclusions

The results from this study lead to the following conclusions on how the screen and sand pack influence the purging time required ($t_{99}$) to obtain a representative geochemical groundwater sample from a multi-level bedrock monitoring well interval:

1. The ratios of hydraulic conductivities between the screen, sand pack, and fracture control the amount of spreading and groundwater velocities in the sand pack. Only a small portion of the sand pack may actually become hydraulically active during pumping.

2. The required purging time (and volume) can be significantly reduced by choosing screen and sand pack materials that have similar hydraulic conductivities. The optimal configuration (shortest purging time) is achieved when ratio of the screen, sand pack, and fracture hydraulic conductivities are close to 1:1:1.

3. A shorter screen does not necessarily reduce purging times unless the flow field from the fracture is truncated by the upper and lower boundaries of the sand pack.

4. The location of fractures with respect to other fractures or the upper and lower boundaries of the sand pack can also act to reduce purging times due to flow field truncation.
The results in this study are best used for understanding the relative relationships in $t_{99}$ rather than absolute values for a given scenario. This is because of the conservative assumptions made in the initial transport conditions and the possible issues associated with using fully-transient conditions in the numerical model.
2.6 References


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Table 2-1: Spatial discretization used in the 2-D domain (unit-thickness) with axisymmetric coordinates. Examples of discretization in z are shown for the cases of a single or multiple fractures intersecting the sand pack.

<table>
<thead>
<tr>
<th>From (m)</th>
<th>To (m)</th>
<th>Starting block size (m)</th>
<th>Multiplier (-)</th>
<th>Maximum block size (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>X</td>
<td>0</td>
<td>0.0254</td>
<td>0.0005</td>
<td>1.05</td>
</tr>
<tr>
<td></td>
<td>0.0508</td>
<td>0.0254</td>
<td>0.0005</td>
<td>1.05</td>
</tr>
<tr>
<td></td>
<td>0.0508</td>
<td>250</td>
<td>0.0005</td>
<td>1.05</td>
</tr>
<tr>
<td></td>
<td>0.001*</td>
<td>0.001</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Y</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Z\textsuperscript{a}</td>
<td>1.5</td>
<td>0</td>
<td>0.0002</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>1.5</td>
<td>3</td>
<td>0.0002</td>
<td>2</td>
</tr>
<tr>
<td>Z\textsuperscript{b}</td>
<td>1</td>
<td>0</td>
<td>0.0002</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>1.5</td>
<td>0.0002</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.5</td>
<td>0.0002</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>3</td>
<td>0.0002</td>
<td>2</td>
</tr>
</tbody>
</table>

A) an example of the gridding scheme in z for the case of a single fracture placed at z = 1.5 m in a 3 m high domain
B) an example of the gridding scheme in z for the case of two fractures placed at z = 1 and 2 m in a 3 m high domain
* ensures nodes are placed at 0.001 m so that 0.001 m-thick screen can be defined
Table 2-2: Numerical model input parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value or Range</th>
<th>Parameter</th>
<th>Value or Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow simulation</td>
<td>transient</td>
<td>Pump location</td>
<td>typically at the same location in z as the fracture in single-fracture cases</td>
</tr>
<tr>
<td>Initial head</td>
<td>0.0</td>
<td>Fracture aperture</td>
<td>200 – 1000 microns</td>
</tr>
<tr>
<td>Specified head at x = 250 m</td>
<td>0.0</td>
<td>Fracture storativity</td>
<td>1x10^{-5}</td>
</tr>
<tr>
<td>Flow solver convergence criteria</td>
<td>1x10^{-10}</td>
<td>Fracture longitudinal dispersivity</td>
<td>0.05 m</td>
</tr>
<tr>
<td>Well screen and casing radius</td>
<td>0.0254 m</td>
<td>Fracture transverse longitudinal dispersivity</td>
<td>0 m</td>
</tr>
<tr>
<td>Length of screen and casing</td>
<td>3- 6 m</td>
<td>Matrix K (isotropic)</td>
<td>1x10^{-10} m/s</td>
</tr>
<tr>
<td>Solute free-solution diffusion coefficient</td>
<td>1x10^{-10} m²/s</td>
<td>Matrix porosity</td>
<td>0.001</td>
</tr>
<tr>
<td>Transport solver convergence criteria</td>
<td>1x10^{-15}</td>
<td>Matrix longitudinal dispersivity</td>
<td>0.0005 m</td>
</tr>
<tr>
<td>Concentration control</td>
<td>0.05</td>
<td>Matrix transverse and vertical transverse dispersivity</td>
<td>0.0001 m</td>
</tr>
<tr>
<td>Initial concentration in screen and sand pack</td>
<td>0 (arbitrary units)</td>
<td>Matrix storativity</td>
<td>1x10^{-5}</td>
</tr>
<tr>
<td>Specified concentration in the aquifer (matrix and fracture)</td>
<td>1 (arbitrary units)</td>
<td>Screen properties</td>
<td>discussed in 2.2.2.3</td>
</tr>
<tr>
<td>Pumping rate</td>
<td>0.1 – 10 L/min</td>
<td>Sand pack properties</td>
<td>discussed in 2.2.2.3</td>
</tr>
</tbody>
</table>
Table 2-3: Properties of sand pack materials. A) Cumulative weight percent passed for a suite of commercially available sand pack blends. The maximum screen slot or fracture aperture that each grade is compatible with is shown. B) Estimated values of hydraulic conductivity for sand pack materials based on the grain size distribution and the Hazen Method.

A)

<table>
<thead>
<tr>
<th>Sand Pack Grade</th>
<th>ASTM E11 Sieve # and open mm</th>
<th>Max. Slot Size</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>4.75 3.35 2.36 1.70 1.18 0.85 0.60 0.42 0.30 0.25 0.21</td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>100 95 40 5 2 1</td>
<td>0.25 0.010</td>
</tr>
<tr>
<td>B</td>
<td>100 99 35 5 1</td>
<td>0.30 0.012</td>
</tr>
<tr>
<td>C</td>
<td>100 99 50 5 1</td>
<td>0.42 0.016</td>
</tr>
<tr>
<td>D</td>
<td>100 95 45 5 1</td>
<td>0.60 0.023</td>
</tr>
<tr>
<td>E</td>
<td>100 95 55 10 1</td>
<td>0.85 0.033</td>
</tr>
<tr>
<td>F</td>
<td>100 99 55 5 1</td>
<td>1.18 0.045</td>
</tr>
<tr>
<td>G</td>
<td>99 50 10 1</td>
<td>1.70 0.067</td>
</tr>
</tbody>
</table>

B)

<table>
<thead>
<tr>
<th>Sand Pack Grade</th>
<th>d_{10} (mm)</th>
<th>Size and class (based on d_{50})</th>
<th>C</th>
<th>Range in K (x10^{-3} m/s)</th>
<th>Mid-point of K range (x10^{-3} m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.3</td>
<td>medium sand</td>
<td>80-120</td>
<td>0.720 - 1.08</td>
<td>0.90</td>
</tr>
<tr>
<td>B</td>
<td>0.44</td>
<td>coarse sand</td>
<td>120-150</td>
<td>2.32 – 2.90</td>
<td>2.61</td>
</tr>
<tr>
<td>C</td>
<td>0.62</td>
<td>coarse sand</td>
<td>120-150</td>
<td>4.61 – 5.77</td>
<td>5.19</td>
</tr>
<tr>
<td>D</td>
<td>0.88</td>
<td>v. coarse sand</td>
<td>120-150</td>
<td>9.29 – 11.6</td>
<td>10.5</td>
</tr>
<tr>
<td>E</td>
<td>1.18</td>
<td>v. fine pebble</td>
<td>120-150</td>
<td>16.7 – 20.9</td>
<td>18.8</td>
</tr>
<tr>
<td>F</td>
<td>1.75</td>
<td>v. fine pebble</td>
<td>120-150</td>
<td>36.7 – 45.9</td>
<td>41.3</td>
</tr>
<tr>
<td>G</td>
<td>2.36</td>
<td>v. fine pebble</td>
<td>120-150</td>
<td>66.8 – 83.5</td>
<td>75.2</td>
</tr>
</tbody>
</table>
Table 2-4: Estimated hydraulic conductivities for varying slot sizes on a 0.0508 m (2’’)
diameter screen based on 3 rows of slots with standard slot penetration of 0.0254 m (1’’)
minimum inside length and 6.35x10^{-3} m (0.25’’) spacing.

<table>
<thead>
<tr>
<th>Slot Size</th>
<th>( \times 10^{-3} \text{ m/s} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{inches} )</td>
<td>0.01</td>
</tr>
<tr>
<td>( \text{millimetres} )</td>
<td>0.254</td>
</tr>
<tr>
<td>( \text{m}^2 \text{ open area} / \text{m (x10}^{-3}) )</td>
<td>2.794</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.018</td>
</tr>
<tr>
<td>( K_{\text{screen}} \text{ (x10}^{-3} \text{ m/s}) )</td>
<td>0.896</td>
</tr>
</tbody>
</table>
Table 2-5: Compatible screen and sand pack materials based on slot size and the retention of 99% of the grains (shaded boxes). Screen and sand pack combination that are compatible with 500 and 750 micron fractures are denoted using $a$ and $b$, respectively.

<table>
<thead>
<tr>
<th>Sand Pack Grade</th>
<th>Slot size in millimetres</th>
<th>0.254</th>
<th>0.330</th>
<th>0.508</th>
<th>0.711</th>
<th>1.016</th>
<th>1.295</th>
<th>1.626</th>
<th>2.591</th>
<th>3.251</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>$a$, $a$, $a$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>E</td>
<td>$a$, $b$, $a$, $b$, $a$, $b$, $a$, $b$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>$a$, $b$, $a$, $b$, $a$, $b$, $a$, $b$, $a$, $b$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>G</td>
<td>$a$, $b$, $a$, $b$, $a$, $b$, $a$, $b$, $a$, $b$, $a$, $b$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 2-6: Hydraulic conductivity ratios for well construction materials for the case of a single A) 500 micron fracture, and B) 750 micron fracture intersecting the interval. The cases where the flow field is truncated by the boundaries of the sand pack, resulting in a reduction in $t_{99}$, are noted by gray shading. The pumping rate is 1 L/min.

### A) 500 micron fracture

<table>
<thead>
<tr>
<th>Slot size (mm)</th>
<th>Sand grade</th>
<th>Screen</th>
<th>Sand pack</th>
<th>Fracture (500 µm)</th>
<th>$K_{screen}$:$K_{sand}$:$K_{fracture}$</th>
<th>Flow limiter</th>
<th>$t_{99}$ (min) for $n_{sand} = 0.2$, 3 m screen</th>
<th>$t_{99}$ (min) for $n_{sand} = 0.2$, 6 m screen</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.254</td>
<td>D</td>
<td>0.896</td>
<td>10.5</td>
<td>182</td>
<td>1 : 11.7 : 202.9</td>
<td>Screen</td>
<td>73.1</td>
<td>74.9</td>
</tr>
<tr>
<td></td>
<td>E</td>
<td>0.896</td>
<td>18.8</td>
<td>182</td>
<td>1 : 21.0 : 202.9</td>
<td>Screen</td>
<td>61.5</td>
<td>104.2</td>
</tr>
<tr>
<td></td>
<td>F</td>
<td>0.896</td>
<td>41.3</td>
<td>182</td>
<td>1 : 46.1 : 202.9</td>
<td>Screen</td>
<td>36.7</td>
<td>133.9</td>
</tr>
<tr>
<td></td>
<td>G</td>
<td>0.896</td>
<td>75.2</td>
<td>182</td>
<td>1 : 83.9 : 202.9</td>
<td>Screen</td>
<td>55.1</td>
<td>52.1</td>
</tr>
<tr>
<td>0.330</td>
<td>D</td>
<td>1.97</td>
<td>10.5</td>
<td>182</td>
<td>1 : 6.3 : 92.4</td>
<td>Screen</td>
<td>71.7</td>
<td>68.7</td>
</tr>
<tr>
<td></td>
<td>E</td>
<td>1.97</td>
<td>18.8</td>
<td>182</td>
<td>1 : 9.6 : 92.4</td>
<td>Screen</td>
<td>61.5</td>
<td>104.2</td>
</tr>
<tr>
<td></td>
<td>F</td>
<td>1.97</td>
<td>41.3</td>
<td>182</td>
<td>1 : 21.0 : 92.4</td>
<td>Screen</td>
<td>46.1</td>
<td>143.2</td>
</tr>
<tr>
<td></td>
<td>G</td>
<td>1.97</td>
<td>75.2</td>
<td>182</td>
<td>1 : 38.2 : 92.4</td>
<td>Screen</td>
<td>58.6</td>
<td>54.6</td>
</tr>
<tr>
<td>0.508</td>
<td>D</td>
<td>7.17</td>
<td>10.5</td>
<td>182</td>
<td>1 : 15.5 : 25.4</td>
<td>Screen</td>
<td>34.4</td>
<td>34.4</td>
</tr>
<tr>
<td></td>
<td>E</td>
<td>7.17</td>
<td>18.8</td>
<td>182</td>
<td>1 : 26.0 : 25.4</td>
<td>Screen</td>
<td>42.1</td>
<td>40.1</td>
</tr>
<tr>
<td></td>
<td>F</td>
<td>7.17</td>
<td>41.3</td>
<td>182</td>
<td>1 : 5.8 : 25.4</td>
<td>Screen</td>
<td>57.6</td>
<td>54.6</td>
</tr>
<tr>
<td></td>
<td>G</td>
<td>7.17</td>
<td>75.2</td>
<td>182</td>
<td>1 : 10.5 : 25.4</td>
<td>Screen</td>
<td>77.3</td>
<td>76.2</td>
</tr>
<tr>
<td>0.711</td>
<td>D</td>
<td>19.7</td>
<td>18.8</td>
<td>182</td>
<td>1 : 1.1 : 9.7</td>
<td>Sand Pack</td>
<td>29.6</td>
<td>29.6</td>
</tr>
<tr>
<td></td>
<td>E</td>
<td>19.7</td>
<td>41.3</td>
<td>182</td>
<td>1 : 2.1 : 9.2</td>
<td>Screen</td>
<td>36.6</td>
<td>35.6</td>
</tr>
<tr>
<td></td>
<td>F</td>
<td>19.7</td>
<td>75.2</td>
<td>182</td>
<td>1 : 3.8 : 9.2</td>
<td>Screen</td>
<td>47.5</td>
<td>46.5</td>
</tr>
<tr>
<td>1.016</td>
<td>F</td>
<td>57.3</td>
<td>41.3</td>
<td>182</td>
<td>1 : 1.4 : 4.4</td>
<td>Sand Pack</td>
<td>27.6</td>
<td>28.6</td>
</tr>
<tr>
<td></td>
<td>G</td>
<td>57.3</td>
<td>75.2</td>
<td>182</td>
<td>1 : 1.3 : 3.2</td>
<td>Screen</td>
<td>32.5</td>
<td>32.5</td>
</tr>
<tr>
<td>1.295</td>
<td>G</td>
<td>119</td>
<td>75.2</td>
<td>182</td>
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### B) 750 micron fracture

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<th>Flow limiter</th>
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Figure 2-1: Cross-section of an open well (left) and multi-level monitoring well (right) in a bedrock aquifer. The larger aperture fractures will dominate the water chemistry in the borehole (indicated by the size of the arrows and colouring). Not to scale.
Figure 2-2: A) Conceptual model cross-section of a sampling interval intersected by a single fracture in a confined aquifer. B) Implementation of the three-dimensional conceptual model in a two-dimensional, unit-thickness numerical domain. Axisymmetric coordinates are used to simulate radial flow to a single pumping well. Not to scale.
Figure 2-3: Schematic for gridding in the numerical model. The arrow indicates the direction of coarsening away from a boundary (fracture plane, sand pack-aquifer interface, etc.). The dashed line shows where planes of symmetry are in the domain due to the discretization. Not to scale.
Figure 2-4: Estimated required purge times to achieve 99% fractional contribution of formation water in the pump discharge for two different fracture apertures and a variety of screen and sand pack combinations. The pumping rate is 1 L/min. When the length of the screen is 3 m (A), the pump and fracture are located at $z = 1.5$ m. When the length of the screen is 6 m (B), the pump and fracture are located at $z = 3$ m. The solid line in B) shows the general decrease in $t_{99}$ when the same sand pack grade is paired with increasingly larger screen slots. The dashed line in B) shows the general increase in $t_{99}$ when the same screen slot size is paired with increasingly coarser sand pack grades. Cases where the flow field from the fracture is being truncated by the upper and lower boundaries of the sand pack are shown in bolder colours in A) and B). This results in the opposite trends in $t_{99}$, shown by the solid and dashed lines in B), for the non-truncated cases.
Figure 2-5: The influence of sand pack porosity (n) on the required purged time necessary for achieving 99% fractional contribution of formation water in the pump discharge, $t_{99}$, for the case of a 750 micron fracture intersecting a 3 m interval at $z = 1.5$ m. The pump intake is located at $z = 1.5$ m and the pumping rate is 1 L/min. The difference in $t_{99}$ ranges between 19 and 33% for each sand pack-screen combination.
Figure 2-6: Concentration breakthrough curves in the pump discharge when the pumping rate is varied between 0.1 and 10 L/min. The sand pack grade and slot size are F (n = 0.2) and 0.508 mm, respectively. The fracture and pump are placed at z = 3 m.
Figure 2-7: Concentration breakthrough curves in the pump discharge when A) the location of a single 750 micron fracture is varied along the length of the 6 m screen, and B) the aperture of single fracture located at $z = 3$ m is changed between 400 and 1000 microns. The sand pack grade and slot size are F ($n = 0.2$) and 0.508 mm, respectively. The pump intake is located at $z = 3$ m and the pumping rate is 1 L/min.
Figure 2-8: Concentration breakthrough curves in the pump discharge when multiple equivalent-aperture, equally-spaced fractures (cumulative transmissivity equal to a single 750 micron fracture) intersect a 6 m interval. The sand pack grade and slot size are F (n = 0.2) and 0.508 mm, respectively. The pumping rate is 1 L/min with the pump intake located at z = 3 m.
Chapter 3

Discretizing a Discrete Fracture Model for Simulation of Radial Transport

3.1 Introduction

Solute transport in fractured rock is of particular concern in groundwater environments impacted by anthropogenic activities where there are sensitive nearby receptors, such as domestic wells, rivers and lakes that are used as a drinking water supply or are sensitive aquatic habitats. The rate of migration and degree of dispersion and matrix diffusion are important factors in evaluating the travel time between source and receptor (Abelin et al. 1991; Novakowski and Lapcevic 1994). Consideration for radial solute transport is important when a pump (injection or withdrawal) is employed, such as the case of wastewater injection, domestic water wells, and tracer experiments.

Domestic water well receptors are of particular concern because of potential contaminant-related human health risks and compliance with regulatory drinking water standards. Monitoring wells may be employed to provide direct access to the aquifer for groundwater sampling purposes at a particular location away from a known contaminant source, or solute concentrations can be estimated through analytical or numerical methods. The estimation of solute concentration in a passive, finite volume well receptor in a steady flow field can be calculated by converting time-concentration point data using Palmer (1988). A mass balance approach with a first-order boundary condition at the well-aquifer interface is used to describe tracer entering, mixing and exiting the borehole. The formulation was developed for porous media but can be adapted to bedrock aquifers albeit for one fracture only.
Tracer experiments have been employed to investigate transport parameters in fractured bedrock settings by the nuclear, environmental, and petroleum industries for over thirty years (Bodin et al. 2003). The complexities of fracture networks and heterogeneous transport commonly observed in fractured rock often make large-scale tracer experiments costly and difficult to implement (Abelin et al. 1991). As a result, many tracer experiments in the literature are those conducted in a single fracture (Lapcevic et al. 1999; Novakowski et al. 2004; Novakowski et al. 2006) or a well-defined fracture zone (Novakowski 1992a; Himmelsbach et al. 1998; Hoehn et al. 1998; Becker and Shapiro 2003), typically on the scale of <50 m. There are numerous ways in which these tests can be performed, the most common of which are tracer injection in divergent or convergent flow fields (Gelhar et al. 1985). The benefit of the divergent flow field method is that only a single tracer is necessary, and numerous monitoring wells can be used to determine the spatiotemporal distribution of the solute in the formation (Novakowski 1992a).

Numerous analytical and numerical models have been developed for the interpretation of radial transport in steady divergent flow fields in a single fracture or homogeneous porous medium (Chen 1985; Hseih 1986; Valocchi 1986; Chen 1987; Raven et al. 1988; Novakowski 1992a; Andersson et al. 2004; Huang and Goltz 2006; Liou 2009). Novakowski (1992a) provides analytical solutions for the resident concentration in two scenarios involving a single fracture: 1) borehole-to-borehole, where both the injection borehole and the observation borehole have a finite volume; 2) borehole-to-point, where the injection borehole has a finite volume and the observation borehole volume is negligible. These scenarios consider a pulse injection at the source and matrix diffusion in the fracture. Both the injection and observation boreholes are assumed to be well-mixed (physical static mixers may be employed to homogenize tracer
concentrations in boreholes in field tests), and a Cauchy boundary condition is included in the mass balance formulation of the inlet boundary condition, based on mathematical development (Novakowski 1992b) and laboratory experiments (Novakowski 1992c). A third case where both the injection and observation well have negligible volumes with a constant source was also presented, and used as a verification by Chen (1987).

Numerical models offer the ability to study more complex flow and transport scenarios than analytical solutions because they can incorporate heterogeneity in both flow and transport properties. Complex fracture networks, layered sediments, time-dependent boundary conditions, matrix diffusion, user-defined tracers, and fully-transient scenarios are all possible and easy to implement in three-dimensional (3-D) numerical flow and transport models like HydroGeoSphere (Therrien et al. 2006), FRAC3DVS (Therrien et al. 2005), TOUGH2 (Pruess et al. 1999), SWIFT (HSI-GeoTrans 2000) and FEFLOW (Diersch 2009). Despite their capabilities, few examples of field-scale tracer experiment or general radial transport interpretation in fractured rock (single or multiple fracture systems) using suitable numerical models are found in the literature (Park et al. 2004; Liou 2007).

HydroGeoSphere (HGS) from Therrien et al. (2006) provides the ability to simulate a variety of injection and observation well configurations, including passive, finite-volume observation wells and nodes. Boreholes are implemented as one-dimensional (1-D) strings of nodes within the 3-D domain using a common node approach. The pump intake can be placed at any node defining the well screen. Flow and transport in the well are treated as analogous to a finite diameter pipe using the equations derived in Sudicky et al. (1995), Therrien and Sudicky (2000), and Therrien
et al. (2006). Dispersion along the axis of the borehole is accounted for using the formulation from Lacombe et al. (1995). The borehole concentration is determined using a flux-averaged approach, and is not based on an assumption of the nature of the mixing process (no mixing, complete mixing, etc.). This approach may be limited in its applicability to modeling and interpreting real field testing scenarios where low-volume passive observation borehole interval concentrations may be homogenized using physical mixers, as in Novakowski (1992a). Radial flow can be simulated using an axisymmetric coordinate system, but can only be used for point-to-point and borehole-to-point scenarios. Axisymmetric flow and transport modeling was previously identified in Langevin (2008) as an efficient alternative to equivalent 3-D models because of significantly reduced runtimes. Previous work by Weatherill et al. (2008) noted the sensitivity of the transport solution in diffusive and dispersive scenarios to spatial discretization around the fracture-matrix interface in a laboratory scale numerical modeling exercise. However, the application of the high discretization around the fracture-matrix interface at the field scale, and the sensitivity of the transport solution to discretization around the injection well/point in a radial flow field remain unresolved in the literature.

The objective of this chapter is to develop a method for discretization in radial flow fields. HGS is employed to simulate borehole-to-point solute transport conditions with verification by the Novakowski (1992a) semi-analytical solution. The direct application of the numerical model is limited to the borehole-to-point scenario due to differences in how borehole mixing is addressed in the semi-analytical solution. Thus, the transformation of borehole-to-point data from the numerical solution into borehole-to-borehole data using Palmer (1988) will be explored. The scenarios presented are hypothetical, but are similar to ones based on real field data used to
validate the semi-analytical solutions derived in Novakowski (1992a) and Novakowski and Lapcevic (1994). Appropriate spatiotemporal discretization and other model implementation considerations in the numerical model necessary for matching the model output with the semi-analytical solutions are discussed. Particular consideration is given to how far into the matrix away from the fracture actually needs to be highly-discretized to try and reduce the number of elements required in the domain while maintaining good agreement with the semi-analytical solution. In addition, a new mixing model, based on Palmer (1988), is developed for the case of a well-mixed, finite volume observation borehole intersected by multiple fractures in a steady radial flow field. This new mixing model is used as a post-processor to convert numerical model time-concentration point data from a multiple fracture simulation into an equivalent concentration breakthrough curve in a passive observation borehole. The results from this study are useful for developing numerical modeling approaches in radial transport scenarios involving continuous or pulse source injection or pumping conditions in fractured rock, such as tracer experiments, wastewater injection, and domestic well pumping near a source of contamination.

### 3.2 Mixing Model for a Finite-Volume Borehole Intersected by Multiple Fractures

Palmer (1988) previously presented a solution which accounts for mixing as a solute enters and eventually passes through the standing water in a monitoring well. Using a mass balance approach with a first-order boundary condition at the well-aquifer interface to describe solute entering and exiting the borehole, the change in concentration of tracer in the observation interval with time is (Palmer 1988):

$$\frac{dC}{dt} = \frac{q' A}{V_e} [C'(t) - C(t)]$$  \hspace{1cm} (2)
where \( C \) is the concentration leaving the interval (i.e. the concentration of the well-mixed interval), \( q' \) is the apparent flux rate into the well [L T\(^{-1}\)], \( A \) is the cross-sectional area of the interval in the \( r-z \) plane [L\(^2\)], and \( C'(t) \) is the time-dependent concentration [M L\(^{-3}\)] of the tracer entering the well. Equation (2) can be solved yielding a general solution (Palmer 1988):

\[
C(t) = a e^{-at} \int_0^t e^{at} C'(t) dt \quad \text{with} \quad a = \frac{q'A}{V_e} \tag{3}
\]

where \( V_e \) is the volume of water in the observation borehole interval [L\(^3\)]. The apparent flux, \( q' \) [L T\(^{-1}\)] is equal to the product of the actual flux \( q = v\theta \) and the borehole factor \( f \), where \( v \) is the groundwater velocity [L T\(^{-1}\)] and \( \theta \) is porosity [-]. Following Havely et al. (1966), \( f \), in the case of an open borehole, is equal to 2. Thus, \( a \) in Equation (3) can be re-written:

\[
a = \frac{2v\theta A}{V_e} \tag{4}
\]

Equation (4) can be re-written specifically for the case of a single fracture intersecting the borehole by setting \( \theta = 1 \) and \( A = 2r_{wo}(2b) \), giving:

\[
a = \frac{v4r_{wo}(2b)}{V_e} \tag{5}
\]

where \( r_{wo} \) is the radius of the observation well [L], and \( 2b \) is the fracture aperture [L]. The average concentration \( C \) in the observation interval at any time can then be calculated if \( C'(t) \) and all terms in \( a \) are known.

The mathematical development by Palmer (1988) in Equation (2) can be re-formulated to account for multiple fractures intersecting the observation interval, written as:

\[
\frac{dC}{dt} = \frac{\sum_{i=1}^{n} q_i A_i [C_i'(t) - C(t)]}{V_e} \tag{6}
\]
The general solution to Equation (6) is obtained using an integrating factor and the product rule:

\[ C(t) = ae^{-at} \int_0^t e^{at} \sum_{i=1}^{n} C_i(t) \, dt \quad \text{with} \quad a = \frac{\sum_{i=1}^{n} q_i' A_i}{V_e} \]  

(7)

Equation (7) can be modified for the specific case of multiple fractures of different aperture intersecting the borehole interval at specific distance \( r \) from an injection well in a radial flow field using:

\[ q_i' = f q_i = f v_i \theta_i = f \frac{Q_i}{A_i'} \theta_i \]  

(8)

The volumetric flow contribution of an individual fracture, \( Q_i \), to the total in-flow rate into the observation borehole, \( Q_T \) (equal to the flow rate in the injection well), is proportioned by the cubic law, which is simplified to:

\[ Q_i = \frac{(2b_i)^3}{\sum_{i=1}^{n} (2b_i)^3} Q_T \]  

(9)

\[ Q_T = Q_1 + Q_2 + \cdots + Q_n \]

The cross-sectional area of the fracture in the \( r-z \) plane, \( A_i' \), is a ring, written as:

\[ A_i' = 2\pi r (2b_i) \]  

(10)

Substituting Equations (9) and (10) into Equation (8) with \( \theta_i = 1 \) and \( f = 2 \) gives:

\[ q_i' = 2 \frac{\sum_{i=1}^{n} (2b_i)^3}{2\pi r (2b_i)} Q_T = \frac{(2b_i)^2 Q_T}{\pi r \sum_{i=1}^{n} (2b_i)^3} \]  

(11)

The cross-sectional area of an individual fracture at the borehole (in the \( r-z \) plane) is:

\[ A_i = 2r_w (2b_i) \]  

(12)
The substitution of Equations (11) and (12) into Equation (7) gives the final expression for the concentration of a well-mixed, finite-volume observation borehole intersected by multiple fractures at any time under steady flow conditions. $C'_i(t)$ at a given $r$ in each fracture can be evaluated using a numerical flow and transport model.

### 3.3 Numerical Modeling Methods

The following section describes the domain type, input parameters, grid specification and boundary conditions, injection well/node and source definition, and general modeling outline used in this study. The scenario involves an injection well/point spaced 10 m apart from an observation point. Point-to-point scenarios refer to cases where the injection and receptor reservoirs have negligible volume (i.e. a short section of borehole isolated by a straddle packer). Borehole-to-point scenarios have an injection well that acts as a reservoir with a significant finite volume. Modeling was conducted using a 32-bit PC with a 2.33 GHz dual-core processor and 4 GB of DDR2 RAM. Appendix C provides the FORTRAN code used to solve the Novakowski (1992a) semi-analytical solution and an example input and output file. Appendix D provides a set of example HydroGeoSphere input files. A brief description of the governing equations for solute transport used in HGS is provided in Appendix A.

#### 3.3.1 Domain Type

Figure 3-1 provides a depiction of equivalent modeling domains that could be used to solve the same steady radial divergent flow and transport problem in HGS. The rectangular domain uses a Cartesian coordinate system, while the cylindrical and wedge domains could be constructed with nodes in a radial coordinate system (as depicted in Figure 3-1) or meshed with triangular elements using a 2-D grid generator. Axisymmetric coordinates can be used to simulate radial flow in a 2-D domain (Langevin 2008) and are implemented in a unit thickness domain (in the $y$-
direction) in HGS (Therrien et al. 2006). This significantly reduces the number of nodes required in the domain compared to the 3-D rectangular domain, particularly when the grid is fined around the fractures and pumping wells. However, this form of domain can only be used in point-to-point and borehole-to-point scenarios. The rectangular (3-D) and axisymmetric (2-D) coordinates are used in this study because they can be constructed using identical gridding procedures.

3.3.2 Input Parameters

The input parameters used in the semi-analytical solutions and equivalent numerical simulations are provided in Table 3-1. Three fracture apertures are considered: 200, 750, and 1500 microns, which represent the range from the smallest to largest fractures that are typically observed in near-surface bedrock aquifers (Becker and Shapiro 2000; Zanini et al. 2000; Novakowski et al. 2006). The injection rate, $Q$, was adjusted for each fracture aperture (using the cubic law) so that the head rise at steady conditions was more than 1 m. The injection rates in Table 3-1 result in a head rise of approximately 1.23 m at the injection well/point and 0.42 m at the observation well/point. The range in effective diffusion coefficients, $D_d$, was based on a portion of those given in Weatherill et al. (2008), which varied from typical values of free-water diffusion coefficients for conservative tracers ($1 \times 10^{-10} \text{ m}^2/\text{s}$) through to low diffusion in highly tortuous rock ($1 \times 10^{-13} \text{ m}^2/\text{s}$). The matrix tortuosity, $\tau$, was calculated for each case using $D_d = D*\tau$. The matrix hydraulic conductivity was typically set to $1 \times 10^{-10} \text{ m/s}$ or impermeable (when diffusion was not considered). Matrix porosity was varied at 1, 5, 10, and 15% – a representative range of what might be expected in most rock types.

3.3.3 Grid Specifications and Boundary Conditions

Interactive grid generation was employed in the numerical model to allow for fining of the grid near fractures and wells in both the 2-D (axisymmetric coordinates) and 3-D (rectangular,
Cartesian coordinates) domains. This is a similar approach to that used by Weatherill et al. (2008). The necessary spatial discretization needed to match HGS output with the analytical solutions will be discussed in the results. Gridding schemes in subsequent results will be discussed in the following terms: $X$, $Y$, and $Z$ are domain lengths along the principal axes; $x$, $y$, and $z$ refers to a distance from the origin along the principal axis; $\Delta x_{\text{min}}$, $\Delta y_{\text{min}}$, and $\Delta z_{\text{min}}$ are the starting element sizes away from the starting $x$, $y$, or $z$ coordinate; $m_x$, $m_y$, and $m_z$ are the multiplication factors which determine the rate element sizes increase away from the initial elements; and $\Delta x_{\text{max}}$, $\Delta y_{\text{max}}$, and $\Delta z_{\text{max}}$ are the maximum element sizes allowed. The use of the axisymmetric coordinate system requires that $Y = 1$ m, $\Delta y_{\text{min}} = \Delta y_{\text{max}} = 1$ m, and $m_y = 1$. Point-to-point and borehole-to-point simulations were performed using the 2-D axisymmetric coordinate system capabilities in the numerical model. Equivalent 3-D rectangular domains were also attempted for the same scenarios using identical gridding procedures (the same grading used in $x$ was used in $y$).

Initial head and concentration in all HGS simulations were equal to 0 m and 0 (arbitrary concentration units), respectively. Flow boundary conditions in the 2-D domain were all no-flow with the exception of a specified head condition of 0 m at $x = X$. Specified head boundaries of 0 m were used at $x = 0$, $x = X$, $y = 0$, and $y = Y$ m, and no-flow flow boundaries were used at the top and bottom of the domain ($z = 0$ and $z = Z$ m) in the 3-D models. A specified concentration of 0 was applied to all the outer boundaries in both domain types.

The numerical model first solves for steady-state flow and then conducts the transport simulation. The flow solver convergence criteria was set at $1 \times 10^{-10}$. Timestepping for the transport solution
was dictated by a concentration control (CC), which creates an adaptive time array based on the user-defined maximum concentration change at any node in the domain. The CC was treated as a variable when matching numerical results with the semi-analytical solutions. The transport solver convergence criteria was set to $1 \times 10^{-15}$ and fully implicit transport time weighting was used.

### 3.3.4 Injection Well/Node and Source Definition

Point-to-point simulations in HGS employed the use of a well node as the injection point (radius = $1 \times 10^{-5}$ m). The well node was located in the same plane as the fracture. Borehole-to-point simulations were conducted using a finite diameter injection well (radius = 0.038 m) with a 0.5 m-long screen (volume of injection interval is equal to 2.268 L). The pumping node within the well was placed at the point of intersection with the fracture.

Point-to-point simulations were conducted only using constant-source injection in this study. Thus, the chosen injection node was given a concentration of 1 (arbitrary concentration units) for the duration of the simulation. Pulse-source injections were considered in the borehole-to-point scenario. Unlike the semi-analytical solution, the numerical model does not have a Dirac source function for mass injection. Instead, a specified concentration time panel was used to simulate the pulse of mass by injecting the equivalent amount of mass ($M_t$) calculated to be in the injection well of known volume ($V_i$) at $t = 0$ in the semi-analytical solution using the relationship:

$$M_t = CQ t_i$$  \hspace{1cm} (13)

where $C$ is the concentration of solute in the injection well [M L$^{-3}$], $Q$ is the injection flow rate [L$^3$ T$^{-1}$], and $t_i$ is the duration of the injection [T], and
\[ M_i = C_0 V_i \quad \text{with} \quad C_0 = 1 \quad \text{concentration unit.} \quad (14) \]

3.4 General Modeling Outline

The following summarizes the modeling approach used to determine a suitable spatiotemporal discretization required to fit HGS results to the semi-analytical solutions from Novakowski (1992a), the application of the existing borehole mixing model from Palmer (1988) and the new borehole mixing model for a multi-fracture system presented in this chapter:

1. Spatial discretization in x in a 2-D domain and timestep discretization (using CC) were determined using the simplest case of point-to-point constant-source transport in a steady divergent flow field in a single fracture without matrix diffusion (impermeable matrix). HGS output was compared to the analytical solution until good agreement was achieved for all cases of \(2b\).

2. The addition of matrix diffusion to the previous case required consideration of spatial discretization in z adjacent to the fracture plane. HGS output was compared with the analytical solution until a good fit was achieved for the range of \(2b\) and \(D_\alpha\) of interest.

3. Borehole-to-point simulations started with the spatiotemporal discretization determined in the point-to-point models. Changes to the discretization parameters (initial block size, block size multiplier, maximum block size, and concentration control) in HGS were made according to curve fits with the semi-analytical solutions for the cases of matrix diffusion and no matrix diffusion.

4. An exercise was undertaken to understand how far into the matrix from the fracture actually needs to be discretized using the discretization schemes developed in the previous borehole-to-point simulations. These tests covered the entire range of \(2b\) and
The objective was to determine the minimal number of elements needed to discretize the domain while maintaining good agreement (within 5% at the peak concentration) with the semi-analytical solution.

5. Equivalent borehole-to-point and borehole-to-borehole simulations were attempted in a 3-D domain using the minimal discretization schemes determined in #4. Symmetry in x and y was applied around the centrally-located injection well.

6. The mixing model from Palmer (1988) was applied to the single fracture borehole-to-point time-concentration data from the semi-analytical solution and #3, and compared to the borehole-to-borehole semi-analytical solution.

7. The new mixing model presented in this chapter was applied to HGS borehole-to-point output from multi-fracture simulations to produce borehole-to-borehole concentration breakthrough curves in the observation interval. Discretizations determined in previous simulations were maintained in the multi-fracture scenarios presented. The influence of multiple fractures, matrix porosity, and fracture longitudinal dispersivity on concentration breakthrough curves was tested.

3.5 Results
The following sections show the results from the general modeling outline described in 3.4.

3.5.1 Point-to-Point
Figure 3-2A shows good agreement between HGS and the semi-analytical solution for the case of no matrix diffusion using the following discretization: \(X = 1000\) m, \(Y = 1\) m, \(Z = 0.5\) m, \(\Delta x_{\text{min}} = 0.01\) m, \(m_x = 1.05\), \(\Delta x_{\text{max}}\) is not specified (elements were not limited to a maximum length), and \(CC = 0.01\) (1% of peak concentration). The influence of explicitly defining \(\Delta x_{\text{max}}\) was not explored here. The same discretization scheme works for all cases of fracture aperture. The
match is sensitive to the combination of initial block size, block size multiplier, and domain length in the x-direction.

The addition of matrix diffusion in the simulation requires consideration for spatial discretization in z (Figure 3-2B and C). Discretization was tested for the case of $\theta_m = 1\%$ for each combination of fracture aperture and effective diffusion coefficient. A good fit between HGS and the semi-analytical solution is achieved in all cases with $\Delta z_{\text{min}} = 2b$ and $CC = 0.01$. The block size multiplier in z, $m_z$, is case-dependent. For example, when $2b = 200$ microns with $D_d = 1 \times 10^{-10}$ m$^2$/s, a good fit is obtained when $m_z = 2$. In comparison, when $2b = 200$ microns with $D_d = 1 \times 10^{-13}$ m$^2$/s, $m_z$ could be increased to 5 while maintaining nearly the same quality of fit as with $m_z = 2$. No maximum $m_z$ (that had significant adverse impacts on the curve match) was noted in the $2b = 750$ and 1500 micron tests ($m_z$ tested from 2 to 100). The benefit of the increase in $m_z$ is the subsequent decrease in computational runtime in HGS. For example, the runtime for the case of $2b = 750$ microns and $D_d = 1 \times 10^{-10}$ m$^2$/s was reduced from approximately 60 s ($m_z = 2$) to 18 s ($m_z = 100$). However, because the simulation runtimes are still short using $m_z = 2$, and to simplify the process in creating new HGS simulations, a single discretization that satisfies all cases is applied in the following form: $\Delta x_{\text{min}} = 0.01$ m, $m_x = 1.05$, $\Delta z_{\text{min}} = 2b$, $m_z = 2$, and $CC = 0.01$.

3.5.2 Borehole-to-Point

Figure 3-3 shows the results of borehole-to-point simulations in HGS compared to the semi-analytical solutions for the case of no matrix diffusion (A), a constant fracture aperture of 200 microns with $\theta_m = 1\%$ and varying $D_d$ (B), and constant $D_d$ with $\theta_m = 1\%$ and varying fracture aperture (C). The spatial discretization in the 2-D domain is the same as was derived in the point-
to-point models shown in Figure 3-2 and presented in 3.5.1. The timestep discretization is reduced by an order of magnitude using \( CC = 0.001 \) to achieve a better fit with the semi-analytical solutions.

The mass injected into the system for the case of a 0.038 m-diameter well with a 0.5 m screen is 2.268 kg (assuming \( C_0 = 1 \) in (13) and (14)). The length of the injection time panel varies between tests conducted in different fracture apertures due to the different required flow rates (see Table 3-1). Additional numerical modeling shows that the specified injection time panel used to simulate the Dirac is non-unique. Thus, a variety of injection concentrations, injection rates and subsequent injection time intervals can be used if the total mass is maintained. However, the injection time panel must also remain short relative to the timing of the peak concentration at the observation point to preserve the quality of the fit between the numerical model and the semi-analytical solution. Long injection time panels result in a time delay shift in the concentration breakthrough curve. The limits of an appropriate injection time panel were not tested.

All modeling simulations to this point have used spatial discretization schemes that employ an initial block size and block size multiplier to discretize away from the fracture in the z-direction. There was no limit on the maximum block size allowed, thus the block sizes continued to increase in size towards the upper and lower boundaries of the domain. The purpose of increasing discretization around the fracture is to reduce error in the transport solution when matrix diffusion is involved. Table 3-2 shows the results of the discretization required in the z-direction for every combination of fracture aperture, effective diffusion coefficient, and matrix porosity. The gridding procedure outlined in 3.4.1 is modified to a common scheme of: \( \Delta z_{\text{min}} = \)
0.0002 m and \( m_x = 2 \) (the most discretized case). This is applied until the distance away from the fracture is equal to 1, 2, 4, 6, 8, 10, 20, 40, 60, 80, and 100 initial block sizes; the remaining domain is one block. Concentration control was treated as a variable between fracture aperture cases, but is held constant at a value that worked for every matrix porosity and effective diffusion coefficient (see Table 3-2). Discretizing further into the domain than what is shown in Table 3-2 results in the same solution, but uses more elements, and thus increases the simulation runtimes. Discretizing less into the matrix than what is shown in Table 3-2 results in more than a 5% difference between the numerical results and the semi-analytical solution. The results show three trends: 1) more discretization is required with high values of \( D_d \) values for a given fracture aperture and matrix porosity, 2) more discretization is needed in cases with higher matrix porosity for a given fracture aperture and \( D_d \), and 3) more discretization is needed for smaller aperture fractures for a given matrix porosity and \( D_d \). Concentration control was modified to 0.0005 (for the 200 micron fracture) and 0.0001 (for the 750 and 1500 micron fracture) to maintain a good fit between the numerical model and the semi-analytical solution. Interestingly, only 10 of 48 cases shown required more than one block of 0.0002 m on either side of the fracture to maintain a good fit with the semi-analytical solution.

The reproducibility of the borehole-to-point results using a 2-D domain with axisymmetric coordinates was tested in a 3-D rectangular domain. By using the same spatial and timestep discretization as in Table 3-2 and applying symmetry around the injection borehole, the 3-D domain expands to \( X = Y = 2000 \) m with the injection borehole at \( x = y = 1000 \) m. The domain remains 0.5 m in the z-direction with the single fracture at 0.25 m. The observation point is placed at \( x = 1010, y = 1000, \) and \( z = 0.25 \) m. The amount of mass injected and subsequent
injection time panel is maintained. The numerical model could not run any of the simulations, even with the reduced discretization in the z-direction, because the resultant array sizes exceeded the limits of the model. However, the numerical model did execute successfully if the case was limited to a single fracture that only required one block size of 0.0002 m for discretization in the z-direction (from Table 3-2), and \( m_x \) was changed from 1.05 (as determined in 3.5{Palmer, 1988 #374}.1) to 1.1 or greater. An example result (\( 2b = 750 \) microns, \( D_0 = 1 \times 10^{-11} \text{ m}^2/\text{s} \), \( \theta_m = 5\% \)) is shown in Figure 3-4. Solutions between 2-D (\( m_x = 1.05 \)) and 3-D (\( m_x = 1.1 \)) modeling domains remained within 5\% of the semi-analytical solution. The distinct advantage of the 2-D modeling is that the runtimes are <3 min (1,830 nodes, 728 elements) compared to 10.5 hours for near-equivalent (\( m_x \) is different) 3-D simulations (191,100 nodes, 151,320 elements).

3.5.3 Borehole-to-Borehole

The following borehole-to-borehole results are for the case of \( r = 10 \) m, \( 2b = 750 \) microns, \( D_0 = 1 \times 10^{-11} \text{ m}^2/\text{s} \), \( \theta_m = 5\% \), \( r_w = r_w0 = 0.038 \) m, and \( V_i = V_e = 2.268 \) L. Figure 3-5 shows a comparison between 3-D HGS and semi-analytical borehole-to-borehole simulations. The fit between the models is poor. The HGS borehole-to-borehole output is closer to the borehole-to-point solution.

The observation borehole mixing models from Novakowski (1992a) and Palmer (1988) are compared in Figure 3-6. This was done by converting borehole-to-point from the semi-analytical solution into borehole-to-borehole data using Palmer (1988). The timing of the solute breakthrough is similar, but the difference between the maximum concentrations is almost 20\%.
Figure 3-7 shows the results of converting borehole-to-point HGS results into borehole-to-borehole time-concentration data in the observation well using the Palmer (1988) mixing model. A variety of injection borehole-observation borehole volume ratios are presented. The fit between the converted data and the semi-analytical solution is fair. There appears to be a crossover point with respect to the volume ratio of the injection and observation boreholes (~1:5) at which the converted data either under-estimates or over-estimates the concentration component of the breakthrough curve in the observation borehole compared to the semi-analytical solution.

A variety of scenarios utilizing the new mixing model are shown in Figure 3-8. Flow properties in each are equivalent to a single 750 micron fracture (i.e. the total transmissivity is the same). The fractures have the same aperture and are equally spaced along the length of the injection well screen. Heterogeneity is examined in the two-fracture case by changing matrix porosity (Figure 3-8B) and longitudinal dispersivity (Figure 3-8C). The results show how the concentration breakthrough curve in the observation well can change with the presence of multiple fractures despite the flow conditions being identical. Heterogeneity in the matrix porosity between the two fractures has little influence on the concentration breakthrough curve in these dispersion-dominated scenarios. A difference in fracture longitudinal dispersivity influences both the peak concentration and the timing of breakthrough in the observation well.

### 3.6 Discussion

The results show the importance of spatiotemporal discretization in the numerical simulations. The gridding schemes around the fracture-matrix interface in the z-direction in the field-scale simulations in a radial flow field are similar to those determined in uniform flow field, laboratory-scale simulation in Weatherill et al. (2008). The amount of discretization into the matrix, as shown in Table 3-2, is dependent mainly on the matrix porosity and effective diffusion coefficient.
-- more diffusive cases require more discretization. This study furthers the findings from Weatherill et al. (2008) by also showing how important discretization is in the x-direction away from the injection borehole. Discretization in the x-direction was more demanding than in the z-direction because a block size multiplier of 1.05 was required, and the domain needed to be extended out to 1000 m to avoid boundary effects. Timestep discretization was also important and varied over two orders of magnitude (0.01 to 0.0001), depending on the type of tracer experiment scenario being modeled.

The combination of high discretization in the domain and a large number of timesteps in the transport solution (due to using a concentration control) can make numerical modeling prohibitive due to long computational runtimes or because the required array sizes are larger than those allocated in the numerical model. This was shown to be particularly problematic when attempting to model radial transport in both single- and multiple-fracture scenario in 3-D -- mainly due to the discretization required in x and y rather than in the z-direction around the fracture(s). The numerical model is better suited to point-to-point and borehole-to-point radial transport analysis because the axisymmetric coordinate system can be employed in a 2-D domain of unit-thickness, thus reducing the number of nodes and computational runtime significantly. However, the semi-analytical solution has a distinct benefit over the numerical model for the case of a single fracture since spatiotemporal discretization is of no concern and runtimes are shorter (<2 s). The advantage of the 2-D numerical model is in the ability for multiple fractures to be incorporated into the simulation, which was otherwise unsuccessful in the 3-D simulation attempts that were part of this study. Three-dimensional models have the ability to simultaneously model several observation wells/points, but this is not likely suitable since
dispersion is spatially-dependent. Thus, observation wells at different radii from the well may need to be modeled independently.

The Palmer (1988) borehole mixing model and the multi-fracture borehole mixing model developed in this chapter are useful for converting time-concentration point data in the aquifer into well-mixed, passive observation well data. The difference between the converted data and the borehole-to-borehole semi-analytical solution noted in Figure 3-6 and Figure 3-7 may be attributed to the difference in the boundary conditions used at the well-aquifer interface.

Although the hypothetical third-order inlet boundary condition employed in Novakowski (1992a) is better justified in the laboratory column experiments in Novakowski (1992c), the use of a first-order boundary condition, as in Palmer (1988), may still be valid and a reasonable assumption. The mixing model presented in this chapter is particularly useful for the sensitivity analysis of how the presence of multiple fractures (compared to assuming a single equivalent fracture aperture from an aquifer test) and the heterogeneity of transport properties between fractures influences the concentration breakthrough profiles in an observation borehole (as shown in Figure 3-8) and the subsequent interpretation of transport properties.

The numerical model is also limited in its use in trying to model radial transport where a physical mixing system is used to homogenize borehole concentrations, as in Novakowski (1992a), because the mixing process cannot be accounted for, unless we simulate borehole-to-point transport and use Palmer (1988). However, dipole-dipole tests or other configurations that employ the use of a pump in the observation well may be suitable. Future work should consider the application of the numerical models in a variety of other tracer experiment configurations.
where an analytical or semi-analytical model has been developed and validated. Problems may still arise depending on if the concentration in the observation borehole is calculated using resident, as used in Novakowski (1992a) or flux-averaged (used in HGS) methods, as was shown in Figure 3-5.

3.7 Conclusions

The results, interpretations, and discussion presented in this study lead to the following conclusions on the suitability of using a numerical model to simulate a field-scale divergent steady radial flow tracer experiment:

1. Spatial discretization around the injection well and fracture, and the timestep discretization in the transport solution are crucial in matching the numerical model to a semi-analytical solution. Large discrepancies arise when spatiotemporal discretization is insufficient, resulting in the potential misinterpretation of the transport process. The necessary increased spatiotemporal discretization can be prohibitive due to long computation runtimes and array size requirements, particularly when using a 3-D modeling domain.

2. Numerical models alone are best suited to simulate point-to-point and borehole-to-point radial transport in a single fracture using a 2-D, unit-thickness domain with an axisymmetric coordinate system. There is no advantage to using a numerical model over a semi-analytical model for these cases since the solutions are nearly identical. The semi-analytical solution also has shorter runtimes and does not require consideration for appropriate spatiotemporal discretization. Both models limit the ability to incorporate heterogeneity and to represent real field settings.
3. Numerical models are a valuable tool for generating time-concentration data at a particular distance away from the injection borehole in single- and multiple-fracture cases. The conversion of this point data into passive observation borehole data using and the new mixing model developed in this study, based on Palmer (1988), is particularly useful for the sensitivity analysis on how multiple fractures with heterogeneous transport properties might influence concentration breakthrough curves in observation wells.
3.8 References


Table 3-1: Input parameters for the semi-analytical solutions and the numerical model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fracture aperture ($2b$)</td>
<td>200, 750 and 1500 microns</td>
</tr>
<tr>
<td>Longitudinal dispersivity in fracture ($\alpha_L$)</td>
<td>1 m</td>
</tr>
<tr>
<td>Transverse dispersivity in fracture ($\alpha_T$)</td>
<td>0 m</td>
</tr>
<tr>
<td>Radius of injection ($r_w$) and observation well ($r_{wo}$)</td>
<td>0.038 m</td>
</tr>
<tr>
<td>Radial distance from injection well to observation well/node</td>
<td>10 m</td>
</tr>
<tr>
<td>Volume of injection well ($V_i$) and observation well ($V_e$)</td>
<td>2.268x10^{-3} m³</td>
</tr>
<tr>
<td>Injection Rate ($Q$)</td>
<td>0.2 L/min (200 micron fracture)</td>
</tr>
<tr>
<td></td>
<td>10.5 L/min (750 micron fracture)</td>
</tr>
<tr>
<td></td>
<td>84.4 L/min (1500 micron fracture)</td>
</tr>
<tr>
<td>Free-water diffusion coefficient ($D^*$)</td>
<td>1x10^{-10} m²/s</td>
</tr>
<tr>
<td>Matrix tortuosity ($\tau$)</td>
<td>0.001 to 1 m</td>
</tr>
<tr>
<td>Effective diffusion coefficient ($D_d = D^*\tau$)</td>
<td>1x10^{-10} to 1x10^{-13} m²/s</td>
</tr>
<tr>
<td>Matrix porosity ($\theta_m$)</td>
<td>1, 5, 10, and 15 %</td>
</tr>
</tbody>
</table>
Table 3-2: Discretization in the z-direction away from the fracture necessary for matching numerical model output to the analytical solution. Discretizing further into the matrix results in the same outcome in the breakthrough curve at $r = 10$ m, while less discretization results in differences greater than 5 % between the two solutions.

<table>
<thead>
<tr>
<th>$\theta_m$</th>
<th>$D_m$ (m$^2$/s)</th>
<th># of equivalent initial block sizes*</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>200 microns$^{a}$</td>
</tr>
<tr>
<td>1%</td>
<td>$1 \times 10^{-10}$</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>$1 \times 10^{-11}$</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>$1 \times 10^{-12}$</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>$1 \times 10^{-13}$</td>
<td>1</td>
</tr>
<tr>
<td>5%</td>
<td>$1 \times 10^{-10}$</td>
<td>40</td>
</tr>
<tr>
<td></td>
<td>$1 \times 10^{-11}$</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>$1 \times 10^{-12}$</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>$1 \times 10^{-13}$</td>
<td>1</td>
</tr>
<tr>
<td>10%</td>
<td>$1 \times 10^{-10}$</td>
<td>40</td>
</tr>
<tr>
<td></td>
<td>$1 \times 10^{-11}$</td>
<td>6</td>
</tr>
<tr>
<td></td>
<td>$1 \times 10^{-12}$</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>$1 \times 10^{-13}$</td>
<td>1</td>
</tr>
<tr>
<td>15%</td>
<td>$1 \times 10^{-10}$</td>
<td>40</td>
</tr>
<tr>
<td></td>
<td>$1 \times 10^{-11}$</td>
<td>8</td>
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<td>$1 \times 10^{-12}$</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>$1 \times 10^{-13}$</td>
<td>1</td>
</tr>
</tbody>
</table>

* initial block size = 0.0002 m, total distance into the matrix can be calculated by multiplying the # of equivalent initial block sizes listed in the table by 0.0002 m

$^a$ concentration control = 0.0005

$^b$ concentration control = 0.0001
Figure 3-1: Examples of grids that could be employed to simulate equivalent divergent flow fields in HGS. The grid can be fined around wells and fractures, as shown by the grid lines on selected faces of each example. A central injection well (denoted with Q) exists in each domain with an observation well placed at a given distance away. The number of nodes (and subsequent elements) that defines each equivalently discretized domain decreases from left to right. The 2-D domain (unit thickness) uses axisymmetric coordinates to simulate 3-D radial flow. Two injection wells are needed (at Y=0 and Y=1) in this simulation, both injecting at the same rate as the single injection wells used in the other domains. Note: a finite volume observation borehole cannot be used in the axisymmetric coordinate systems. Only observation points can be used in this case.
Figure 3-2: Comparison of concentration breakthrough curves at \( r = 10 \) m from numerical simulations (symbols) with the semi-analytical solutions (lines) for point-to-point, constant-source injection in a steady divergent flow field (\( \theta_m = 1\% \)). The spatiotemporal discretization required in the numerical model to match the semi-analytical solution is given in each example.
Figure 3-3: Comparison of concentration breakthrough curves at $r = 10$ m from numerical simulations (symbols) with the semi-analytical solutions (lines) for borehole-to-point, pulse-source injection in a steady divergent flow field ($\theta_m = 1\%$).
Figure 3-4: Comparison of numerical model results (2-D and 3-D) with the semi-analytical solution for a borehole-to-point tracer experiment in a steady divergent flow field in a single fracture ($r = 10 \text{ m}$, $2b = 750 \text{ microns}$, $D_0 = 1 \times 10^{-11} \text{ m}^2/\text{s}$, and $\theta_m = 5\%$). Substantial differences in runtimes and subsequent decreases in the quality of fit with the semi-analytical solution are noted when $m_x$ is increased.
Figure 3-5: Comparison of numerical and semi-analytical models for borehole-to-borehole tracer concentration breakthrough curves in a steady convergent flow field at $r= 10$ m for the case of a single fracture ($2b = 750$ microns, $D_d = 1 \times 10^{-11}$ m²/s, $\theta_m = 5\%$, $V_i = V_e = 2.268$ L). The borehole-to-point scenario is provided for reference.
Figure 3-6: Conversion of borehole-to-point analytical solution data to borehole-to-point data using Palmer (1988) for a single fracture ($r = 10\, \text{m}$, $2b = 750\, \text{microns}$, $D_d = 1 \times 10^{-11}\, \text{m}^2/\text{s}$, $\theta_m = 5\%$, $V_l = V_e = 2.268\, \text{L}$).
Figure 3-7: Conversion of borehole-to-point time-concentration data from 2-D numerical simulations to borehole-to-borehole data using the Palmer (1988) mixing model. This is the case of $r = 10$ m, $2b = 750$ microns, $D_0 = 1 \times 10^{-11}$ m$^2$/s, $\theta_m = 5\%$, and $V_i = 2.268$ L. Results are shown for a variety of injection borehole-observation borehole volume ratios.
Figure 3-8: Concentration breakthrough curves in the observation borehole for the cases of A) increasing number of equally-spaced, equivalent aperture fractures, B) two fractures with different matrix porosities, and C) two fractures with different longitudinal dispersivity. All multi-fracture scenarios have a cumulative transmissivity equal to that of a single 750 micron fracture.
Chapter 4

Bacterial Count Variability in Samples Pumped from Bedrock

Monitoring Wells with Sand Pack Multi-level Completions

4.1 Introduction

The co-existence of septic systems and wells in rural settings and the proximity to other sources of groundwater pollution (agricultural and industrial land use) may lead to unsafe drinking water, particularly in environments underlain by bedrock aquifers with thin overburden. Recent work has shown that low permeability surficial material such as clay and silt, which have traditionally been thought to be a protective barrier, may allow the transmission of pollutants from the surface to the aquifer via macropore networks (Jacobsen et al. 1997; Conboy and Goss 2000; Cey et al. 2007). Once in the bedrock rock aquifer, contaminants are transported quickly over widespread areas as a result of high groundwater velocities typically found in fractures (Novakowski et al. 2006). Solute retarding mechanisms may offer some protection to downstream receptors through increased dispersion in the fracture and mass loss into the rock matrix (matrix diffusion). However, the protection offered by matrix diffusion is limited in granites and other low porosity rocks (Foster 1975).

Direct mixing of surface water and septic system effluent with groundwater used as a drinking water source may result in human exposure to pathogenic bacteria (e.g. Salmonella, E. coli), viruses (e.g. norovirus, hepatitis A) and protozoa (e.g. Giardia, Cryptosporidium). Testing water samples specifically for microbial pathogens is inhibited by cost and current analytical methods (Field and Samadpour 2007). Thus, a variety of biological (e.g. bacteria), chemical (e.g. nitrate,
phosphate, organic carbon) and physical (e.g. turbidity) parameters are used to help identify the occurrence of a pollution event, the source of pollution, and the potential for the presence of pathogens.

*E. coli*, total coliforms, fecal coliforms and enterococci (e.g. fecal streptococcus) are common fecal indicator bacteria used as tracers of human and animal waste in groundwater studies (Crane and Moore 1986; Personné et al. 1998; Conboy and Goss 2000; Powell et al. 2003; Foppen and Schijven 2005; Schets et al. 2005; Muniesa et al. 2006; Edge and Hill 2007; van Lieverloo et al. 2007; Levison and Novakowski 2008). Total coliforms and *E. coli* have traditionally been considered as the best fecal indicator bacteria tracers of surface water and human fecal contamination in groundwater, respectively.

Heterotrophic plate count, another standard bacteria test, is used as a method for monitoring the overall bacteriological quality of drinking water and the effectiveness of water treatment in public distribution networks. It is not considered an indicator of water safety because it does not define the types or sources of organisms present (Health Canada 2006). Stelma et al. (2004) have also noted that few heterotrophic bacteria found in potable water are pathogenic. Dissolved organic carbon and turbidity have also been used as proxies of bacterial contamination (Pronk et al. 2006; Allen et al. 2008).

Previous studies have noted a heterogeneous distribution of microbes in porous media and fractured aquifer systems due to the spatial variability in aquifer properties and water chemistry (Alfreider et al. 1997; Lehman et al. 2001; Griebler et al. 2002). The majority of bacteria were
found to exist attached to the surface of particulates in saturated sediment experiments, while a maximum of only 10% remain suspended (Harvey et al. 1984; Hazen et al. 1991; Alfreider et al. 1997). Lehman et al. (2001) noted the opposite distribution with higher counts and diversity in the unattached bacterial communities in relatively deep coreholes in a crystalline bedrock aquifer. Attachment and detachment to and from biofilms and the substratum (Figure 4-1) are the dominant transport mechanisms that control the presence of planktonic bacteria in the bulk fluid (Characklis 1990). The distributions of bacteria between the wellbore and the surrounding aquifer or within the sand pack in the case of a multi-level monitoring well are poorly understood.

Fecal indicator bacteria samples collected from monitoring wells are often assumed to be representative of: 1) water quality and bacterial assemblages in the aquifer during natural flow conditions, and 2) the quality of the drinking water obtained from nearby domestic wells. Low-flow (minimal drawdown) sampling protocols, which were originally designed to prevent sampling-induced turbidity (e.g. Puls and Barcelona 1996), are now widely employed for solutes in most groundwater investigations (Shapiro 2002). Currently, little work has been done in understanding the influence of pumping on observed microbial assemblages and biologically sensitive chemical parameters in groundwater samples (Kwon et al. 2008). It is unclear how low-flow purging methods might work in obtaining a representative sample of bacteria in the aquifer given the uncertainty in the distribution of bacteria in the sand pack or well-aquifer system. Samples collected using these methods may also not be representative of what homeowners are exposed to in their drinking water from bedrock wells because: 1) domestic wells are not usually purged prior to use, 2) domestic well pumps are sized according to household needs and well
capacity and thus typically operate at much higher, fixed flow rates, and 3) domestic bedrock wells are open boreholes, not multi-level completions with sand packs.

The objective of this chapter is to examine the variability of fecal indicator bacteria in discrete groundwater samples due to pumping. Heterotrophic plate counts are used as a proxy for the response of general subsurface bacterial communities to disturbances in the aquifer-well system induced by pumping. Two wells were instrumented as multi-level piezometers in a bedrock aquifer and bacterial enumeration was conducted using standard membrane filtration methods.

### 4.2 Field Method

The following section describes the methods used for sampling experiments conducted between July and October, 2008. An overview of the field setting, and multi-level monitoring well installation is also provided.

#### 4.2.1 Field Setting

Tests were conducted in bedrock monitoring wells currently used for a long-term investigation of the impacts of septic systems on drinking water quality in a small hillside village in eastern Ontario, Canada (Figure 4-2). Glacial till cover (often <1 m regionally, but up to 19 m locally) is underlain by Cambro-Ordovician limestone and sandstone (Nepean sandstone) of variable thickness and Precambrian metasediments and intrusives (Figure 4-3). Water well records filed with the Ontario Ministry of the Environment (MOE) indicate most domestic wells in the village are drilled into the bedrock to depths of 20-25 m with recommended pumping rates between 7.5 and 30 L/min (2-8 gpm).
4.2.2 Monitoring Well Installation

Wells P2 and P7 are 15.24 cm (6”) diameter boreholes that were drilled using air rotary equipment in 2006 and 2008, respectively, and subsequently hydraulically tested using discrete interval slug tests (Figure 4-3) and inspected using a borehole camera. Both wells were completed as multi-level piezometers using 5.08 cm (2”) diameter PVC riser (standpipe) and screen (250 µm horizontal slots with 7 mm spacing, on-centre), well gravel (porosity = 0.3, mean grain diameter ~2.3 mm, referred to as the sand pack in this text) and bentonite. Each multi-level interval was designed so that the screen intersected a discrete fracture feature(s) identified during hydraulic testing (Figure 4-3). The riser was extended to the top of the casing to provide access at the surface. The purpose of the sand pack is to fill the annular space between the screen and the borehole wall while allowing for the uninhibited transmission of water during natural flow and pumping conditions. A minimum of 0.9 m (3 ft) of bentonite was used to “cap” the sand pack, hydraulically isolate the interval from the rest of the borehole, and as the fill material between intervals. The sand pack was extended vertically above and below the screen by ≥0.6 m (2 ft) to minimize potential scouring of the bentonite seal due to pumping. Up to three intervals of this type can be constructed in a 15.24 cm (6”) diameter borehole. However, due to space constraints in the borehole, a 5.08 cm (2”) diameter screen and riser cannot be used in the shallowest interval in the case of a three-interval design because of the presence of the risers from the deeper intervals. We chose to complete the shallow intervals using 2.54 cm (1”) diameter screen and riser rather than leaving the interval open (no screen, riser, sand pack or bentonite) to avoid the groundwater from coming in contact with the steel casing. The top of the sand pack in this case was placed ≥0.6 m from the bottom of the casing, and the bentonite seal was extended well up into the casing. This form of completion in the shallow interval helps to isolate the
interval from any potential surface water that might be short circuiting down the outside of the casing due to an improper casing seal.

These wells are purged on a monthly basis during water quality testing, but are otherwise undisturbed.

4.2.3 Sampling Intervals and Procedures

Five individual tests were conducted only on the middle intervals of wells P2 and P7, denoted as P2-M and P7-M in Figure 4-3. These intervals were specifically chosen for this study because they had shown some evidence of potential septic system contamination in earlier water quality tests conducted using traditional purging protocols (nitrates <2 mg/L, *E. coli* and total coliforms present, see Chapter 5). Water level data suggests a weak hydraulic connection between the two intervals. The objective of using two different sampling points and conducting different tests in each was to verify the reproducibility of the observed bacterial count trends, not to test whether both share the same local contamination source or hydraulic connectedness.

Five different pumping scenarios were chosen to examine a range of pumping-induced flow conditions: 1) constant pumping at a high flow rate to test the influence of high velocity and shear stress, 2) constant pumping at a low flow rate where drawdown and pumping-induced velocities would be at a minimum, 3) intermittent pumping where the pump is on at a high flow rate for two periods of time separated by a period of no pumping (on-off-on) to test for reproducibility in the observed trends, 4) multiple incremental increases in pumping rate to test the for reproducibility in the response to increasingly disturbing conditions compared to the natural flow regime, and 5) variable flow rate change, which is similar to 4, but with a decrease in flow rate and subsequent
stress on the system. The setup details and pumping schedule of each test are summarized in Table 4-1. High-flow (>0.3 L/min) sampling was conducted using a variable speed submersible pump which was lowered down the riser and placed in the screened interval to a maximum depth of approximately 29 m below the top of the casing (mbtoc) as limited by the length of the discharge tube. Low-flow sampling was conducted in P2-M using a peristaltic pump. The location of the intake was limited by the available length of tubing at the time of the test, and was subsequently placed approximately 7.5 mbtoc, which is roughly 5 m above the top of the screen in P2-M.

Flow rate, purge volume and field parameters were continuously monitored using the equipment configuration shown in Figure 4-4. The flow-through-cell could not accommodate the high flow rates from the pump, so a peristaltic pump was used to transfer water from the manifold at a constant and controlled flow rate. A multi-parameter sonde mounted in the flow-through-cell measured and recorded pH, conductivity, temperature, dissolved oxygen (DO) and oxidation-reduction potential (ORP) in real-time. Each parameter was calibrated prior to each test using the methods and calibration standards provided by the manufacturer. Samples were obtained from the manifold discharge while water exiting the flow-through-cell was discharged onto the ground.

Samples were collected at varying time intervals during the course of each test, and were obtained more frequently at the beginning of each to capture early-time responses. Samples for bacterial analysis were collected in new pre-prepared, pre-sterilized 300 mL plastic bottles that were provided and quality-assured by a commercial water quality testing lab. Bottles were uncapped and recapped immediately before and after each sample was taken. Field duplicates and
triplicates were obtained in immediate succession, but were not mixed and homogenized prior to analysis and are thus more useful for examining short-term count variations rather than verifying sampling techniques. All samples were stored in insulated coolers with ice packs in the field and transported to the laboratory the same day. Turbidity samples were collected in high-density polyethylene bottles and analyzed within 8 hours using a LaMotte 2020e turbidimeter on the Formazin/Attenuation calibration mode with the averaging procedures and methods outlined in the manufacturer’s instruction manual. Periodic calibration was performed using polymer standards ranging from 0 to 10 NTU.

The suite of bacterial analyses performed on each sample included *E. coli*, total coliform, fecal coliform, fecal streptococcus and heterotrophic plate count and was conducted by the same commercial laboratory that provided the sampling bottles. The laboratory is a member of the Canadian Association for Environmental Analytical Laboratories and fully accredited for the analysis of these microbiological parameters. All analyses used membrane filtration methods based on those outlined in the Standard Methods for the Examination of Water and Wastewater (Clesceri et al. 2005): total coliform and *E. coli* (SM 9222 B), fecal coliform (SM 9222 D), fecal streptococcus (SM 9230 C), and heterotrophic plate count (SM 9215 D). The 95% confidence limits for the membrane filter coliform counts were taken from Table 9222: II (for counts ≤20/100 mL) or estimated using the normal distribution equations (c ± 2s(c)^{1/2} for counts >20/100 mL), as outlined in Clesceri et al. (2005). The same confidence intervals are applied to the fecal streptococci results, which is a similar enumeration method.
4.3 Results
The results from the five tests conducted in P2-M and P7-M are shown in Figure 4-5 to Figure 4-9. Each figure includes fecal indicator bacteria and heterotrophic plate counts, pumping rate and the specific conductance for each test. Specific conductance is shown in all figures as it was a good representation of the trends found in the other field parameters (temperature, pH, DO and ORP) observed during pumping. Early-time field parameter measurements reflect the stabilization of the sensor to being submerged in the sample and are not truly representative of the changes in the purged water itself. The adjustment period attributed to the initial stabilization is identified in the specific conductance graphs by a dashed line (Figure 4-5 to Figure 4-9).

Turbidity measurements are only shown for tests for which a turbidimeter was used. The purge volume is shown with respect to the equivalent well volumes for each test (Figure 4-5 to Figure 4-9). The pore volume of the sand pack is included in this calculation (along with the initial volume in the screen and riser) as to incorporate all of the components of the multi-level installation and help distinguish between the fractional contributions of the aquifer and original well contents to pump discharge. The definition of a well volume varies in the literature, but has included the pore volume in the sand pack in previous studies (Pohlmann and Alduino 1992).

Some total coliform results were given a value of overgrown (OG) by the commercial laboratory, meaning there were too many other types of bacteria (not specifically identified) in the sample that interfered with their ability to do a proper count. It does not imply that total coliform counts in these samples are >400 cts/100 mL (the upper detection limit).

4.3.1 Key Observations
The following are interpreted from Tests 1-5 shown in Figure 4-5 to Figure 4-9.
1. The presence of fecal indicator bacteria is more evident (a greater number of positive tests results) in samples collected prior to the removal of three to five equivalent well volumes.

2. The highest counts of fecal indicator bacteria were observed at the onset of pumping events. Counts quickly reduced by an order of magnitude (or more in some cases) to levels at or near the method detection limit (1 cts/100 mL). Some of the changes were limited to within the 95% confidence intervals established for the enumeration method.

3. The presence of a given fecal indicator bacteria in a single sample is poorly correlated with the presence of all/other fecal indicators being present in the same sample.

4. Like fecal indicator bacteria, heterotrophic plate counts were highest at the onset of pumping and rapidly decreased by two to three log-units to stabilized concentrations near the method detection limit (10 cts/1 mL).

5. Bacterial counts were influenced by changes in pumping rate. This was best observed in the heterotrophic plate counts in Tests 3-5 (Figure 4-7 to Figure 4-9). Heterotrophic plate counts quickly re-stabilized to levels near those observed at previous pumping rates.

6. The pumping rate did not correlate well with the magnitude of observed bacterial concentrations in the samples.

7. Specific conductance stabilized early during the tests, typically prior to the purging of three well volumes.

8. Turbidity levels remained low (<3 NTU) during the tests (Figure 4-6 and Figure 4-8) with most readings below 1 NTU. Like bacterial samples, turbidity was highest at the onset of pumping and decreased quickly to stable levels near the detection limit (0.05
Some turbidity increase was noted following the pumping rate increases in Test 4 (Figure 4-8). Rapid re-stabilization to near the detection limit was noted; the same trend was observed in the bacterial data.

4.4 Discussion

The results from the five field tests clearly show that bacterial counts can be variable during purging in a bedrock multi-level monitoring well. This discussion will offer an interpretation of these results in the context of conceptual models of flow and bacterial distribution in the subsurface. Implications for water quality interpretation and sampling protocols, as well as the limitations of the concentration-based approach are discussed.

4.4.1 Flow and Transport Conceptual Model

Bacteria are transported to the borehole via advection in fractures under natural and pumping flow regimes. A conceptual model of flow to and within an open and multi-level well in a bedrock aquifer is shown in Figure 4-10. Flow into the borehole is dominated by the most significant hydraulic features, thus a water sample will reflect that of the fractures with the highest transmissivity, regardless of the position of the pump (Shapiro 2002).

Numerical modeling was conducted using HydroGeoSphere (Therrien et al. 2006) to better understand the nature of flow in the sand pack and the influence of multi-level completions on obtaining representative aquifer samples. The modeling scenarios included a variety of pumping rates, screen and sand pack hydraulic properties, and discrete bedrock fractures, similar to those in this study. The results of this work are not directly incorporated into this manuscript, but are used to help with the formulation of the flow and bacterial mobilization conceptual models and results interpretation in the following discussion. The sand pack in the multi-level well (Figure
4-10b) introduces complexities to the flow system during pumping because the groundwater has to negotiate through its pore spaces between the fracture and the well screen. Modeling results show only a discrete zone within the sand pack is hydraulically active during pumping, the extent of which is dependent on the hydraulic properties of the sand pack and screen and the nature of the fractures that intersect the borehole.

Pumping induces a change in the local groundwater gradient around the well causing increases in the velocity and subsequent shear stresses at the interface between the bulk fluid and the biofilm or substratum. Previous colloid transport and water distribution system studies have shown an increase in turbidity and bacterial counts (detached bacteria) in water samples in response to pumping, which is attributed to changes in shear stress (Backhus et al. 1993; McMath et al. 1999). The influence of pumping on groundwater velocities in the aquifer remains local to the borehole. The highest velocities in the vicinity of the multi-level occur at the interface between the sand pack and the screen, and the fracture and sand pack, when there is a reduction in porosity and hydraulic conductivity. Thus, pumping should have its greatest influence on bacterial detachment on the inner surface of the well screen, from zones in the sand pack between the screen and fractures, and from the surface of fractures in the aquifer in close proximity to the borehole. Straining and exclusion in the sand pack and fractures due to changes in pore throat size and connectivity may effectively reduce bacterial counts and control bacterial community profiles observed in pumped groundwater samples, as has been noted in previous field and column studies in fractured and granular media (e.g. Malard et al. 1994; Cumbie and McKay 1999; Bradford et al. 2003; Foppen et al. 2005).
Four hypothetical concentration profiles are presented in Figure 4-11 for a time series of samples collected at a constant pumping rate (Q) based on different bacterial sources (planktonic or attached) and locations of bacteria in the subsurface (proximal or distal to the borehole). The variability and magnitude of the bacterial counts in purged samples is influenced by the pumping rate, location of the source, the nature of detachment, and dilution in the fracture.

In the case where bacteria come from the screen or sand pack in the wellbore (Figure 4-11a and b) the peak concentration occurs at early-time because the travel distance to the pump is short. Planktonic mass in the screen is finite, and is quickly removed during pumping (Figure 4-11a). The higher the pumping rate the quicker this occurs. Initial concentrations in the samples reflect that of the screen storage prior to pumping. The shape of the concentration curve for when all of the planktonic bacteria are located in the pores of the sand pack is similar to that of the case for the screen, except the initial concentration is zero because the bacteria have yet to be mobilized to the screen (Figure 4-11a). The maximum concentration is delayed because of the required travel time from the pores in the sand pack to the pump intake in the screen. Concentrations return to zero once the biomass in the sand pack has been purged.

The difference between the planktonic and attached/biofilm-related concentration profiles is attributed to the amount of biomass in the reservoir and the nature of detachment. If previously defined ratios of planktonic to attached bacteria in saturated sediments hold true (Harvey et al. 1984; Hazen et al. 1991; Alfreider et al. 1997) then biofilms will be a greater source per unit volume of sand pack. While maximum bacterial concentrations in pumped samples may not differ between sources, the total biomass removed over time may be larger from biofilms, as
illustrated by the difference in area under the curves in Figure 4-11a and b. Higher pumping rates result in increased shear stresses in the system causing detachment rates to increase. The maximum concentration arrival will be quicker and the magnitude will be greater when the pumping rate is higher because the travel time is reduced and fewer bacteria will be able to remain attached (Figure 4-11b). The tailing at late time (Figure 4-11b) represents the continual detachment of bacteria, which unlike planktonic bacteria in the first case may never be fully removed from the sand pack. The magnitude of bacterial concentrations is much lower at this point because the more easily detachable biomass has already been removed.

Two points distinguish what may be expected when the bacteria are mobilized from a biofilm in an adjacent fracture (Figure 4-11c) compared to the wellbore (Figure 4-11b): 1) a time delay due to additional travel distance to the pump intake, and 2) higher concentrations and more biomass removed over time. The latter is due to the increase in surface area in a fracture available for attachment/biofilm growth with distance from the borehole.

The final case shows the anticipated concentration profile when the bacteria are being mobilized from a distal source out into a fracture (Figure 4-11d). Here the magnitude of the bacterial concentrations is diminished due to dilution. The peak concentration of bacteria occurs at later time, and higher pumping rates will result in shorter travel times.

4.4.2 Field Sampling Results Interpretation

Based on the previous discussion, we interpret the bacterial trends from the field study to be dominated by a combination of planktonic and attached sources in the borehole and adjacent fractures. Peak concentrations in the early-time samples are likely the combination of planktonic
bacteria and weakly attached bacteria in the screen and pore spaces of the sand pack. As pumping continues, the bacterial counts rapidly decrease because: 1) the planktonic component is flushed from the screen sand pack, and 2) the amount of proximal weakly attached bacteria is quickly depleted. Fecal indicator bacteria trends often coincide with that of the heterotrophic plate count results, suggesting both may come from the same combination of planktonic and attached sources in the subsurface.

The heterotrophic plate count results in Tests 3-5 (Figure 4-7 Figure 4-9) suggest that local attached sources are not being fully depleted during pumping and that the concentrations observed in a time series of samples are a representation of the adjustment of detachment rates to a given flow regime. An increase in pumping rate increases the velocity and subsequent shear stresses in the sand pack and proximal fracture causing the removal of bacteria that had previously remained attached. A re-stabilization back to lower counts occurs as the bacteria that will become detached due to the higher flow rate are removed. Decreasing the flow rate, as shown in Test 5 (Figure 4-9), does not necessarily lower the magnitude of the steady-state heterotrophic plate counts. This is because the detachment rates have already stabilized to a higher-stress environment.

While the heterotrophic plate counts show significant changes due to new flow regimes, the fecal indicator bacteria are often only observed in the samples collected following the start of the first pumping interval. This emphasizes just how minor a component the fecal indicator bacteria are in subsurface (i.e. trace microbial contaminants) and that they are not really and interacting/growing component of the subsurface ecosystem. It may also suggest that the fecal
indicator bacteria are more associated with the planktonic component or are weakly attached on the surface of biofilms and mineral surfaces (sand pack grains or fracture surfaces), and are thus flushed out of the system during initial pumping.

The magnitude of bacterial counts at the beginning of the tests did not correlate well with the pumping rate, which was not expected. Heterotrophic plate counts >2000 cts/mL were observed in tests conducted at 0.3 L/min (Test 2), 6 L/min (Test 4), 10 L/min (Test 5), and counts ~1000 cts/mL for similar tests conducted >13 L/min (Tests 1 and 3). The difference is likely to be a reflection of changing bacterial populations in the subsurface possibly due to the influx of new bacteria to the well via natural flow or a reduction in the general population due to a discontinuous nutrient supply that occurred between the dates the tests were performed. The interpretation is also limited by the initial concentrations being at the upper detection limit of the analytical method. It is interesting to note that the same levels of bacterial counts were observed in Test 2 conducted at 0.3 L/min as in the other tests. This test was specifically designed as a low-flow scenario where the pumping-induced velocities and drawdown would be minimal in the wellbore. We interpret these results to show just how easily detachable some bacteria are from surfaces in the borehole. Biofilms and attached cells on the smooth-surface PVC screen and riser walls may be particularly susceptible compared to those on rougher sand grains or fracture walls.

4.4.3 Limitations of the Concentration-based Approach

Our interpretation of bacterial trends is based on the comparison of field data with conceptual models of bacterial concentration trends during the course of well pumping. The plate count method does not differentiate between planktonic and biofilm-detached cells, single or clumps of cells (both would be counted as one colony forming unit), nor does it account for cells that are viable but non-culturatable or dead (McMath et al. 1999; Myers et al. 2007). Thus, the bacterial
counts observed in the groundwater samples may only represent a portion of the biomass in the subsurface.

A microscopy technique would be better suited for distinguishing between single cells and multicell clumps and interpreting their source in groundwater samples. For example, epifluorescence microscopy has been successfully employed for this purpose examining heterotrophic bacteria sloughing in water distribution pipes (McMath et al. 1999). This technique also has the benefit of allowing for the enumeration of cells that plate count methods are unable to, as discussed previously. More importantly, this method may be useful for determining the source of fecal indicator bacteria from the subsurface. If fecal indicator bacteria are dominantly sourced from biofilm detachment then the question becomes: are the associated pathogens also surviving in the biofilms and becoming detached during pumping? If not, the interpretation of the health risk based on fecal indicator bacteria concentrations alone is misleading.

4.4.4 Implications for Sampling Protocol and Water Quality Interpretation

The most significant finding is that fecal indicator bacteria counts can remain variable during pumping and are more likely to be better detected in samples taken prior to the removal of 3-5 well volumes. The variation in fecal indicator bacteria concentrations during pumping can change the general interpretation of drinking water quality. In many tests the significant presence of fecal indicator bacteria was only noted in samples collected prior to the purging of three well volumes. In the same cases, the stabilized counts were often at the method detection limit (i.e. interpreted as being absent) for the rest of the pumping period. This meant that the water quality interpretation changed from non-compliant to compliant with respect to the current drinking water standards in Ontario (MOE 2002) depending on the timing of the sample.
Single samples, taken at any point during purging, are not likely to be representative of the variability and magnitude of the bacterial concentrations in the groundwater being pumped from the well, particularly at early-time. The act of purging 3-5 well volumes or until chemical field parameters stabilize could result in a significant reduction in fecal indicator bacteria that would likely be observed in subsequent samples. This in turn could lead to misrepresentation of the drinking water quality using the fecal indicator bacteria concentration method. We suggest a multi-sample approach is more suitable when sampling for fecal indicator bacteria for the purpose of assessing drinking water quality, with an emphasis on sampling during the purging interval prior to the removal of 3-5 well volumes or the stabilization of chemical field parameters.

The influence of increased surface area available for attachment and biofilm growth in the monitoring well due to the presence of the sand pack on observed bacterial concentrations in pumped samples remains in question. Future work should consider if infrequently used multi-level monitoring wells with sand packs are suitable for inferring water quality using bacteriological parameters in nearby open and frequently pumped bedrock residential wells.

4.5 Conclusions

The results from this study lead to the following conclusions about bacterial counts in pumped groundwater samples and the subsequent water quality interpretation using fecal indicator bacteria:

1. The pumping rate did not correlate well with the magnitude of observed bacterial concentrations in the samples.
2. Bacterial concentrations in groundwater samples remain variable during the course of pumping. The highest concentrations of bacteria occur at the onset of pumping prior to the complete purge of the wellbore as defined in conventional sampling protocols.

3. Samples are dominated by planktonic and detached cells sourced in the screen storage, sand pack, and adjacent fractures.

4. Multiple samples and other enumeration techniques would provide better, more accurate and more useful data for assessing the source of bacteria in the subsurface and the potential exposure to pathogens using fecal indicator bacteria.
4.6 References


Table 4-1: Objectives and details of five tests conducted to observe the variability of bacteria in samples during pumping.

<table>
<thead>
<tr>
<th>Test #</th>
<th>Interval Name</th>
<th>Sampling Date (2008)</th>
<th>Interval Sampling Depths (mbtoc)</th>
<th>Objective</th>
<th>Pump Type and Intake Location (mbtoc)</th>
<th>Pumping Schedule</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>P7-M</td>
<td>July 16</td>
<td>22.816 – 28.410</td>
<td>High-flow, constant</td>
<td>Submersible, in screen</td>
<td>0-480 min: 13 L/min</td>
</tr>
<tr>
<td>2</td>
<td>P2-M</td>
<td>October 29</td>
<td>12.725 – 21.692</td>
<td>Low-flow, constant</td>
<td>Peristaltic, ~7.5</td>
<td>0-360 min : 0.3 L/min</td>
</tr>
</tbody>
</table>
| 3      | P7-M          | August 28            | 22.816 – 28.410                  | Intermittent pumping, constant (on-off-on) | Submersible, in screen | 1) 0-100 min: 14.5 L/min  
2) 100-160 min : 0 L/min  
3) 160-260 min: 14.5 L/min |
| 4      | P7-M          | September 24         | 22.816 – 28.410                  | Multiple increases in flow rate | Submersible, in screen | 1) 0-100 min: 6 L/min  
2) 100-200 min : 12 L/min  
3) 200-300 min: 17 L/min |
| 5      | P2-M          | August 28            | 12.725 – 21.692                  | Flow rate change | Submersible, in screen | 1) 0-100 min: 10 L/min  
2) 100-105 min: 4.5-16 L/min  
3) 105-200 min : 4.5 L/min |
Figure 4-1: Bacteria transport mechanisms in a hydraulically active pore space: a) detachment of single cells or multi-cell fragments from the substratum or biofilm, b) attachment of single cells or multi-cell fragments to the surface of a biofilm or substratum, c) advection, and d) motility. Not to scale.
Figure 4-2: Location map of the study area in eastern Ontario and the bedrock monitoring well array that is part of a larger groundwater study examining the impacts of septic systems on drinking water quality in a small rural village. Squares indicate monitoring wells used for this study. The local groundwater flow direction is northwest.
Figure 4-3: Surficial and bedrock geology, hydraulic characterization and multi-level completion intervals in monitoring wells P2 and P7. Results from slug tests performed using straddle packers shows that flow in the bedrock aquifer is controlled by discrete fracture features. Multi-level intervals were designed to isolate different fractures and allow for the observation of the vertical profile of hydraulic head and water quality in the aquifer. Intervals P2-M and P7-M were used in this study.
Figure 4-4: Schematic of the equipment setup used to monitor field parameters, flow and purge volume, and collect water samples during the pumping of bedrock monitoring wells.
Figure 4-5: Results from Test 1 in well P7-M. Pumping was conducted at 13 L/min. The detection limits are 1 cts/100 mL and 10 cts/mL for fecal indicator bacteria and heterotrophic plate count, respectively. The vertical bars represent the upper and lower limits of the 95% confidence interval for membrane filter coliform counts.
Figure 4-6: Results from Test 2 in well P2-M. Pumping was conducted at 0.3 L/min. The
detection limits are 1 cts/100 mL, 10 cts/mL and 0.05 NTU for fecal indicator bacteria,
heterotrophic plate count and turbidity, respectively. The vertical bars represent the upper
and lower limits of the 95% confidence interval for membrane filter coliform counts.
Figure 4-7: Results from Test 3 in well P7-M. Intermittent pumping (on-off-on) was conducted at 14.5 L/min. The pump remained off for 60 minutes between pumping events. The detection limits are 1 cts/100 mL and 10 cts/mL for fecal indicator bacteria and heterotrophic plate count, respectively. The vertical bars represent the upper and lower limits of the 95% confidence interval for membrane filter coliform counts.
Figure 4-8: Results from Test 4 in well P7-M. Pumping was increased abruptly to double and triple the original flow rate following 100-min intervals at a constant flow rate. The detection limits are 1 cts/100 mL, 10 cts/mL and 0.05 NTU for fecal indicator bacteria, heterotrophic plate count and turbidity, respectively. The vertical bars represent the upper and lower limits of the 95% confidence interval for membrane filter coliform counts.
Figure 4-9: Results from Test 5 in well P2-M using variable flow rates. Overgrown (OG) was reported for total coliform counts when colonies of other bacteria present interfered with being able to count properly. It does not necessarily imply that the total coliform count is greater than 400 cts/100 mL. The detection limits are 1 cts/100 mL and 10 cts/mL fecal indicator bacteria and heterotrophic plate count, respectively. The vertical bars represent the upper and lower limits of the 95% confidence interval for membrane filter coliform counts.
Figure 4-10: Flow conceptual model to and within a) an open well and b) a bedrock well multi-level interval in a bedrock aquifer during pumping. Only one interval is depicted in the multi-level well. Flow to the well is dominated by the fractures with the highest transmissivity (aperture differences denoted by the weight of the line, relative flow contribution shown by the size of arrow). The magnified view shows the tortuous flow paths through the sand pack between the fracture and the screen slots. Flow within the well moves vertically and converges to the pump intake. Legend: 1) piezometric surface, 2) pump intake, 3) standpipe, 4) bentonite hydraulic seal, 5) sand pack, 6) screen slot, 7) fractures with different apertures, 8) flow paths, 9) bottom of the well, and 10) bedrock. Not to scale.
Figure 4-11: Conceptual concentration profiles for bacterial concentrations in groundwater samples taken during constant pumping rates, Q, based on the location (proximal or distal) and source of bacteria (planktonic or biofilms) in the subsurface. Pumping rate, source distance, detachment rate and dilution all influence the magnitude and temporal distribution of observed bacterial counts in purged groundwater samples.
Chapter 5

The Potential for Anthropogenic Contamination of Groundwater in a Bedrock Aquifer having Variable Overburden Cover in a Semi-urban Setting

5.1 Introduction

Fractured bedrock aquifers are an important drinking water resource in many locations around the world, however, a lack of suitable overburden can leave them vulnerable to contamination (Powell et al. 2003; Novakowski et al. 2006c). For example, it is estimated that there are 750,000 wells in Ontario (Novakowski et al. 2006a), many of which are in fractured bedrock settings in the eastern and northern parts of the province having little or no overburden cover. The degradation of groundwater quality is often attributed to anthropogenic contaminant sources, including agriculture and septic systems (Fetter 2001). The potential for human consumption of contaminated groundwater in most rural settings is compounded by the co-presence of private wells and septic systems and close proximity to agricultural activity.

The adverse impact of septic systems on groundwater quality has been a concern for decades due to the potential health risks associated with nitrate and pathogenic microorganisms in the effluent. Investigations of groundwater contamination are often conducted in saturated or unsaturated porous media, and are focused on the scale of a single septic system (Robertson and Cherry 1992; Aravena et al. 1993; Gerritse et al. 1995; Harman et al. 1996; Wilhelm et al. 1996; Shadford et al. 1997; MacQuarrie et al. 2001; Robertson 2003) or a few septic systems in a subdivision or small area (Alhajjar et al. 1988; Zhan and McKay 1998; Robertson 2003; Wilcox et al. 2005). Few studies have examined the impacts of septic systems on water quality on a village or regional
scale (Hinkle et al. 2005; Verstraeten et al. 2005; Rosen and Thomas 2006), or in bedrock terrains (Powell et al. 2003).

Pharmaceuticals and personal care products (PPCPs) have also recently become emerging contaminants of concern around the globe (Seiler et al. 1999; Ternes et al. 1999; Kolpin et al. 2002; Metcalf et al. 2003a; Metcalf et al. 2003b; Zuccato et al. 2005). PPCPs can be defined as “any product used by individuals for personal health or cosmetic reasons or used by agribusiness to enhance growth or health of livestock” (US EPA 2010). This covers thousands of chemical compounds, including prescription and over-the-counter therapeutic drugs, veterinary drugs, soap and shampoo antimicrobial or medicinal ingredients, cosmetics, and caffeine. Following their application, many of the pharmaceutical compounds are not completely eliminated in the user’s body (human or animal) and are subsequently excreted through urine and feces unaltered or only slightly transformed (Heberer 2002). Many of these compounds continue to be persistent during conventional sewage treatment (Ternes et al. 1999; Metcalf et al. 2003b; Servos et al. 2005) and are released into the environment through many pathways, including leaking municipal sewer pipes, municipal sewage treatment plant discharge, agricultural runoff from fields where treated sewage sludge or animal manure is applied, and septic systems (Heberer 2002; US EPA 2010). The effects of long-term, low-dose exposure of humans and other organisms to these compounds remains to be determined. Servos et al. (2007) notes that the extent of exposure in the Canadian environment is poorly documented. Internationally, the state of the science is still in the phase of developing analytical methods and quantifying these compounds in various aquatic matrices. Only a few studies have focused on PPCPs in septic systems and receiving groundwaters (Seiler et al. 1999; Hinkle et al. 2005; Verstraeten et al. 2005; Godfrey et al. 2007), and the fate and transport of these compounds in the fractured rock setting has yet to be explored.
Recent studies have shown that low permeability surficial materials such as clay and silt, which have traditionally been thought to be a protective barrier, may still allow the transmission of surface pollutants to deeper within the subsurface via macropore networks (Jacobsen et al. 1997; Conboy and Goss 2000; Cey et al. 2007). Once in a bedrock aquifer, contaminants may become quickly widespread as the result of preferential pathways which have high groundwater velocities such as open fractures (Novakowski et al. 2006b). Dilution during recharge and solute retarding mechanisms may offer some protection to downstream receptors through dispersion in the fracture network and mass loss into the matrix by diffusion. However, matrix diffusion is limited when groundwater velocities are high and/or the porosity of the rock is low (Foster 1975).

The objective of this study is to determine if the water quality in the underlying bedrock aquifer having variable overburden cover is being adversely impacted by anthropogenic activity in a semi-rural setting and to try and ascertain what and where the sources are. Eight bedrock monitoring wells were instrumented as multi-level piezometers in an unserviced lakeside village surrounded by undeveloped and agricultural land. A multiparameter sampling program involving nutrients, chloride, fecal indicator bacteria, and 40 PPCPs was used to track anthropogenic effects. The response of monitoring well water levels to recharge and local pumping events, and groundwater stable isotopes ($\delta^2$H and $\delta^{18}$O) were used to infer hydraulic connections in the fracture network. Chemical, isotopic, and bacterial analyses were conducted using conventional methods.

5.2 Geography and Geology of the Study Area

Field investigations for this study were conducted between 2005 and 2009 in a hillside village along the south of a large Lake (the Lake) in eastern Ontario, Canada (Figure 5-1). Figure 5-1 shows that the village consists of two main parts (collectively referred to as the Site): 1) the original, higher-density town-proper portion (the Main Village) on the north side of the highway.
(dating back to the early 1800s), and a newer, lower-density subdivision (the Subdivision) to the southeast (homes typically built between 1960 and 1990). The combined population of both portions and additional rural housing in the area is less than 500 persons. A land use map is provided in Figure 5-2. Numerous small-scale beef and dairy cattle farms are present in the surrounding environs with associated pasture, hay, and straw fields.

Residents rely fully on on-site servicing for water supply and wastewater disposal. There are an estimated 110 private wells at the Site and many more in the surrounding environs. Provincial water well records indicate most are drilled bedrock wells constructed prior to the 1980s with typical depths ranging between 10 and 25 m. A few overburden wells are present and still in use in the Village. The number of septic systems is similar to the number of wells. The average system was constructed in the 1970s and ~35% of homeowners claim to have the settling tanks pumped out every two years (Ng 2005). Raised-bed leaching fields are common in the Subdivision because of thin overburden, and are also used in large-capacity applications at the community hall and health centre (see Figure 5-2 for locations). The health centre septic system is of particular concern because it is in constant use and is constructed in an area with thin overburden cover that is potentially upgradient from local water well receptors. The two churches located in the Main Village and a few neighbouring properties use holding tanks due to topographic, overburden thickness, and land slope restrictions.

Figure 5-1 shows 5 m topographic contours at the Site. The topography is closely controlled by the structure and character of the underlying bedrock (Wynne-Edwards 1967). The Village is generally flat near the Lake, but is bordered on the western and southern flanks by a 25 m topographic rise. The Subdivision slopes gradually to the Lake with a change in elevation of 15 m. Appendix E provides additional figures showing regional surface topography and surface
water features. The surface water divide is generally within three kilometres to the east and south of the Site and locally mimics the shape of the Lake shoreline.

Surficial geology is dominated by Quaternary glacial moraine deposits, and is described on the regional scale as thin (less than 0.45 m thick) and discontinuous sandy till overlying bedrock (Henderson 1967). Postglacial muck and peat deposits are found along the shoreline of the Lake and are common in the surrounding, higher-elevation areas overlying till deposits in close proximity to bedrock outcrop.

Bedrock geology (see figures in Appendix E) is complex as the Site is located at the contact between the Paleozoic sediments that are part of the Ottawa-St. Lawrence Lowland to the northeast, and the Precambrian Frontenac Axis (Wynne-Edwards 1967). The Paleozoic sediments are flat-lying and consist of (in stratigraphic order from oldest to youngest) the Nepean Formation (buff, fine- to coarse-grained quartz sandstone, partially calcareous towards the upper contact) and the March Formation (brown to buff, irregularly bedded, interbedded quartz sandstone, sandy dolostone, and dolostone). The flat-lying Paleozoic sediments are unconformably underlain by Grenville Series Precambrian metasediments and igneous intrusives. In general, the structure of the Precambrian basement is dominated by a series of northeast-trending, upright, similar folds with shallow or moderate plunge to the northeast (Wynne-Edwards 1967). Wynne-Edwards (1967) notes the unconformity can consist of a quartz-cobble conglomerate overlying fresh Precambrian rock, but is more often found as a deep zone of altered Precambrian rock overlain by sandstone without the basal conglomerate, particularly when the underlying rock type is marble (crystalline limestone and dolostone). This crumbled and oxidized zone sits directly below the Nepean Formation and is likely a regolith or fossil soil (Wynne-Edwards 1967).
5.3 Methods
The following is a general outline of the methodologies used for monitoring well installation, hydraulic testing, site instrumentation, overburden sampling, groundwater sampling, and analytical methods for a variety of chemical, isotopic, and biological parameters. Appendix F provides a more detailed description of some methods.

5.3.1 Site characterization
Eight 0.1524 m (6 inch) diameter monitoring wells were drilled between 2006 and 2008 (locations provided in Figure 5-1) using an air rotary percussion rig. The steel casing was typically installed no more than 2 m into bedrock to allow for hydraulic testing and groundwater sampling at shallow depths. Rock chip samples were collected every 1.5 m during drilling to determine subsurface geology.

Hydraulic testing was conducted immediately following drilling to locate significant fracture features and determine their hydraulic properties. Straddle packer sets (packer spacing ranging between 1.1 and 1.325 m) and conventional slug tests or constant-head tests were used in combination to produce a contiguous vertical transmissivity profile for each borehole. A submersible borehole camera was also used to examine the quality of the borehole prior to hydraulic testing, and to provide better resolution on the location and orientation (horizontal or inclined) of specific fracture features.

All boreholes were completed as multi-level piezometers designed to isolate transmissive features identified during hydraulic testing. Up to three intervals (designated as shallow (-S), mid (-M), and deep (-D) in the well interval nomenclature) were constructed in each borehole using conventional screen and sand pack materials and installation methods. Twenty-three intervals
were constructed in this manner, however, P8-D was not water-bearing upon completion and P3-S was abandoned partway through the study due to subsidence.

Overburden sampling and depth to refusal tests were conducted at 17 locations on the Site (see Appendix G) in July, 2007 using a truck-mounted auger. Soil samples were collected every 1.5 m and the depth to the water table was measured using an electronic water level meter. A standard set of sieves (75 $\mu$m to 19 mm) was used to determine the grain size distribution and classify samples using the Unified Soil Classification System (American Society for Testing and Materials 2007). Hydraulic conductivity was inferred from ranges reported in Table 3.7 from Fetter (2001) for different types of unconsolidated sediment types.

Precipitation events and ambient air temperature were recorded using an onsite tipping bucket rain gauge with built-in event logger and thermocouple. Pressure transducers were installed in most monitoring well intervals to record hydraulic head on 15-minute intervals. A dedicated barometric pressure transducer was also deployed and used for the barometric correction of hydraulic head data during post-processing. The combination of the local rain gauge and the distribution of pressure transducers throughout the site allowed for the detailed examination of the system response to precipitation events. Hourly meteorological data provided by Environment Canada (rain, snow, total precipitation, air temperature, snow pack thickness) for a nearby weather station were used to help monitor hydraulic responses in the wells due to the melting of the snow pack during various parts of the winter and spring months. The collection time interval for the pressure transducers was changed to five seconds for a 24-hour test during a period without precipitation in August, 2008 to examine high-resolution baseflow trends and hydraulic responses to local pumping events in nearby domestic wells.
Recharge estimates in shallow bedrock monitoring intervals (P1-S, P6-S, and P7-S) were conducted using the Water Table Fluctuation (WTF) Method from Healy and Cook (2002). The value of specific yield used for the estimates was determined by calculating the primary porosity from the hydraulic testing data. Primary porosity for a particular multi-level interval was calculated by dividing the sum of the intersecting fracture apertures by the total length of the interval (or the length of the tested sections in the case of P7-S). Recharge was calculated for various time periods by accumulating all the peak water level responses including those on the back side of recession curves.

5.3.2 Groundwater Sampling and Analysis
Groundwater samples were obtained from multi-level intervals using dedicated polyethylene tubing fitted with a foot valve or a submersible pump. Each interval was purged until field parameters stabilized and at least one well volume was removed prior to the collection of the sample. Table 5-1 provides a detailed schedule of sampling events. Analytes included major ions and nutrients (ammonia, chloride, dissolved organic carbon (DOC), nitrate-N, nitrite-N, and total phosphorus), stable isotopes (δ^{18}O and δ^{2}H in water), and bacteria (E. coli, total coliform, fecal coliform, and fecal streptococci). Samples were collected, preserved, stored, and analyzed using conventional field and laboratory methods. Appendix F provides a more details on the analytical methods.

Groundwater samples were also collected for the analysis of 40 pharmaceutical and person care products (PPCPs). Appendix F provides a list of these compounds along with background information on the common use, example trade name, CAS number, and chemical formula for each. The PPCPs cover a wide range of therapeutic uses, including: antibiotics; chest pain, hypertension and blood circulation; cholesterol reducers; pain killers, fever reducers, and anti-inflammatory; and psychiatric and anticonvulsants.
Environment Canada’s National Laboratory for Environmental Testing (NLET) in Burlington, ON conducted the analysis for a suite of acid pharmaceuticals (acetaminophen, bezafibrate, clofibrate, diclofenac, fenoprofen, fenofibrate, gemfibrozil, ibuprofen, indomethacin, ketoprofen, naproxen, salicylic acid, and triclosan) using NLET Method 3500. Groundwater samples were collected in 1 L amber glass bottles with a Teflon®-lined cap. Samples collected in February, 2007 and September, 2008 were preserved at 4±3 °C with 100 mL of dichloromethane and 10 mg/L mercuric chloride. The preservation method was changed to 4±3 °C at pH <2 (2-4 mL 50% H₂SO₄) for samples collected in May, 2009 due to a recognized misprint in the NLET Schedule of Services (2008). Concentrations were measured using gas capillary chromatography and negative-ion chemical ionization mass spectrometry detection. The method detection limit for each compound is provided in Appendix F.

Antibiotic (sulfonamide group – sulfacetamide, sulfadiazine, sulfadimethoxine, sulfaguanidine, sulfamerazine, sulfamethazine, sulfamethoxazole, sulfapyridine, and sulfathiazole) concentration analysis on groundwater samples collected in September, 2008 was conducted at a research laboratory at Environment Canada in Burlington, ON using techniques developed by Balakrishnan et al. (2006). Groundwater samples were collected in 1 L low density polyethylene bottles and frozen. Solid phase extraction was used to concentrate the target compounds. Analysis was conducted using a Quattro Ultima tandem liquid chromatography triple quadrupole mass spectrometer equipped with a Z-Spray electrospray ionization source in positive-ion mode. The mass spectrometer apparatus was attached to an Alliance 2695 high performance liquid chromatography system. The method detection limit for each compound is provided in Appendix F.
PPCP analyses for groundwater samples collected in May, 2009 were conducted by NLET. The methods employed for the acid pharmaceutical component of the suite are the same as those discussed previously. All other analyte concentrations were measured from samples collected in 1 L low density polyethylene bottles that were frozen for preservation. Solid phase extraction methods to concentrate the target compounds were adapted from Hao et al. (2006) and Miao et al. (2004). Liquid chromatography tandem mass spectrometry was used to analyze the samples. The type of column and gradient conditions at the time of injection are specific to the type of analyte, and some methods are still in testing at NLET (Sverko 2010). The method detection limit for each compound is provided in Appendix F.

5.4 Results
The following outlines the results from the field program conducted at the Site between 2007 and 2009. This includes the results from the geological and hydrogeological characterization, precipitation and hydraulic response monitoring, and chemical and bacterial sampling events.

5.4.1 Surficial and Bedrock Geology
Figure 5-3 provides a composite diagram of surficial and bedrock geology, hydraulic testing, and multi-level completion intervals for the eight monitoring wells. The observed depth to bedrock at the Site ranges between approximately 0 and 11 m. The thickest overburden is noted in the low-lying portions of the Main Village towards the Lake while the thinnest is found in the surrounding, higher-elevation areas. Appendix G provides detailed information and results from the augering survey including the grain size distribution curves. Refusal depths using the auger coincide with boulder layers noted during the drilling of the monitoring wells and in the local historical water well records, not competent bedrock. All soil samples classify as silty sand and clayey sand. Hydraulic conductivity is expected to range between $1 \times 10^{-8}$ to $1 \times 10^{-6}$ m/s (Fetter 2001). Provincial water well records indicate the presence of high clay content in the sediments.
between the boulder lags and the bedrock. The measured depth to the water table in the overburden ranged between 1.2 and 3.6 mbgs in the Main Village.

Bedrock geology is shown in Figure 5-3 and is also shown in detailed monitoring well schematics in Appendix H and geologic cross-sections in Appendix I. The traces of the geological cross-section presented in Appendix I are shown in Figure 5-1. The cross-sections, which include data from historical residential water well records, show an undulating bedrock surface, particularly along C-C’ (note the vertical exaggeration equals 5). The topography of the Precambrian basement is also variable. The weathered zone is preserved between the marble and overlying Paleozoic sediments in portions of the Site (see cross-sections D-D’ and E-E’ in Appendix I).

5.4.2 Hydraulic Testing, Gradient, and Flow Direction

Figure 5-3 provides a composite of the results from the hydraulic testing conducted in monitoring wells at the Site. Detailed borehole schematics, which include submersible camera and drill operator observations, are presented in Appendix H. In general, only a few fractures observed with the borehole camera were identified as water producing features by the driller or hydraulic testing. Conductive fractures in the Paleozoic sediments are noted at nearly regular intervals of 2 to 4 m (Figure 5-3). Test interval transmissivities range from approximately $4 \times 10^{-8}$ m$^2$/s to $2.5 \times 10^{-3}$ m$^2$/s. Discrete features are often quite distinguishable in the vertical transmissivity profiles because they are separated by testing intervals with transmissivities that are several orders of magnitude lower (best shown in P6 and P7). Few vertical fractures are noted in the Paleozoic sediments using the submersible camera, however, the general increase and uniformity in the transmissivity measurements across several contiguous testing intervals may indicate their presence.
The weathered zone at the Paleozoic-Precambrian contact shows few discrete fractures (Figure 5-3). Test interval transmissivities range from approximately $1 \times 10^{-7}$ m$^2$/s to $1 \times 10^{-4}$ m$^2$/s with the highest often noted at the contact with the underlying marble. The Precambrian marble and igneous intrusives have sparse and irregularly-spaced fractures compared to the overlying Paleozoic sediments. Major fracture features often occur in zones and/or are inclined, as noted in the submersible camera observations and by the nature of the vertical transmissivity profiles. Test interval transmissivities range from approximately $1.6 \times 10^{-9}$ m$^2$/s to $2.5 \times 10^{-3}$ m$^2$/s. The dominant fracture feature transmissivities in the Precambrian basement are on the same order of magnitude as those in the overlying Paleozoic sediments. The hydraulic conductivity of these preferential flow pathways (up to $2 \times 10^{-3}$ m/s) is upwards of three to five orders of magnitude greater than the estimates for the overburden at the Site.

Water levels in monitoring wells vary between $<1$ m and 5 m below ground surface with the exception of a few artesian cases (P2-D, P4-S and P4-D). Calculations of hydraulic gradient and flow direction using the three- and four-point graphical method are provided in Appendix J and are based on water levels observed on May 7, 2009 in shallow and mid intervals. The magnitude of the groundwater gradient ($\nabla h$) ranges between 0.022 and 0.078, which are steep and similar to local topographic changes. The direction of groundwater flow varies between 319° and 357° (NW to N), roughly mimics surface topography in the vicinity of the wells, and is in the direction of the Lake.

5.4.3 Hydraulic Response to Recharge/Pumping Events

Table 5-2 provides a summary of monitoring interval flow characteristics with respect to head differential, response to local pumping events, and response to recharge events. The observations are based on the six-month (December 1, 2008 to May 31, 2009), one-month (October, 2008) and one-day (noon on August 25 to noon on August 26, 2008) data provided in Appendix K. The
classification schemes in Table 5-2 involving a magnitude of head change are based on natural
breaks in the data. Adjectives describing the timing of the response to recharge are qualitative.

Response to local pumping events is classified in Table 5-2 as strong (max. $\Delta h >0.3$ m), moderate
(max. $\Delta h =0.1-0.3$ m), weak (max. $\Delta h <0.1$ m), and none (no change noted). Only 5 of the 20
monitored intervals show no response to pumping in local residential wells based on data from all
three monitoring timeframes. These intervals are either deep multi-level completions (P1-D, P2-D,
P6-D, and P7-D) and/or they have a head differential of more than 1 m compared to the other
intervals in the same well (P2-D, P7-S). Response to a local pumping event (based on the one-
day dataset) is noted in 10 intervals (P2-S, P2-M, P3-M, P3-D, P4-S, P4-D, P6-S, P6-M, P8-S,
and P8-M). Four other intervals indicate that the hydraulic response due to local pumping is
either weakly correlated with what is observed in an adjacent vertical multi-level interval (P1-S
and P1-M), or the intervals are responding to different domestic pumps (P5-S and P5-M).

Hydraulic response to precipitation/recharge events is classified in terms of the magnitude and
timing using the six-month dataset (December, 2008 to May, 2009). In particular, the hydraulic
responses coinciding with the melting of the snow pack and rainfall in mid-February, and the
rainfall in late-March and early-April are used as reference events. The magnitude of the
response is classified in Table 5-2 as strong (max. $\Delta h = 1-3$ m), moderate (max. $\Delta h = 0.5-1$ m),
and weak (max. $\Delta h <0.5$ m). A qualitative classification system is used to describe the timing of
the response to precipitation/recharge. “Immediate” refers to quick responses that have sharp
peaks. “Moderately delayed” also refers to a relatively quick response but the peaks are more
rounded and the signal is somewhat subdued. “Strongly delayed” refers to responses where there
is not an immediate and drastic change in water level but rather a longer-term, much reduced
gradual increase following multiple contiguous precipitation events. Intervals that exhibit this
sort of timing typically show greater variability in hydraulic head on a daily basis due to local pumping than responses to precipitation/recharge events during a longer timeframe.

Only 2 of 20 intervals (P1-S and P7-S) are classified as being strong and immediate responders to recharge events. These two intervals are both completed in limestone and sandstone in the shallow subsurface and have more than 1 m in head differential between lower intervals within their respective wells. Nine of 20 intervals (P1-M, P1-D, P4-S, P4-D, P6-S, P6-M, P6-D, P7-M, and P7-D) classify as having strong hydraulic head changes that are moderately delayed following a recharge event. These intervals are commonly mid and deep completions in sandstone or igneous intrusives. Seven of 20 intervals (P2-S, P2-M, P2-D, P5-S, P5-M, P8-S, and P8-M) show moderate response with moderately delayed timing. These intervals are mainly those completed in igneous intrusives or intersect the weathered zone. The remaining 2 of 20 intervals (P3-M and P3-D) show a weak and strongly delayed response to recharge and are completed in the marble.

5.4.4 Recharge Estimates

The following WTF method analysis utilizes precipitation and hydraulic head data (see Appendix K) from October, 2008 (for monitoring intervals P1-S and P7-S) and March 26 to May 31, 2009 (for monitoring intervals P1-S, P6-S and P7-S). The local rain gauge recorded a total of 84 mm of precipitation during October, 2008. The total head rise was 1.68 m in P1-S and 5.98 m in P7-S. Total precipitation from the nearby weather station between March 26 and May 31, 2009 was 318 mm. The total observed head rise in P1-S, P6-S, and P7-S was 6.52 m, 2.06 m, and 2.25 m, respectively. The specific yield (primary porosity) estimates are 3.6x10^{-4} (P1-S), 2.3x10^{-4} (P6-S), and 1.7x10^{-4} (P7-S). The estimated recharge using the October, 2008 data is 0.6 mm (P1-S) and 1.0 mm (P7-S), which is approximately 0.7% to 1.2% of the precipitation. Recharge estimates using all three observation intervals and the March 26 to May 31, 2009 precipitation data are 2.3
mm (P1-S), 0.5 mm (P6-S), and 0.4 mm (P7-S). These recharge estimates equate to 0.7%, 0.2%, and 0.1% of the precipitation for the period, respectively.

5.4.5 Stable Isotopes
Isotopic values in groundwater samples ranged between -70 and -85 ±1‰ VSMOW for δ²H (mean = -77 ‰) and -12.4 and -9.9 ±0.1‰ VSMOW for δ¹⁸O (mean = -11.3 ‰). Figure 5-4 provides a histogram of δ²H and δ¹⁸O. Each plot gives the range in isotopic values in groundwater samples collected from each interval (including analytical error). The position of the symbol shows the mean value and the number indicates how many samples were collected. The fill colour corresponds to the rock type the sampling interval is collected in. The amount-weighted mean annual value of precipitation for Ottawa from Birks et al. (2003) is provided for reference. The histogram of δ²H data shows three groupings: Group 1 (4 of 22 intervals) ranges from -80 to -86 ‰ VSMOW with the highest frequency of values at -82 ‰ VSMOW; Group 2 (15 of 22 intervals) ranges from -74 to -80 ‰ VSMOW with the highest frequency of values at -76 ‰ VSMOW; Group 3 (3 of 22 intervals) ranges from -69 to -74 ‰ VSMOW with the highest frequency of values at -71 ‰ VSMOW. While isotopic values for a particular interval may range across more than one grouping, the majority fall into just one. The grouping number for each interval is included in Table 5-2. The δ¹⁸O data is limited to a narrow range and the histogram shows more of a unimodal distribution. Additional cross-plots and other isotopic information are provided in Appendix L.

5.4.6 Nutrients and Chloride
Table 5-3 provides the results of nitrate concentrations in groundwater. Thirty-eight of 140 samples collected had nitrate concentrations above the analytical method detection limit (0.05 to 0.2 mg/L-N). The highest concentration observed was 2.85 mg/L-N and none of the samples had nitrate concentrations greater than the Ontario Drinking Water Standard of 10 mg/L-N. In
general, nitrate is detected in the shallow and mid intervals in the monitoring wells; the highest concentrations are noted in mid intervals (P2-M, P6-M).

Nitrite, ammonia, total phosphorus, and dissolved organic carbon (DOC) concentrations are presented in Appendix M. Concentrations of all analytes are low and typically less than the detection limits. The maximum concentrations of nitrite, ammonia, and total phosphorus are 0.5 mg/L-N, 0.2 mg/L, and 0.06 mg/L, respectively. DOC is present in all samples (only sampled once on February 21, 2008) at low concentrations ranging between 0.72 and 2.39 mg/L.

Chloride concentrations are provided in Table 5-4. A general increase is noted in most intervals from January, 2008 to July, 2008. The highest chloride concentrations are noted in P5 (up to 478 mg/L) and the lowest in P6 (up to 5.6 mg/L).

Field parameters, sulphate and fluoride results are provided for reference in Appendix N. Dissolved oxygen concentrations ranged between 0.1 and 7.7 mg/L.

5.4.7 Bacteria
Total coliform, *E. coli* and fecal streptococci results are provided in Tables 5-5 to 5-7. The presence of total coliform, fecal streptococci or *E. coli* is noted in every sampling interval at some time during the study. Fecal coliform was not detected in any of the samples (only a single collection on September 4, 2008). The highest total coliform count observed was 300 cts/100 mL in the January 7, 2008 sampling of P3-S. The highest *E. coli* count was 25 cts/100 mL noted in the July 2, 2008 sample from P7-S. The highest fecal streptococci count was 114 cts/100 mL observed in the July 2, 2008 sample from P7-S. Overgrown (OG) refers to when other bacteria interfere with the proper enumeration of the target bacteria in the laboratory. The presence of any particular indicator bacteria in a sample does not correlate well with the co-presence of another.
5.4.8 Pharmaceuticals and Personal Care Products

The concentrations of PPCPs measured in groundwater are reported in Table 5-8. Fourteen of 40 target compounds were detected: sulfacetamide, sulfadimethoxine, sulfaguanidine, sulfamethoxazole, sulfapyridine, sulfathiazole, gemfibrozil, triclosan, fenoprofen, ibuprofen, salicylic acid, amitriptyline HCl, and carbamazepine. It should be noted that sulfadimethoxine is used in veterinary applications.

The presence of any one of the 40 target compounds is detected in 16 of the 21 sampling intervals. Nine of these 16 intervals are the shallow multilevel completions, 3 are mid, and 4 are deep. The only intervals in which PPCPs were tested but not detected include P4-D, P5-M, P5-D, and P8-M. Intervals P4-D and P8-M were sampled twice (but not necessarily analyzed for the same compounds) while P5-M and P5-D were only sampled once. Concentrations range between trace amounts near the method detection limit (typically <5 ng/L) and 168 ng/L.

The concentrations of acid pharmaceuticals detected in the February and September, 2008 samples may be questionable due to improper preservation methods noted by the laboratory. These data are still useful, but are best suited to a presence/absence analysis rather than an interpretation based on absolute concentration.

5.5 Discussion

The following presents a conceptual model of groundwater flow and contaminant transport based on results from the field studies conducted at the Site. The conceptual model is a necessary precursor to understanding contaminant concentrations at the Site. The source(s) of contamination, spatial and temporal distribution of contaminants in the subsurface, and the implications of bedrock aquifer vulnerability to surface contaminant sources are discussed.
5.5.1 Conceptual Model

Figure 5-5 provides a simplified conceptual model in cross section for groundwater flow and contaminant transport at the Site. The cross-section is oriented parallel to regional groundwater flow and is not to scale (vertical exaggeration is on the order of 5:1 to 10:1). The conceptual model is based on a balance of the results presented in Section 5.4, and can be summarized in the following main points:

- Borehole hydraulic testing results show highly transmissive preferential pathways exist as horizontal to near-horizontal bedding plane/sheeting fractures in the Paleozoic sediments (numerous) and inclined or random-oriented fractures in the Precambrian basement rocks (few);
- The fracture network is complex with a variety of different orientations and connections, particularly when considered in three dimensions, as evidenced by the hydraulic testing results and variable hydraulic response to recharge and local pumping events;
- Hydraulic, isotopic, and contaminant data suggest vertical fracture connectivity in the system is limited, but sufficient enough to allow anthropogenic contaminants to enter and migrate to the deeper subsurface;
- Regional surficial and bedrock geology information, and observations of disconnected surface water features and the use of raised-bed septic systems in the surrounding environs indicates overburden is thin and of low permeability in the upland areas;
- Sieve analysis of samples from the upper portions of the thicker overburden deposits underlying the Village show appreciable amounts of fines and the estimated hydraulic conductivity is low. Higher permeability sandy lens and boulder lags may be present and act as preferential flow and contaminant transport pathways;
- Contaminants may also enter the bedrock system through thicker overburden deposits depending on the nature of the overburden material, flow paths, and the presence of fractures at the overburden-bedrock interface.
5.5.2 Contaminant Sources

The objective of the groundwater sampling was to use nutrients, fecal indicator bacteria, and PPCPs as tracers to establish the presence and source(s) of contamination in the bedrock aquifer at the Site. Nutrient levels remained low throughout the sampling period and do not directly support either septic systems or agriculture as a source. The presence of fecal indicator bacteria (E. coli and fecal streptococci) and total coliform counts confirms that fecal contamination and surface water are adversely impacting groundwater quality, respectively. However, the presence/absence of fecal indicator bacteria in the samples is more relevant to the determination of potability and does not distinguish between human and animal sources. Of relevance to the present work, however, is the concurrent investigation at the Site by Trimper (2010) which detected human enteric viruses (Adenovirus, Adenovirus type 40, Hepatitis A virus, and Rotavirus) in groundwater samples collected during four sampling events conducted between July, 2008 and May, 2009 from a subset of the monitoring intervals.

The variety of PPCPs detected in groundwater samples and their spatial distribution provides the best evidence that multiple septic systems, including the large capacity raised-bed leaching field at the health centre and off-Site leaching fields, are contributing to groundwater contamination. The specific impact of the health centre septic system on groundwater quality in the Main Village is likely negligible due to the estimated groundwater flow direction (N to NW). The co-presence of sulfadimethoxine, an antimicrobial used to treat coccidia in farm animals, in wells P1, P2 and P7 suggests an additional contribution from nearby agricultural sources (beef and dairy farms) located to the east and southeast of the Site based on flow direction.

Elevated chloride concentrations detected in many of the monitoring intervals of wells located in the Main Village (P1, P2, P3, P5, and P7) are mainly attributed to the application of road de-icing salts to the highway that transects the Site (maintained by the Ontario Ministry of Transportation,
MTO). Chloride might also be sourced from septic systems since other indicators are present, however, the relative contribution is unknown. According to the MTO subcontractor responsible for maintaining the highway, plowing and salting commences following the accumulation of 2 cm of snow on the highway. A combination of brine and rock salt is applied at a rate of 130 kg/km when snow and ice are present, which is reduced to 100 kg/km when only snow is present. Local road winter maintenance in the Main Village and Subdivision is performed by the Township. Plowing is the most common method and is required less frequently than for the highway. A 97/3 sand/salt mixture is only applied to local roads when required for traction. The combination of thicker, low permeability overburden within the Main Village and the difference in the amount of road salt applied would suggest that the chloride contribution from local roads to groundwater pollution in the bedrock aquifer is likely negligible compared to that from the highway. The infiltration of the road salt into the bedrock aquifer via fractures in the outcrop-bordered ditches present along extensive lengths of the highway in the vicinity of the Main Village is interpreted.

**5.5.3 Spatiotemporal Distribution of Contaminants and Tracers**

Recharge, although estimated to be low relative to the amount of precipitation, is a dominant factor in controlling the introduction of surface contaminants into the deeper bedrock system. Variability in recharge, both seasonally and spatially across an area can add to the heterogeneity of a bedrock system because the infiltrating waters act as both a transmitter and diluter of contaminants (Iqbal and Krothe 1995; Levison and Novakowski 2009). The nature of the fracture network itself causes dispersion in three-dimensions, resulting in varying and reduced contaminant concentrations and complexities in understanding the temporal and spatial distribution of contaminants at the Site. The complexities of recharge and flow in the fracture network are reflected in the stable isotope dataset. While many of the groundwater samples collected from the multilevel network plot near the amount-weighted average of annual precipitation (Figure 5-4), there are several outliers, including samples from mid and deep
intervals. This is indicative of preferential pathways and/or the mixing of different recharge waters (Clark and Fritz 1997).

The presence of contaminants in shallow bedrock monitoring intervals does not necessarily imply the source(s) is (are) proximal to the borehole. For example, septic systems located in the Main Village are likely to have a limited impact on the underlying bedrock aquifer water quality due to the thickness of the overburden and the lack of vertical connectivity noted in the underlying fracture network. The thicker overburden is of low permeability, resulting in longer retention times and an increased potential for attenuation. This may be different in the upland areas where the overburden is thin, however, a vertical connection must still be present. Thus, a significant lateral component to the transport pathway from source to receptor is interpreted.

The detection of contaminants in the mid and deep intervals of monitoring wells located in the Main Village suggest the sources are likely located in the surrounding upland areas in order for the pollutants to migrate to such depths given the limited vertical connectivity of the fracture network. The location of the contributing sources is likely limited to within 3 km to the east and south of the Site because of the surface water divide (see Section 5.2). The presence of *E. coli* in these intervals indicates recent fecal contamination (WHO 2006) and that transport is rapid based on previously published survival rates ranging between a few weeks in soil (Mawdsley et al. 1995) to up to 300 days in fractured rock aquifers (Malard et al. 1994). As depicted in the conceptual model in Figure 5-5, these upland areas are recharge zones with co-present septic system leaching fields, thin overburden, plentiful bedrock exposure, and agriculture.

Consistently low concentrations of nutrients are likely the result of dilution during recharge and dispersion in the bedrock aquifer. For the case of nitrate, the presence of DO in the groundwater indicates aerobic conditions exist in the bedrock system; therefore, attenuation through
heterotrophic denitrification is limited and also indicates the potential for nitrification of ammonium in the subsurface. Nitrate concentrations remained well below the drinking water standard of 10 mg/L-N (MOE 2002; WHO 2006; US EPA 2009) and do not indicate potability concerns at the Site. In comparison, other studies in fractured bedrock and porous media aquifers have shown elevated and spatiotemporally variable concentrations of nitrate in groundwater that may exceed the drinking water standard in areas impacted by septic systems and agricultural sources (Robertson and Cherry 1992; Harman et al. 1996; Verstraeten et al. 2005; Wilcox et al. 2005; Levison and Novakowski 2009).

Current microbial drinking water quality standards are 0 CFU/100 mL (CFU = colony forming unit; membrane filtration methods count the number of colony-forming units and the results can be equivalently expressed as counts/100 mL abbreviated to cts/100 mL) for both total coliforms and \textit{E. coli} (MOE 2002; US EPA 2009). The widespread and regular detection of fecal indicator bacteria across the site at sampling depths up to ~37 metres below ground surface demonstrates that the groundwater at the Site is noncompliant with these standards and that the bedrock aquifer is vulnerable to microbial contamination. Powell et al. (2003) notes similar results in two sandstone aquifers in the United Kingdom where the presence of fecal indicator bacteria was observed at even greater depths of up to 91 m. Low counts or the absence of fecal indicator bacteria in some groundwater samples in this study may be more of a result of the sampling method than source dilution in the aquifer, as shown by Kozuskanich et al. (2010) (Chapter 4). Thus, the results may be biased towards non-detects because of the purging process prior to the collection of a single sample. The correlation between bacterial counts or absence/presence and chemical concentrations is poor. In a similar study conducted in an agricultural watershed, Levison and Novakowski (2009) attribute the comparable spatiotemporal dissimilarities in the distribution of chemical and bacterial analytes to differences in the transport processes. It should
be noted that the results from this study are not subject to the uncertainties of domestic well surveys where poor well completion quality might be an issue in biasing the results.

In general, PPCP concentrations in groundwater from this study reported in Table 5-8 are within a similar range (1 to ~100 ng/L) as reported in other groundwater (Seiler et al. 1999; Godfrey et al. 2007) and surface water (Daughton and Ternes 1999; Lissemore et al. 2006; Servos et al. 2007) studies conducted in Ontario and other parts of North America. Their ubiquity in the environment is generally not interpreted because they are not airborne contaminants. Unlike the relatively consistent nutrient output from a household septic system, PPCPs may be quite variable according to their therapeutic use. For example, an antibiotic might be used for relatively short time to treat a specific infection in an individual. The same antibiotic could also be used within the larger population if the ailment is contagious (e.g. pink eye or strep throat). Other drugs, such as cholesterol-reducers and painkillers, may be used on an on-going basis, particularly in an aging population. Thus, using PPCPs to try to understand contaminant transport between an individual septic system and down-gradient receptor may be difficult at the field scale. Pharmaceuticals specific to rare disease treatment may be of use for this purpose, but requires user-specific data that are not public information.

5.6 Conclusions

The results from this study lead to the following conclusions on flow and transport and the potential for adverse impacts on bedrock aquifer water quality from anthropogenic surface sources in areas with thin or inadequate overburden, and the methods used to identify and differentiate contaminant sources:

1. Contaminants released at surface in areas with thin or inadequate overburden can migrate quickly and deeply via a complex bedrock fracture network into the aquifer that is relied on as a potable drinking water resource.
2. Recharge plays a crucial role in moving surface contaminants into the deeper subsurface. It also acts to dilute contaminants and create additional heterogeneity in the transport through the fractured bedrock system.

3. PPCP analysis provides detail on the types of sources (both septic systems and agriculture) and confirms there are multiple contributors present (based on the distribution and variety of compounds detected). This interpretation could not otherwise be definitely established using traditional methods including nutrient concentrations and fecal indicator bacteria counts.

4. PPCP concentrations in samples from the bedrock aquifer are similar to those measured in previous groundwater and surface water studies conducted in Ontario and other parts of North America.

5. Although limited in use for source determination, fecal indicator bacteria provide a consistent and cost-effective method for determining the potential for adverse public health impacts due to groundwater consumption in this setting because drinking water standards have been established.
5.7 References


Ng, J. 2005. Integrated stormwater management for lakeside villages: a study of Portland, ON. Master's, Department of Civil Engineering, Queen's University, Kingston.


Table 5-1: Groundwater sampling schedule.

<table>
<thead>
<tr>
<th>Sampling Date</th>
<th>Nutrients and Major Ions</th>
<th>Isotopes</th>
<th>Bacteria</th>
<th>PPCPs</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ammonia</td>
<td>chloride</td>
<td>DOC</td>
<td>nitrate - N</td>
</tr>
<tr>
<td>22-Feb-07</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
</tr>
<tr>
<td>03-Apr-07</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
</tr>
<tr>
<td>03-May-07</td>
<td></td>
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<td></td>
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<tr>
<td>23-May-07</td>
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<td>19-Jul-07</td>
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<tr>
<td>10-Sep-07</td>
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<td>14-Nov-07</td>
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<td>07-Jan-08</td>
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<tr>
<td>07-Apr-08</td>
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<tr>
<td>07-May-09</td>
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</table>
Table 5-2: Classification of monitoring well intervals by head differential, response to local pumping events, response to recharge, and mean $\delta^{2}H$. The dataset used for each category is indicated by the superscript.

<table>
<thead>
<tr>
<th>Well Interval</th>
<th>Bedrock Geology</th>
<th>Transmissivity ($m^2/s$)*</th>
<th>&gt;1m Head Differential Noted Between Upper and Lower Interval(s)</th>
<th>Response to Local Pumping $^{1,2,3}$</th>
<th>Response to Pumping Event Also Noted in Upper and Lower Interval(s) $^{1}$</th>
<th>Response to Recharge Events $^{2}$: Magnitude, Timing</th>
<th>Isotope Grouping using $\delta^{2}H$</th>
</tr>
</thead>
<tbody>
<tr>
<td>P1-S</td>
<td>Sandstone</td>
<td>$1.3x10^{-3}$</td>
<td>Yes (lower)</td>
<td>[ ]</td>
<td>Weak or different pump</td>
<td>[ ]</td>
<td>3</td>
</tr>
<tr>
<td>P1-M</td>
<td>Sandstone</td>
<td>$1.0x10^{-3}$</td>
<td>No</td>
<td>[ ]</td>
<td>Weak or different pump</td>
<td>[ ]</td>
<td>3</td>
</tr>
<tr>
<td>P1-D</td>
<td>Sandstone</td>
<td>$3.3x10^{-4}$</td>
<td>No</td>
<td>[ ]</td>
<td>No</td>
<td>[ ]</td>
<td>3</td>
</tr>
<tr>
<td>P2-S</td>
<td>Igneous intrusive</td>
<td>$6.3x10^{-5}$</td>
<td>No</td>
<td>[ ]</td>
<td>Yes</td>
<td>[ ]</td>
<td>2</td>
</tr>
<tr>
<td>P2-M</td>
<td>Igneous intrusive</td>
<td>$1.5x10^{-2}$</td>
<td>No</td>
<td>[ ]</td>
<td>Yes</td>
<td>[ ]</td>
<td>2</td>
</tr>
<tr>
<td>P2-D</td>
<td>Igneous intrusive</td>
<td>$1.0x10^{-5}$</td>
<td>Yes (higher)</td>
<td>[ ]</td>
<td>No</td>
<td>[ ]</td>
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<tr>
<td>P3-M</td>
<td>Weathered</td>
<td>$9.1x10^{-5}$</td>
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<td>[ ]</td>
<td>Yes</td>
<td>[ ]</td>
<td>2</td>
</tr>
<tr>
<td>P3-D</td>
<td>Marble</td>
<td>$1.2x10^{-5}$</td>
<td>No</td>
<td>[ ]</td>
<td>Yes</td>
<td>[ ]</td>
<td>2</td>
</tr>
<tr>
<td>P4-S</td>
<td>Marble</td>
<td>$7.7x10^{-5}$</td>
<td>No</td>
<td>[ ]</td>
<td>Yes</td>
<td>[ ]</td>
<td>2</td>
</tr>
<tr>
<td>P4-D</td>
<td>Marble</td>
<td>$1.3x10^{-2}$</td>
<td>No</td>
<td>[ ]</td>
<td>Yes</td>
<td>[ ]</td>
<td>2</td>
</tr>
<tr>
<td>P5-S</td>
<td>Sandstone/weathered</td>
<td>$1.6x10^{-4}$</td>
<td>No</td>
<td>[ ]</td>
<td>Different pump</td>
<td>[ ]</td>
<td>2</td>
</tr>
<tr>
<td>P5-M</td>
<td>Marble</td>
<td>$8.2x10^{-5}$</td>
<td>No</td>
<td>[ ]</td>
<td>Different pump</td>
<td>[ ]</td>
<td>2</td>
</tr>
<tr>
<td>P6-S</td>
<td>Sandstone</td>
<td>$4.1x10^{-4}$</td>
<td>No</td>
<td>[ ]</td>
<td>Yes</td>
<td>[ ]</td>
<td>1</td>
</tr>
<tr>
<td>P6-M</td>
<td>Igneous intrusive</td>
<td>$2.5x10^{-3}$</td>
<td>No</td>
<td>[ ]</td>
<td>Yes</td>
<td>[ ]</td>
<td>1</td>
</tr>
<tr>
<td>P6-D</td>
<td>Igneous intrusive</td>
<td>$8.3x10^{-4}$</td>
<td>No</td>
<td>[ ]</td>
<td>Yes</td>
<td>[ ]</td>
<td>1</td>
</tr>
<tr>
<td>P7-S</td>
<td>Limestone/sandstone</td>
<td>$4.3x10^{-4}$</td>
<td>Yes (higher)</td>
<td>[ ]</td>
<td>No</td>
<td>[ ]</td>
<td>3</td>
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<tr>
<td>P7-M</td>
<td>Sandstone</td>
<td>$1.8x10^{-3}$</td>
<td>No</td>
<td>[ ]</td>
<td>No</td>
<td>[ ]</td>
<td>2</td>
</tr>
<tr>
<td>P7-D</td>
<td>Sandstone</td>
<td>$8.3x10^{-4}$</td>
<td>No</td>
<td>[ ]</td>
<td>No</td>
<td>[ ]</td>
<td>2</td>
</tr>
<tr>
<td>P8-S</td>
<td>Sandstone</td>
<td>$4.1x10^{-4}$</td>
<td>No</td>
<td>[ ]</td>
<td>Yes</td>
<td>[ ]</td>
<td>2</td>
</tr>
<tr>
<td>P8-M</td>
<td>Weathered</td>
<td>$2.5x10^{-3}$</td>
<td>No</td>
<td>[ ]</td>
<td>Yes</td>
<td>[ ]</td>
<td>2</td>
</tr>
</tbody>
</table>

Notes:
1) One-day data
2) One-month data
3) Six-month data
* from hydraulic testing results

$\square$ = strong (max. $\Delta h >0.3$ m)
$\square$ = moderate (max. $\Delta h = 0.1-0.3$ m)
$\square$ = weak (max. $\Delta h < 0.1$ m)
$\square$ = none
$\bullet$ = strong (max. $\Delta h =1-3$ m)
$\star$ = moderate (max. $\Delta h =0.5-1$ m)
$\triangle$ = weak (max. $\Delta h <0.5$ m)
Table 5-3: Nitrate concentrations (mg/L-N) in groundwater samples. The current Ontario drinking water standard is 10 mg/L NO₃-N. Results greater than the method detection limit are highlighted.

<table>
<thead>
<tr>
<th>Date</th>
<th>P1-S</th>
<th>P1-M</th>
<th>P1-D</th>
<th>P2-S</th>
<th>P2-M</th>
<th>P2-D</th>
<th>P3-S</th>
<th>P3-M</th>
<th>P3-D</th>
<th>P4-S</th>
<th>P4-D</th>
<th>P5-S</th>
<th>P5-M</th>
<th>P5-D</th>
<th>P6-S</th>
<th>P6-M</th>
<th>P6-D</th>
<th>P7-S</th>
<th>P7-M</th>
<th>P7-D</th>
<th>P8-S</th>
<th>P8-M</th>
</tr>
</thead>
<tbody>
<tr>
<td>22-Feb-07</td>
<td>ND / 0.05</td>
<td>ND / 0.05</td>
<td>ND / 0.05</td>
<td>0.09</td>
<td>ND / 0.05</td>
<td>ND / 0.05</td>
<td>ND / 0.05</td>
<td>ND / 0.05</td>
<td>ND / 0.05</td>
<td>ND / 0.05</td>
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<tr>
<td>04-Apr-07</td>
<td>0.13</td>
<td>ND / 0.05</td>
<td>ND / 0.05</td>
<td>ND / 0.05</td>
<td>0.46</td>
<td>ND / 0.05</td>
<td>ND / 0.05</td>
<td>ND / 0.05</td>
<td>ND / 0.05</td>
<td>ND / 0.05</td>
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<tr>
<td>23-May-07</td>
<td>0.1</td>
<td>ND / 0.1</td>
<td>ND / 0.1</td>
<td>2.2</td>
<td>1.4</td>
<td>ND / 0.1</td>
<td>ND / 0.1</td>
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<td>19-Jul-07</td>
<td>ND / 0.08</td>
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<td>ND / 0.08</td>
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<td>1.03</td>
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<td>10-Sep-07</td>
<td>ND / 0.1</td>
<td>ND / 0.1</td>
<td>ND / 0.1</td>
<td>0.8</td>
<td>ND / 0.1</td>
<td>ND / 0.1</td>
<td>0.2</td>
<td>ND / 0.1</td>
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<tr>
<td>14-Nov-07</td>
<td>0.3</td>
<td>ND / 0.1</td>
<td>ND / 0.1</td>
<td>0.1</td>
<td>0.6</td>
<td>ND / 0.1</td>
<td>ND / 0.1</td>
<td>0.1</td>
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<tr>
<td>07-Jan-08</td>
<td>0.75</td>
<td>ND / 0.05</td>
<td>ND / 0.05</td>
<td>0.37</td>
<td>1.42</td>
<td>ND / 0.05</td>
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<tr>
<td>21-Feb-08</td>
<td>0.39</td>
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<td>1.46</td>
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<td>07-Apr-08</td>
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<td>1.60</td>
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</tbody>
</table>

Notes:
ND / ## = not detected, method detection limit given
Blank cells indicate a sample was not collected
Table 5-4: Chloride concentrations (mg/L) in groundwater samples.

| Date      | P1-S | P1-M | P1-D | P2-S | P2-M | P2-D | P3-S | P3-M | P3-D | P4-S | P4-D | P5-S | P5-M | P5-D | P6-S | P6-M | P6-D | P7-S | P7-M | P7-D | P8-S | P8-M |
|-----------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 22-Feb-07 | 55.2 | 60.6 | 16.5 | 97.9 | 147.6| 26.7 | 173.4| 166.9| 157.0|
| 04-Apr-07 | 112.4| 6.1  | 16.6 | 110.5| 156.1| 11.0 | 152.1| 149.6|
| 07-Jan-08 | 154.0| 41.6 | 28.5 | 137.0| 158.0| 11.0 | 172.0| 185.0| 191.0| 34.9 | 37.5 | 183.0| 107.0| 107.0| 4.6  | 5.4  | 5.2  |
| 21-Feb-08 | 149.0| 30.1 | 47.3 | 182.3| 165.5| 11.7 | 181.8| 183.5| 36.6 | 37.0 | 352 J| 198.2| 217 J | 4.7  | 5.6  | 5.3  |
| 07-Apr-08 |      | 174.3| 187.9| 12.9 |      |      | 438 J| 193.2| 216 J | 4.6  | 5.3  | 4.9  |
| 27-May-08 | 56.9 | 55.0 | 20.7 | 177.0| 200 J| 13.3 | 178.0| 189.0| 32.0 | 31.4 | 454 J| 198.0| 225 J | 4.1  | 5.1  | 4.8  |
| 02-Jul-08 | 79.0 | 58.0 | 19.0 | 196.0| 181.0| 12.0 | 169.0| 173.0| 30.0 | 30.1 | 478 J| 209 J | 439 J | 4.2  | 5.1  | 5.0  | 174.0| 48.2 | 16.1 | 50.6 | 35.9 |

**Notes:**
- J = estimated value based on calibration curve extrapolation
- Blank cells indicate a sample was not collected
Table 5-5: Total coliform counts (cts/100 mL) in groundwater samples. Analytical detection limits depend on sample dilution. Samples with coliforms present are highlighted.

| Date       | P1-S | P1-M | P1-D | P2-S | P2-M | P2-D | P3-S | P3-M | P3-D | P4-S | P4-D | P5-S | P5-M | P5-D | P6-S | P6-M | P6-D | P7-S | P7-M | P7-D | P8-S | P8-M |
|------------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 22-Feb-07  | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 2    | ND   | 1    | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    |
| 03-May-07  | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    |
| 23-May-07  | 1    | 22   | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    |
| 19-Jul-07  | ND   | 1    | 19   | ND   | 1    | 40   | 57   | 5    | OG   | OG   | 10   | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    |
| 10-Sep-07  | 14   | 31   | 2    | 20   | 6    | 21   | ND   | 1    | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    |
| 14-Nov-07  | OG   | 3    | 1    | 1    | 6    | 4    | 4    | ND   | 1    | 7    | OG   | 2    | OG   | 10   | OG   | ND   | 1    | ND   | 1    | ND   | 1    |
| 07-Jan-08  | ND   | 1    | ND   | 1    | 9    | 1    | ND   | 100  | ND   | 100  | 300  | 112  | ND   | 1    | 38   | 3    | 100  | ND   | 100  | 17   | ND   | 1    | 1    |
| 21-Feb-08  | 2    | ND   | 2    | ND   | 2    | 10   | ND   | 2    | ND   | 2    | ND   | 2    | ND   | 2    | ND   | 2    | ND   | 2    | ND   | 2    | ND   | 2    |
| 07-Apr-08  | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    | ND   | 1    |
| 27-May-08  | ND   | 1    | 2    | ND   | 2    | 17   | ND   | 1    | ND   | 1    | ND   | 2    | ND   | 1    | ND   | 2    | ND   | 1    | ND   | 1    | ND   | 1    |
| 02-Jul-08  | ND   | 2    | ND   | 1    | ND   | 1    | OG   | 134  | 33   | ND   | 2    | 31   | 2    | ND   | 1    | ND   | 2    | ND   | 1    | ND   | 2    | 4    | OG   |
| 04-Sep-08  | OG   | ND   | 1    | 13   | OG   | 1    | ND   | 1    | OG   | 1    | 4    | ND   | 1    | ND   | 10   | OG   | ND   | 1    | 5    | 1    | 2    | ND   |

Notes:
- ND / ## = not detected, method detection limit given
- OG = overgrown
- Blank cells indicate a sample was not collected
Table 5-6: *E. coli* counts (cts/100 mL) in groundwater samples. Analytical detection limits depend on sample dilution. Samples with *E. coli* present are highlighted.

<table>
<thead>
<tr>
<th>Date</th>
<th>P1-S</th>
<th>P1-M</th>
<th>P1-D</th>
<th>P2-S</th>
<th>P2-M</th>
<th>P2-D</th>
<th>P3-S</th>
<th>P3-M</th>
<th>P3-D</th>
<th>P4-S</th>
<th>P4-D</th>
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<th>P5-M</th>
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<th>P7-S</th>
<th>P7-M</th>
<th>P7-D</th>
<th>P8-S</th>
<th>P8-M</th>
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<td>19-Jul-07</td>
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<td>ND / 1</td>
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<td>07-Jan-08</td>
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<td>02-Jul-08</td>
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</tbody>
</table>

Notes:
ND / ## = not detected, method detection limit given
OG = overgrown
Blank cells indicate a sample was not collected

Table 5-7: Fecal streptococci counts (cts/100 mL) in groundwater samples. Analytical detection limits depend on sample dilution. Samples with fecal streptococci present are highlighted.

<table>
<thead>
<tr>
<th>Date</th>
<th>P1-S</th>
<th>P1-M</th>
<th>P1-D</th>
<th>P2-S</th>
<th>P2-M</th>
<th>P2-D</th>
<th>P3-S</th>
<th>P3-M</th>
<th>P3-D</th>
<th>P4-S</th>
<th>P4-D</th>
<th>P5-S</th>
<th>P5-M</th>
<th>P5-D</th>
<th>P6-S</th>
<th>P6-M</th>
<th>P6-D</th>
<th>P7-S</th>
<th>P7-M</th>
<th>P7-D</th>
<th>P8-S</th>
<th>P8-M</th>
</tr>
</thead>
<tbody>
<tr>
<td>27-May-08</td>
<td>ND / 1</td>
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<td>02-Jul-08</td>
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<td>ND / 1</td>
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<td>ND / 1</td>
<td>OG</td>
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<td>114</td>
<td>13</td>
<td>2</td>
<td>4</td>
<td>ND / 1</td>
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</table>

Notes:
ND / ## = not detected, method detection limit given
OG = overgrown
Blank cells indicate a sample was not collected
Table 5-8: Pharmaceuticals and personal care products detected in groundwater samples. Examples of PPCP concentrations reported in the literature focus on Canadian and other North American studies.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Feb 2007&lt;sup&gt;1&lt;/sup&gt; (ng/L)</th>
<th>Sep 2008&lt;sup&gt;2&lt;/sup&gt; (ng/L)</th>
<th>May 2009&lt;sup&gt;3&lt;/sup&gt; (ng/L)</th>
<th>Examples of Previously Reported Values in the Literature (ng/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Antibiotics</strong></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>Sulfacetamide</td>
<td>P5-S / trace</td>
<td></td>
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<tr>
<td>Sulfadimethoxine</td>
<td>P1-S / trace; P1-M / trace; P2-D / trace; P7-S / trace; P7-D / 27.5</td>
<td></td>
<td>ND</td>
<td></td>
</tr>
<tr>
<td>Sulfaguanidine</td>
<td>P5-S / trace</td>
<td></td>
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<tr>
<td>Sulfamerazine</td>
<td>P4-S / trace</td>
<td></td>
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<tr>
<td>Sulfamethoxazole</td>
<td></td>
<td>P7-S / 6.40</td>
<td></td>
<td>1) 871: max. effluent concentration from 8 WWTPs in Calgary, AB, Canada (Chen et al. 2006) 2) 2.8: median concentration detected in Southern Ontario agricultural surface waters (Lissemore et al. 2006) 3) 1900: max. concentration in 139 U.S. streams (Kolpin et al. 2002) 4) 10 – 450: range in concentrations detected in groundwater downgradient from a high school septic field (Godfrey et al. 2007)</td>
</tr>
<tr>
<td>Sulfapyridine</td>
<td></td>
<td>P3-M / 91.1; P3-D / 96.1</td>
<td>P3-M / 33.6; P3-D / 43.9</td>
<td></td>
</tr>
<tr>
<td>Sulfathiazole</td>
<td>P1-S / 6.85</td>
<td></td>
<td>ND</td>
<td>1.4: median detected concentration in Southern Ontario agricultural surface waters (Lissemore et al. 2006)</td>
</tr>
<tr>
<td>Triclosan</td>
<td>ND</td>
<td>P1-M / 3.42</td>
<td>ND</td>
<td>34: maximum concentration detected in Ontario river water (Servos et al. 2007)</td>
</tr>
<tr>
<td><strong>Cholesterol Reducers</strong></td>
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<tr>
<td>Gemfibrozil</td>
<td>P1-S / 11.9; P1-M / 10.5; P1-D / 17.6; P2-S / 15.2; P2-M / 2.3; P2-D / 19.7; P3-S / 10.5</td>
<td></td>
<td>ND</td>
<td>1) 965 / 436: max. influent / effluent from 12 WWTPs along Thames River, Canada (Lishman et al. 2006) 2) 137: mean concentration in surface waters receiving urban inputs in Southern Ontario (Lissemore et al. 2006) 3) 19.2: Ontario river water (Servos et al. 2007)</td>
</tr>
<tr>
<td><strong>Pain Killers, Fever Reducers and Anti-inflammatories</strong></td>
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<tr>
<td>Fenoprofen</td>
<td>ND</td>
<td>P7-S / 64.2</td>
<td></td>
<td>1) 16500 / 733: max. influent / effluent from 12 WWTPs along Thames River, Canada (Lishman et al. 2006) 2) 1150: max. effluent from 8 WWTPs in Calgary, AB, Canada (Chen et al. 2006) 3) 93: max. concentration in Hamilton Harbour, ON, Canada (Metcalfe et al. 2003b) 4) 8: surface water (Daughton and Ternes 1999) 5) detected: Ontario lake water (Servos et al. 2007) 6) 150: Ontario river water (Servos et al. 2007)</td>
</tr>
<tr>
<td>Ibuprofen</td>
<td>ND</td>
<td>P7-S / 4.70</td>
<td>P7-S / 2.89</td>
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</tr>
<tr>
<td>Compound</td>
<td>Feb 2007(^1) (ng/L)</td>
<td>Sep 2008(^2) (ng/L)</td>
<td>May 2009(^3) (ng/L)</td>
<td>Examples of Previously Reported Values in the Literature (ng/L)</td>
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<td>------------------------------</td>
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<td>---------------------------------------------------------------</td>
</tr>
<tr>
<td>Salicylic acid</td>
<td>P1-S / 6.6</td>
<td>ND</td>
<td>ND</td>
<td>1) &lt;50: surface water (Zweiner et al. 2001)</td>
</tr>
<tr>
<td></td>
<td>P1-M / 10.1</td>
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<td>2) 50 – 1510: sewage water (Zweiner et al. 2001)</td>
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<td>P1-D / 48.5</td>
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<td>P2-M / 5</td>
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<tr>
<td></td>
<td>P2-D / 120</td>
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<td>P3-S / 19.9</td>
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<td>P3-M / 12.8</td>
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<td>P3-D / 168</td>
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<td>Psychiatric and Anticonvulsants</td>
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<td>Amtriptyline HCl</td>
<td>P1-S / 0.88</td>
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<td>1) 1900 / 700: max. / median influent concentration in 14 Canadian STPs (Metcalfe et al. 2003a)</td>
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<tr>
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<td>P2-D / 0.82</td>
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<td>2) 2300 / 700: max. / median effluent concentration in 14 Canadian STPs (Metcalfe et al. 2003a)</td>
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<tr>
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<td>P3-M / 0.94</td>
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<td>3) 301: max. concentration in Hamilton Harbour, ON, Canada (Metcalfe et al. 2003b)</td>
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<tr>
<td></td>
<td>P5-S / 37.2</td>
<td></td>
<td></td>
<td>4) 925: max. effluent concentration from 8 WWTP in Calgary, AB, Canada (Chen et al. 2006)</td>
</tr>
<tr>
<td></td>
<td>P6-S / 0.88</td>
<td></td>
<td></td>
<td>5) 1: median concentration detected in Southern Ontario agricultural surface waters (Lissemore et al. 2006)</td>
</tr>
<tr>
<td></td>
<td>P8-S / 1.42</td>
<td></td>
<td></td>
<td>6) 16.2: mean concentration in surface waters receiving urban inputs in Southern Ontario (Lissemore et al. 2006)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>7) 60 - 120: range in concentrations detected in groundwater downgradient from a high school septic field (Godfrey et al. 2007)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>8) detected: domestic well (Seiler et al. 1999)</td>
</tr>
<tr>
<td>Carbamazepine</td>
<td>P2-M / 0.93</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>P7-S / 4.18</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Notes:**
- P1-D / ### = multilevel interval name / compound concentration
- trace = the compound was detected at levels below the method detection limit, but satisfied the requirements for retention time, and parent and daughter-product mass balance.
- ND = not detected
- Blank cells indicate the compound was not a target analyte

WWTP = wastewater treatment plant
STP = sewage treatment plant

1) Intervals sampled: P1-S, P1-M, P1-D, P2-S, P2-M, P2-D, P3-S, P3-M, P3-D
2) Intervals sampled: P1-S, P1-M, P1-D, P2-S, P2-M, P2-D, P3-M, P3-D, P4-S, P4-D, P5-S, P5-M, P5-D, P6-S, P7-S, P7-M, P7-D, P8-S
3) Intervals sampled: P1-S, P1-M, P1-D, P2-S, P2-M, P2-D, P3-M, P3-D, P4-S, P4-D, P5-S, P6-S, P6-M, P6-D, P7-S, P7-M, P7-D, P8-S
Figure 5-1: Location and topographic map of the Site. The locations of eight monitoring drilled specifically for this study and cross-section traces are shown.
Figure 5-2: Land use map for the Site and the surrounding environs.
Figure 5-3: Composite of geology, hydraulic testing results (horizontal black bars) and multi-level completion intervals (vertical white bars). All elevations are with respect to mean sea level.
Figure 5-4: Histogram of δ²H and δ¹⁸O measured in groundwater samples collected from eight monitoring wells at the Site. Each plot provides the range in results for a sampling interval (including analytical error), shown by the bar. The symbol indicates the mean of the results for each interval, the number of samples collected, and the rock type the sampling interval is completed in. The amount-weighted mean annual value of precipitation from the Ottawa observation station from Birks et al. (2003) is provided for reference.
Figure 5-5: Conceptual model of groundwater flow and contaminant transport at the Site. The cross-section is oriented parallel to the direction of regional groundwater flow. The thickness of the lines representing the fractures infers relative aperture and transmissivity. Conceptual contaminant transport pathways are shown with dots. Regional flow is shown by the blue block arrows. Not to scale. Vertical exaggeration is on the order of 5:1 to 10:1.
Chapter 6

General Discussion

The primary objective of this research was to investigate bacterial and other anthropogenic contamination in a village setting (Chapter 5). The results of bacterial concentrations in pumped groundwater samples raised questions about what the variability might be during pumping, thus prompting a focused study on this matter (Chapter 4). The development of a conceptual model for the interpretation of bacterial concentration trends required an understanding of flow through the screen and sand pack during pumping, which was analyzed using a numerical model (Chapter 2). The use of a fully-transient numerical model in Chapter 2 raised concerns about the discretization of the solution domain since an analytical or semi-analytical solution could not be used for verification. This led to a separate investigation on the discretization of a discrete fracture simulation of radial transport (Chapter 3). Thus, the pumping manuscript (Chapter 2) and the discretization manuscript (Chapter 3) are linked and are necessary precursors to the bacterial manuscript (Chapter 4) and the village-scale study (Chapter 5), which are also linked.

The topics investigated in the previous chapters show the complexities of modeling, sampling, and field-scale efforts in characterizing flow and contaminant transport in fractured bedrock aquifers. One of the major challenges in modeling solute transport in discrete fracture and pumping scenarios is the implementation and verification of appropriate spatial discretization around the well and fracture, and the timestep discretization in the solution. While a semi-analytical model was used for verification purposes in Chapter 3, a sensitivity analysis of the discretization parameters had to suffice for the fully transient case presented in Chapter 2.
Another numerical modeling limitation is the verification of solute transport scenarios where heterogeneity is incorporated. Heterogeneity may be in the form of multiple fractures or different rock matrices with different flow and transport properties, and time-dependent parameters. As a result, fully transient numerical simulations may be better suited for the purpose of examining relative differences between scenarios rather than obtaining absolute results.

The presence of the sand pack and screen and the flow of groundwater to wells through preferential pathways such as fractures make piezometers installations in fractured bedrock wells a complex system. Chapter 2 provides better insight into the nature of flow from the fracture to the pump. Areas of stagnation may be present in the borehole, and traditional rules-of-thumb on the volume of water to be purged prior to sample collection are unfounded. Bacterial sampling, as discussed in Chapter 4, is further complicated by the potential formation of biofilms in the borehole, sand pack, and fractures and the transport mechanisms that differ from those of solutes. Regardless of the target analyte, it is important to consider what the sample is intended to represent. Low-flow purging methods have become common place in groundwater sampling, but may not be suitable for ascertaining what may be pumped from nearby residential boreholes for human consumption. There can be significant differences between how monitoring wells and residential wells are constructed and used. For example, a residential well pump cycles on-and-off depending on demand and typically operates at much higher flow rates than those used in low-flow purging. Also, the sand pack adds a significant amount of surface area around the well screen compared to an open borehole. It remains unclear how suitable sampling from multi-level piezometers is when the objective is to use fecal indicator bacteria to determine the potability of groundwater in nearby residential wells since the results may be influenced by detachment from
biofilms located in the pore space of the sand pack. However, the presence of any fecal indicator bacteria in groundwater samples, no matter where the bacteria come from in the well-aquifer system, shows the aquifer is being polluted by fecal sources and fulfills the primary objective of determining if the groundwater is suitable for human consumption.

The village-scale field investigation presented in Chapter 5 provides an example of the complexities of fractured bedrock aquifer systems and the challenge of characterizing flow and contaminant transport in these settings. A variety of methods including the installation of a monitoring well network, hydraulic characterization, a multiparameter groundwater sampling program, and the development of a conceptual model were all necessary in order to understand the presence, distribution and origin of the contamination. The presence of PPCPs in the groundwater has implications for additional potential public health risks associated with the reliance on private servicing in this setting. It is of upmost importance that the sensitivity of fractured bedrock aquifers to anthropogenic contamination be considered in the development and implementation of land-use and zoning plans and in the siting of a new septic systems and water supply wells around existing development and on undeveloped land.
Chapter 7

Summary and Conclusions

The collective objective of this research was to further the understanding of modeling, sampling, and the potential for anthropogenic contamination in fractured bedrock aquifers. The need for such research stems in part from source water protection efforts for both municipal systems and private wells. The following provides a summary and the specific conclusions from the two modeling studies and the two field investigations presented in Chapters 2 to 5. Lastly, recommendations for future investigations are presented.

7.1 The Influence of Sand Packs and Screens on Obtaining Representative Geochemical Groundwater Samples from Multi-level Monitoring Wells in Bedrock Aquifers – A Numerical Approach

A groundwater flow and solute transport numerical model was employed to examine the influence of the screen and sand pack on the collection of a representative geochemical sample from a discretely fractured bedrock aquifer. The optimization of screen and sand pack combinations was explored for the potential of reducing purging times and volumes in practice. Simulations accounted for the location of the fractures along the well screen, fracture aperture, screen length, and the pumping rate. The variability in the simulated required purging times (t_{99} - the time required to achieve a 99% fractional contribution from the formation to pump discharge) can be explained by: 1) the hydraulic conductivities of the components of the system (fracture, sand pack, and screen), 2) the truncation of the flow field from the fracture to the screen by the upper or lower boundary of the sand pack or the flow field from another fracture, and 3) time-dependent drawdown. Specific conclusions are as follows:
1. The ratios of hydraulic conductivities between the screen, sand pack, and fracture control the amount of spreading and groundwater velocities in the sand pack. Only a small portion of the sand pack may actually become hydraulically active during pumping.

2. The required purging time (and volume) can be significantly reduced by choosing screen and sand pack materials that have similar hydraulic conductivities. The optimal configuration (shortest purging time) is achieved when ratio of the screen, sand pack, and fracture hydraulic conductivities are close to 1:1:1.

3. A shorter screen does not necessarily reduce purging times unless the flow field from the fracture is truncated by the upper and lower boundaries of the sand pack.

4. The location of fractures with respect to other fractures or the upper and lower boundaries of the sand pack can also act to reduce purging times due to flow field truncation.

5. The results in this study are best used for understanding the relative relationships in $t_{09}$ rather than absolute values for a given scenario. This is because of the conservative assumptions made in the initial transport conditions and the possible issues associated with using fully-transient conditions in the numerical model.

7.2 Discretizing a Discrete Fracture Model for Simulation of Radial Transport

Consideration for radial solute transport is important when a pump (injection or withdrawal) is employed, such as the case of wastewater injection, domestic water well extraction near a source of contamination, and tracer experiments. The objective was to develop a method for discretizing a discrete fracture radial transport model with the direct application to analyzing tracer tests. Point-to-point and borehole-to-point numerical simulations were verified by the Novakowski (1992a) semi-analytical solution. Particular consideration was given to how far into the matrix away from the fracture needs to be highly-discretized to maintain good agreement with the semi-
analytical solution and reduce the number of required elements. In addition, a new borehole mixing model, based on Palmer (1988), is developed for the case of multiple intersecting fractures. This new mixing model is used as a post-processor to convert numerical model time-concentration point data from a multiple fracture simulation into an equivalent concentration breakthrough curve in a passive observation borehole. The results, interpretations, and conclusions from this study lead to the following conclusions on the suitability of using a numerical model to simulate a field-scale divergent steady radial flow tracer experiment:

1. Spatial discretization around the injection well and fracture, and the timestep discretization in the transport solution are crucial in matching the numerical model to a semi-analytical solution. Large discrepancies arise when spatiotemporal discretization is insufficient, resulting in the potential misinterpretation of the transport process. The necessary increased spatiotemporal discretization can be prohibitive due to long computation runtimes and array size requirements, particularly when using a 3-D modeling domain.

2. Numerical models alone are best suited to simulate point-to-point and borehole-to-point radial transport in a single fracture using a 2-D, unit-thickness domain with an axisymmetric coordinate system. There is no advantage to using a numerical model over a semi-analytical model for these cases since the solutions are nearly identical. The semi-analytical solution also has shorter runtimes and does not require consideration for appropriate spatiotemporal discretization. Both models limit the ability to incorporate heterogeneity and to represent real field settings.

3. Numerical models are a valuable tool for generating time-concentration data at a particular distance away from the injection borehole in single- and multiple-fracture
cases. The conversion of this point data into passive observation borehole data using and the new mixing model developed in this study, based on Palmer (1988), is particularly useful for the sensitivity analysis on how multiple fractures with heterogeneous transport properties might influence concentration breakthrough curves in observation wells.

7.3 Bacterial Count Variability in Samples Pumped from Bedrock Monitoring Wells with Sand Pack Multi-level Completions

Current groundwater sampling protocols are typically designed for solutes, but are also used for bacterial sampling. Bacteria are commonly used as indicators of surface water and fecal contamination in groundwater. It is unclear how low-flow purging methods might work in obtaining a representative sample of bacteria in the aquifer given the uncertainty in the distribution of bacteria in the sand pack and well-aquifer system. A field investigation was conducted to examine the variability for fecal indicator bacteria (E. coli, total coliform, fecal coliform, fecal streptococci) and heterotrophic plate counts in groundwater samples in a variety of pumping regimes. Two bedrock monitoring wells located in a semi-urban setting were constructed as multi-level piezometers and bacterial enumeration was conducted using standard membrane filtration methods. One- to two-log decreases in bacterial counts were noted during pumping. Bacteria in the samples were interpreted as being a combination of planktonic and attached sources in the borehole and adjacent fractures. The results from this study lead to the following conclusions about bacterial counts in pumped groundwater samples and the subsequent water quality interpretation using fecal indicator bacteria:

1. The pumping rate did not correlate well with the magnitude of observed bacterial concentrations in the samples.
2. Bacterial concentrations in groundwater samples remain variable during the course of pumping. The highest concentrations of bacteria occur at the onset of pumping prior to the complete purge of the wellbore as defined in conventional sampling protocols.

3. Samples are dominated by planktonic and detached cells sourced in the screen storage, sand pack, and adjacent fractures.

4. Multiple samples and other enumeration techniques would provide better, more accurate and more useful data for assessing the source of bacteria in the subsurface and the potential exposure to pathogens using fecal indicator bacteria.

7.4 The Potential for Anthropogenic Contamination of Groundwater in a Bedrock Aquifer having Variable Overburden Cover in a Semi-urban Setting

A field investigation was conducted to examine how anthropogenic contaminant sources in a semi-rural setting, where both septic systems and agriculture are present, might be impacting groundwater quality in an underlying bedrock aquifer having variable overburden cover. Eight monitoring wells were instrumented as multi-level piezometers in an unserviced lakeside village. A multiparameter sampling program involving nutrients, chloride, fecal indicator bacteria, stable isotopes, and 40 pharmaceutical and personal care products (PPCPs) was used to track anthropogenic effects. To our knowledge, this is the first study to report PPCPs in a bedrock aquifer. A conceptual model was developed to better understand the observed contaminant concentrations. The results indicate that the transport pathways in the bedrock system are complex and septic systems, agriculture, and road salting are sources of contamination. Specific conclusions are as follows:
1. Contaminants released at surface in areas with thin or inadequate overburden can migrate quickly and deeply via a complex bedrock fracture network into the aquifer that is relied on as a potable drinking water resource.

2. Recharge plays a crucial role in moving surface contaminants into the deeper subsurface. It also acts to dilute contaminants and create additional heterogeneity in the transport through the fractured bedrock system.

3. PPCP analysis provides detail on the types of sources (both septic systems and agriculture) and confirms there are multiple contributors present (based on the distribution and variety of compounds detected). This interpretation could not otherwise be definitely established using traditional methods including nutrient concentrations and fecal indicator bacteria counts.

4. PPCP concentrations in samples from the bedrock aquifer are similar to those measured in previous groundwater and surface water studies conducted in Ontario and other parts of North America.

5. Although limited in use for source determination, fecal indicator bacteria provide a consistent and cost-effective method for determining the potential for adverse public health impacts due to groundwater consumption in this setting because drinking water standards have been established.

7.5 Recommendations

The results from Chapter 2 show that the optimal configuration (shortest purging time) is achieved when the ratio of the screen, sand pack, and fracture hydraulic conductivities are close to 1:1:1. Physical laboratory scale models would be particularly useful in validating these results. Similar tests of different screen and sand pack combinations may be difficult to conduct in the
field setting because of the required initial and specified concentration conditions assumed in the model. However, field tests might be useful for examining potential issues with turbidity and sedimentation in multi-level wells constructed in different rock types with varying degrees of weathering. Future modeling efforts simulating a fully-transient flow and solute transport scenario should consider ways to confirm the spatiotemporal discretization is correct since an analytical or semi-analytical solution cannot be used for verification.

As shown in Chapter 3, the transport solution from a discrete fracture numerical model can be greatly influenced by the spatiotemporal discretization employed. Verification using an analytical or semi-analytical model is crucial. Future efforts should consider a similar verification approach and the application of the numerical models in a variety of other tracer experiment configurations where an analytical or semi-analytical solution has been developed and validated. The implementation of radial transport simulations in a 3-D domain may be limited by the array sizes being larger than those allocated by the numerical model because of required spatiotemporal discretization. Allocated array sizes are likely to increase, and runtimes will decrease as computer programming languages and hardware continue to develop (use of parallel codes to perform many calculations simultaneously using multi-core processors, etc.).

Based on the results from Chapter 4, it is evident that bacterial concentrations remain variable during pumping. Membrane filtration is not the best suited method for determining bacterial sources in the subsurface (planktonic or attached) in part because it does not account for dead bacteria or distinguish between single cells or multi-cell clumps. Thus, future studies focused on determining the source of fecal indicator bacteria from the subsurface in groundwater samples
should consider a microscopy technique as an alternative enumeration method. Future research
should continue to investigate the variability of bacterial counts on pumped groundwater samples.
Groundwater sampling protocols need to recognize and address the differences in the transport
mechanisms between bacteria and solutes and users need to recognize that low-flow purging and
other common sampling methods may not be suitable for what the samples are intended to be
representative of. A multi-sample approach, which is proposed in this study, may be more
suitable when sampling for fecal indicator bacteria for the purpose of assessing drinking water
quality, with an emphasis on sampling throughout the purging process.

From the research presented in Chapter 5, it is evident that fractured bedrock aquifers with
variable overburden cover are easily impacted by surface anthropogenic contaminant sources.
Fecal contaminants in particular have the potential to adversely impact human health if the
groundwater is used as a drinking water supply. PPCPs are a very useful anthropogenic tracer
because the source is not ambiguous as can be the case for nutrients and fecal indicator bacteria
membrane filtration counts. Future research should continue to examine the presence,
spatiotemporal variability, and transport mechanisms of PPCPs in a variety of aqueous matrices,
including groundwater in fractured bedrock aquifers. Additionally, concurrent advances in other
fields such as pharmacology, toxicology, and epidemiology are needed to understand the effects
of long-term, low-dose human exposure to these compounds on human populations and
potentially develop drinking water standards accordingly. Land use planning and source water
protection plans need to recognize the sensitivity of fractured bedrock aquifers to contamination.
Distal sources may be influencing local water quality because of the potential for high
groundwater velocities, the nature of the fracture networks, and the variability in overburden cover beyond the lot- or village-scale.
Appendix A

HydroGeoSphere Mathematical Formulation and Example Input Files

(Chapter 2 supplement)
**Mathematical Development**

The subsurface flow and transport model *HydroGeoSphere* (HGS) (Therrien et al. 2006), was used to simulate flow and transport to a well. The following provides a brief description of the principal governing equations for transport in the fractures and porous matrix. The notation used in this Appendix follows that of the HGS documentation (Therrien et al. 2006).

For the conditions of steady, saturated flow, with a conservative, non-decaying tracer, three-dimensional solute transport in the porous matrix is represented in HGS by the advection dispersion equation as follows:

\[-\nabla \cdot (\mathbf{q} \mathbf{C} \mathbf{D} \mathbf{C}) \pm Q_t = \frac{\partial (RC)}{\partial t}\]

(1)

where \(\nabla\) is the gradient operator in three dimensions, \(\mathbf{C}\) is the solute concentration, and \(Q_t\) is the solute source or sink term for the boundary conditions. The fluid flux, \(\mathbf{q}\), is given by:

\[\mathbf{q} = -\mathbf{K} \cdot \nabla (\psi + z)\]

(2)

where \(\psi\) and \(z\) are the pressure and elevation heads, respectively. From Equation (2), the hydraulic conductivity tensor, \(\mathbf{K}\), is given by:

\[\mathbf{K} = \frac{\rho g}{\mu} \mathbf{k}\]

(3)

where \(\rho\) is the density of water, \(g\) is the gravitational acceleration constant, \(\mu\) is the viscosity of water, and \(\mathbf{k}\) is the permeability tensor of the porous medium, which is assumed to be isotropic for the simulations in this study.

From Equation (1), the hydrodynamic dispersion tensor, \(\mathbf{D}\), is given by Bear (1972):

\[\mathbf{D} = (\alpha_L - \alpha_T) \frac{\mathbf{qq}}{|\mathbf{q}|} + \alpha_T |\mathbf{q}| \mathbf{I} + \tau D^* \mathbf{I}\]

(4)

where \(\alpha_L\) and \(\alpha_T\) are the longitudinal and transverse dispersivities, respectively, \(|\mathbf{q}|\) is the magnitude of the Darcy flux, \(\tau\) is the matrix tortuosity, \(D^*\) is the free-solution diffusion coefficient of the solute, and \(\mathbf{I}\) is the identity tensor.

The retardation factor, \(R\), given in Equation (1) is given by:

\[R = 1 + \frac{\rho_b}{\theta_m} K_d\]

(5)
where $\rho_b$ and $\theta_m$ are the bulk density and the porosity of the matrix, respectively, and $K_d$ is the distribution coefficient, taken from experimentally determined adsorption isotherms.

In HGS, transport in discrete fractures is coupled with that of the porous matrix via the common node method, whereby concentrations in the fracture and matrix are the same at the interface, therefore requiring no explicit solute exchange term. From Tang et al. (1981), Sudicky and McLaren (1992), and Therrien and Sudicky (1996), two-dimensional solute transport is given as:

$$-\nabla^* \cdot (q_f C_f - D_f \nabla C_f) = \frac{\partial (R_f C_f)}{\partial t}$$  \hspace{1cm} (6)$$

where $\nabla^*$ is the gradient operator in two dimensions (fractures represented as 2-D planar elements in HGS), $C_f$ is the concentration in the fracture, and $D_f$ is the hydrodynamic dispersion tensor for the fracture, similar to Equation (4). The fluid flux in the fracture, $q_f$, is given by:

$$q_f = -K_f \cdot \nabla^* (\psi_f + z_f)$$ \hspace{1cm} (7)$$

where $\psi_f$ and $z_f$ are the hydraulic and elevation heads in the fracture, respectively, and the hydraulic conductivity of an idealized fracture with no aperture variability is given by:

$$K_f = \frac{\rho g}{12 \mu} (2b)^2$$ \hspace{1cm} (8)$$

where $2b$ is the fracture aperture. From Equation (6) above, the retardation factor for the fracture is:

$$R_f = 1 + \frac{2K'_d}{(2b)}$$ \hspace{1cm} (9)$$

where $K'_d$ is the distribution coefficient for the fracture surface.

Wells are implemented in HGS as a 1-D string of nodes within a 3-D gridded domain. The equation describing 1-D flow along the axis of a borehole having a finite diameter and storage capacity and penetrating a variably-saturated aquifer is (Therrien and Sudicky 2000):

$$-\nabla \cdot (\pi r_w^2 q_w) + Q_w \delta(l - l') - P_w \Gamma_w = \pi \frac{\partial}{\partial t} \left[ \left( \frac{r_w^2}{L_s} + r_s^2 S_{ww} \right) \psi_w \right]$$ \hspace{1cm} (10)$$

where the fluid flux $q_w$ [L T$^{-1}$] is given by:

$$q_w = -K_w k_{rw} \nabla (\psi_w + z_w)$$ \hspace{1cm} (11)$$
and where $\nabla$ is the one-dimensional gradient operator along the length direction, $l$, of the well, $r_s$ and $r_w$ are the radius of the well screen and well casing, respectively, $L_s$ is the total length of the screen, $P_w$ is the wetted perimeter of the well, $k_{rw}$ is the relative permeability of the well, and $S_{ww}$ is its saturation. The pressure and elevation heads in the well screen are given by $\psi_w$ and $z_w$, respectively, the discharge or recharge rate per unit length $Q_w$ is applied at location $l'$ in the well screen and $\delta(l - l')$ is the Dirac delta function. $\Gamma_w$ is the fluid exchange rate between the subsurface domain and the well.

The hydraulic conductivity of the well $K_w$ is obtained from the Hagen-Poiseuille formula for flow through a long cylindrical pipe (Sudicky et al. 1995):

$$K_w = \frac{r_s^2 \rho g}{8 \mu}$$

The term on the right side of Equation (10) represents the storage coefficient of the well bore, which is composed of a term accounting for the storage from the compressibility of the fluid and a term describing the transient volume of the well due to the changing water level in the casing during pumping/injection. HydroGeoSphere redistributes the storage contribution caused by the change in water level in the casing to all nodes along the well screen, based on Sudicky et al. (1995). The mass balance in the borehole is completed on the left side of Equation (10) with source/sink terms accounting for injection/withdrawal and exchange with the aquifer.

The relative permeability and saturation functions are used in the case where water level drops below the top of the casing. The simulations used in this Chapter only consider cases where the water level remains above the top of the casing. The reader is directed to Therrien et al. (2006) for more information for how HydroGeoSphere simulates the portion of the well above the water level.

One-dimensional transport along the axis of the well is described by:

$$-\nabla \cdot \pi r_s^2 (q_w C_w - S_{ww} D_w \nabla C_w) + \pi r_s^2 [\lambda_w C_w]_{par} - Q_w (C_w - C_{inj}) \delta(l - l')$$

$$-\pi r_s^2 \Omega_w = \pi r_s^2 \frac{\partial C_w}{\partial t}$$

$$\text{(13)}$$

where $C_w$ and $C_{inj}$ are the solute concentration in the well and injection water, respectively, $\lambda_w$ is the first order decay constant of the solute in the well, and $\Omega_w$ is the solute exchange rate of the well with the subsurface domain. The dispersion coefficient for the well, $D_w$ is defined as (Lacombe et al. 1995):

$$D_w = \frac{r_s^2 a_w^2}{48D^*} + D^*$$

$$\text{(14)}$$

This appendix is not intended to be a comprehensive review of the theory which supports the formulation of HGS, but is presented to provide the relevant governing transport equations under the conditions used for this study. For more detailed information see Therrien et al. (2006).
GROK Input File:

Radial flow and transport in a axisymmetric domain
Single fracture
TRANSPORT SOLUTION - STEADY STATE

end title

!---------------------------grid
generate blocks interactive

grade x
0, 0.0254, 0.0005, 1.05, 0.05

grade x
0.0508, 0.0254, 0.0005, 1.05, 0.05

grade x
0.0508, 250, 0.0005, 1.05, 250

grade x
0.001, 0.001, 1, 1, 1

grade y
0, 1, 1, 1, 1

grade z
2.5, 0, 0.0002, 2, 0.1

grade z
2.5, 6, 0.0002, 2, 0.1

end generate blocks interactive

end

!---------------------------simulation

units: kilogram-metre-second

transient flow
do transport
axisymmetric coordinates

!---------------------------porous media

use domain type porous media

properties file sp.mprops

!screen
clear chosen elements
choose elements block
0, 0.001
0, 1
0, 6

new zone
1

clear chosen zones
choose zone number
1
read properties
screen3
! sand pack
clear chosen elements
choose elements block
0.001, 0.0508
0, 1
0, 6

new zone
2
clear chosen zones
choose zone number
2
read properties
sandFa

! matrix
clear chosen elements
choose elements block
0.0508, 250
0, 1
0, 6

new zone
3
clear chosen zones
choose zone number
3
read properties
matrix

!---------------------------flow
clear chosen nodes
choose nodes all
initial head
0

clear chosen nodes
choose nodes x plane
250
1E-10
specified head
1
0, 0, 0

flow solver convergence criteria
1E-10

flow solver maximum iterations
1000000

!---------------------------well
make well
pump1
0, 0, 0
0, 0, 6
1
0, -1.667E-5 !1L/min /1000/60 = 1.667E-5 m/s
0, 0, 3
0.0254
0.0254

make well
pump2
0, 1, 0
0, 1, 6
1
0, -1.667E-5 !1L/min /1000/60 = 1.667E-5 m/s
0, 1, 3
0.0254
0.0254

!-----------------------------------transport species
solute
t free-solution diffusion coefficient
1E-10
end solute

transport solver convergence criteria
1E-15

transport time weighting
1

upstream weighting of velocities
1, 1, 1

!-----------------------------------transport b.c.
!pumping node
clear chosen nodes
choose nodes block
0, 0, 0.0508
0, 1
0, 6
initial concentration
0.0

clear chosen nodes
choose nodes block
0.0508, 250
0, 1
0, 6
specified concentration
1.0, 1E10, 1.0

!---------------------------fracture
use domain type
fracture
properties file
sp.fprops

clear chosen faces
choose faces block
0.0508, 250
0, 1
2.5, 2.5

new zone
1

clear chosen zones
choose zone number
1
read properties
750

!---------------------------output times
maximum timestep
60

output times
1
10
100
1000
3593.5267
end

!---------------------------controls
concentration control
0.05

!---------------------------output
make observation point
obs x = 0
0, 0, 3

make observation point
obs x = 1
1, 0, 3

make observation point
obs x = 5
5, 0, 3

make observation point
obs x = 10
10, 0, 3

make observation point
obs x = 25
25, 0, 3

make observation point
obs x = 50
50, 0, 3

make observation point
obs x = 75
75, 0, 3

make observation point
obs x = 100
100, 0, 3

make observation point
obs x = 250
250, 0, 3

clear chosen nodes
choose node
0, 0, 3
flux output nodes from chosen
detection threshold concentration
0.997
stop run if flux output nodes exceed detection threshold concentration
MPROPS Input File:

<table>
<thead>
<tr>
<th>Screen</th>
<th>Anisotropic</th>
<th>Porosity</th>
<th>Specific Storage</th>
<th>Longitudinal Dispersivity</th>
<th>Transverse Dispersivity</th>
<th>Vertical Transverse Dispersivity</th>
<th>End Material</th>
</tr>
</thead>
<tbody>
<tr>
<td>Screen1</td>
<td>0.961E-3, 0.961E-3, 1E-10</td>
<td>0.018</td>
<td>1.6667E-6</td>
<td>0.0005</td>
<td>0.0001</td>
<td>0.0001</td>
<td></td>
</tr>
<tr>
<td>Screen2</td>
<td>2.10E-3, 2.10E-3, 1E-10</td>
<td>0.023</td>
<td>3.333E-6</td>
<td>0.0005</td>
<td>0.0001</td>
<td>0.0001</td>
<td></td>
</tr>
<tr>
<td>Screen3</td>
<td>7.54E-3, 7.54E-3, 1E-10</td>
<td>0.033</td>
<td>3.333E-6</td>
<td>0.0005</td>
<td>0.0001</td>
<td>0.0001</td>
<td></td>
</tr>
</tbody>
</table>
screen4
k anisotropic 20.4E-3, 20.4E-3, 1E-10
porosity 0.047
specific storage 3.333E-6 !1E-5/3
longitudinal dispersivity 0.0005
transverse dispersivity 0.0001
vertical transverse dispersivity 0.0001
end material
screen5
k anisotropic 58.1E-3, 58.1E-3, 1E-10
porosity 0.064
specific storage 3.333E-6 !1E-5/3
longitudinal dispersivity 0.0005
transverse dispersivity 0.0001
vertical transverse dispersivity 0.0001
end material
screen6
k anisotropic 118E-3, 118E-3, 1E-10
porosity 0.077
specific storage 3.333E-6 !1E-5/3
longitudinal dispersivity 0.0005
transverse dispersivity 0.0001
vertical transverse dispersivity 0.0001
end material
screen7

k anisotropic
2.28e-3, 2.28e-3, 1e-10

porosity
0.092

specific storage
3.333e-6 !1e-5/3

longitudinal dispersivity
0.0005

transverse dispersivity
0.0001

vertical transverse dispersivity
0.0001

end material

!SAND PACK

sandAa

k isotropic
0.90e-3

porosity
0.2

specific storage
3.333e-6 !1e-5/3

longitudinal dispersivity
0.0005

transverse dispersivity
0.0001

vertical transverse dispersivity
0.0001

end material

sandAb

k isotropic
0.90e-3

porosity
0.35

specific storage
3.333e-6 !1e-5/3

longitudinal dispersivity
0.0005

transverse dispersivity
0.0001

vertical transverse dispersivity
0.0001

end material
sandBa
  k isotropic  2.61E-3
  porosity  0.2
  specific storage  3.333E-6  !1E-5/3
  longitudinal dispersivity  0.0005
  transverse dispersivity  0.0001
  vertical transverse dispersivity  0.0001
  end material

sandBb
  k isotropic  2.61E-3
  porosity  0.35
  specific storage  3.333E-6  !1E-5/3
  longitudinal dispersivity  0.0005
  transverse dispersivity  0.0001
  vertical transverse dispersivity  0.0001
  end material

sandCa
  k isotropic  5.19E-3
  porosity  0.2
  specific storage  3.333E-6  !1E-5/3
  longitudinal dispersivity  0.0005
  transverse dispersivity  0.0001
  vertical transverse dispersivity  0.0001
  end material
sandCb
k isotropic
5.19E-3
porosity
0.35
specific storage
3.333E-6 !1E-5/3
longitudinal dispersivity
0.0005
transverse dispersivity
0.0001
vertical transverse dispersivity
0.0001
end material

sandDa
k isotropic
10.445E-3
porosity
0.2
specific storage
3.333E-6 !1E-5/3
longitudinal dispersivity
0.0005
transverse dispersivity
0.0001
vertical transverse dispersivity
0.0001
end material

sandDb
k isotropic
10.445E-3
porosity
0.35
specific storage
3.333E-6 !1E-5/3
longitudinal dispersivity
0.0005
transverse dispersivity
0.0001
vertical transverse dispersivity
0.0001
end material
sandEa
  k isotropic
  18.8E-3
  porosity
  0.2
  specific storage
  1.6667E-6 ! 1E-5/6
  longitudinal dispersivity
  0.0005
  transverse dispersivity
  0.0001
  vertical transverse dispersivity
  0.0001
  end material

sandEb
  k isotropic
  18.8E-3
  porosity
  0.35
  specific storage
  3.333E-6 ! 1E-5/3
  longitudinal dispersivity
  0.0005
  transverse dispersivity
  0.0001
  vertical transverse dispersivity
  0.0001
  end material

sandFa
  k isotropic
  41.3E-3
  porosity
  0.2
  specific storage
  1.6667E-6 ! 1E-5/6
  longitudinal dispersivity
  0.0005
  transverse dispersivity
  0.0001
  vertical transverse dispersivity
  0.0001
  end material
sandFb
k isotropic
41.3e-3
porosity
0.35
specific storage
3.333E-6 !1E-5/3
longitudinal dispersivity
0.0005
transverse dispersivity
0.0001
vertical transverse dispersivity
0.0001
end material

sandGa
k isotropic
75.15E-3
porosity
0.2
specific storage
1.6667E-6 !1E-5/6
longitudinal dispersivity
0.0005
transverse dispersivity
0.0001
vertical transverse dispersivity
0.0001
end material

sandGb
k isotropic
75.15E-3
porosity
0.35
specific storage
3.333E-6 !1E-5/3
longitudinal dispersivity
0.0005
transverse dispersivity
0.0001
vertical transverse dispersivity
0.0001
end material

! MATRIX
!*****************************************************************************
MATRIX
k isotropic
1E-10
porosity
0.001
specific storage
3.333E-6 !1E-5/3
longitudinal dispersivity
0.0005
transverse dispersivity
0.0001
vertical transverse dispersivity
0.0001
end material
FP props input File:

!------------------------------------------
750
aperture
750.E-6
specific storage
1.333E-2  !S=1E-5, b=0.00075, Ss=1.333E-2
longitudinal dispersivity
0.05
transverse dispersivity
0.0
end material
Array Sizes Input File (modified from auto-generated file):

channel flow: 1d elements 50000
channel flow: material zones 20
channel flow bc: zero-depth gradient segments 5000
dual flow bc: flux faces 10000
dual flow bc: flux function panels 10
dual flow bc: flux nodes 10000
dual flow bc: flux zones 10
dual flow bc: head function panels 100
dual flow bc: head nodes 10000
dual: material zones 20
flow: material zones 20
flow bc: drain-type flux nodes 2
flow bc: evaporation faces 10000
flow bc: evaporation nodes 10000
flow bc: evaporation zones 10
flow bc: evaporation function panels 10
flow bc: flux nodes 10000
flow bc: flux faces 10000
flow bc: flux zones 10
flow bc: flux function panels 10
flow bc: free drainage nodes 1000
flow bc: head nodes 10000
flow bc: head function panels 100
flow bc: river-type flux nodes 2
flow bc: specified nodal flowrate 501
flow bc: specified nodal flowrate function panels 100
flow bc: hydrostatic node columns 100
heat transfer permafrost: thawing table 50
heat transfer permafrost: freezing table 50
heat transfer permafrost: thawing-freezing table 50
heat transfer permafrost: temperature function panels 300
fractures: 2d elements 100000
fractures: zones 300
general: list 300
mesh: node connections 100

185
mesh: node sheets in z for layered grids 50
mesh: x grid lines (rectangular) 10000
mesh: y grid lines (rectangular) 1000
mesh: z grid lines (rectangular) 6000
mesh: number of layers 100
mesh: number of sublayers per layer 100
observation wells: nodes 501
output: flux volume nodes 1000
output: flux volumes 10
output: nodes 100
output: times 1000
permafrost: elements 10000
permafrost: function panels 100
seepage face: 3d elements intersecting 1000
seepage face: nodes 1000
solution: target times 3000
surface flow: 2d elements 50000
surface flow: boundary segments 5000
surface flow: hydrographs 20
surface flow: hydrograph nodes 100
surface flow: material zones 20
surface flow bc: critical depth segments 5000
surface flow bc: zero-depth gradient segments 5000
tile drains: 1d elements 10000
tile drains: 3d elements intersecting 10000
tile drains: concentration function panels 100
tile drains: nodes 1000
transport: species 5
transport: species kinetic reactions 2
transport bc: concentration nodes 10000
transport bc: concentration function panels 100
transport bc: flux nodes 10000
transport bc: flux function panels 100
transport bc: immiscible phase dissolution nodes 1000
transport bc: third-type concentration faces 10000
transport bc: third-type concentration function panels 100
transport bc: zero-order source function panels
transport bc: first-order source function panels
wells: 1d elements
wells: 2d fracture elements intersecting
wells: 3d elements intersecting
wells: flux function panels
tiles: flux function panels
wells: injection concentration function panels
wells: nodes
stress: stressed nodes
stress: stress function panels
end
Appendix B
Concentration and Velocity Vector Profiles in the Screen and Sand Pack (Chapter 2 Supplement)
Figure B1: Screen and sand pack combinations (supplemental to Figure 2-4) – 3 m screen, 750 micron fracture at t₀₉. Arrows are scaled velocity vectors.

<table>
<thead>
<tr>
<th>Screen Slot (mm)</th>
<th>0.254</th>
<th>0.330</th>
<th>0.508</th>
<th>0.711</th>
<th>1.016</th>
<th>1.295</th>
<th>1.626</th>
</tr>
</thead>
</table>

D

E

G

Sand Pack Grade

LEGEND

○ pump intake

fracture

Horizontal exaggeration ~ 118
Figure B2: Screen and sand pack combinations (supplemental to Figure 2-4) – 3 m screen, 500 micron fracture at t_{99}. Arrows are scaled velocity vectors.

<table>
<thead>
<tr>
<th>Screen Slot (mm)</th>
<th>0.254</th>
<th>0.330</th>
<th>0.508</th>
<th>0.711</th>
<th>1.016</th>
<th>1.295</th>
<th>1.626</th>
</tr>
</thead>
</table>

Horizontal exaggeration ~ 118
Figure B3: Screen and sand pack combinations (supplemental to Figure 2-4) – 6 m screen, 750 micron fracture at \( t_99 \). Arrows are scaled velocity vectors.

<table>
<thead>
<tr>
<th>Screen Slot (mm)</th>
<th>0.254</th>
<th>0.330</th>
<th>0.508</th>
<th>0.711</th>
<th>1.016</th>
<th>1.295</th>
<th>1.626</th>
</tr>
</thead>
</table>

```
D
```

```
E
```

```
F
```

```
G
```

Horizontal exaggeration ~ 118

Legend:
- ○ pump intake
- purple fracture
Figure B4: Screen and sand pack combinations (supplemental to Figure 2-4) – 6 m screen, 500 micron fracture at t_{99}. Arrows are scaled velocity vectors.

<table>
<thead>
<tr>
<th>Screen Slot (mm)</th>
<th>0.254</th>
<th>0.330</th>
<th>0.508</th>
<th>0.711</th>
<th>1.016</th>
<th>1.295</th>
<th>1.626</th>
</tr>
</thead>
</table>

Horizontal exaggeration ~ 118
Figure B5: Pumping rate (supplemental to Figure 2-6) – 6 m screen (0.508 mm slots), sand pack is grade F (n = 0.2), 750 micron fracture and pump are located at z = 3 m, concentration profile at t_99. Arrows are scaled velocity vectors.

<table>
<thead>
<tr>
<th>Q (L/min)</th>
<th>t_99 (min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>690</td>
</tr>
<tr>
<td>0.5</td>
<td>143</td>
</tr>
<tr>
<td>1.0</td>
<td>62</td>
</tr>
<tr>
<td>5.0</td>
<td>12</td>
</tr>
</tbody>
</table>
Figure B6: Single fracture location (supplemental to Figure 2-7A) – 6 m screen (0.508 mm slots), sand pack is grade F (n = 0.2), 750 micron fracture, pumping rate = 1 L/min, concentration profile at t_{99}. Arrows are scaled velocity vectors.

Horizontal exaggeration ~ 118
Figure B7: Fracture aperture (supplemental to Figure 2-7B) – 6 m screen (0.508 mm slots), sand pack is grade F (n = 0.2), 750 micron fracture, pumping rate = 1 L/min, concentration profile at t_{99}. Arrows are scaled velocity vectors.

Horizontal exaggeration ~ 118
Figure B8: Fracture aperture (supplemental to Figure 2-7B) – transient progression of concentration and velocity vector profiles in the screen and sand pack for different intersecting fracture apertures. Arrows are scaled velocity vectors.
Figure B9: Multiple equivalent-aperture fractures (supplemental to Figure 2-8) – total fracture transmissivity equals that of a 750 micron fracture, 6 m screen (0.508 mm slots), sand pack is grade F (n = 0.2), concentration profile at $t_{99}$. Arrows are scaled velocity vectors.

$1$ fracture $t_{99} = 62$ min

$2$ fractures $t_{99} = 119$ min

$3$ fractures $t_{99} = 138$ min

$4$ fractures $t_{99} = 113$ min

$5$ fractures $t_{99} = 104$ min

Horizontal exaggeration ~ 118
Appendix C

FORTRAN Code and Example Input and Output Files for Novakowski (1992) Semi-Analytical Solution (Chapter 3 Supplement)
FORTRAN Code:

Program RTRANS

This program solves for mass transport under divergent radial flow conditions for discontinuous inlet and outlet boundary conditions. The solution is for resident concentrations. This code is designed for the case of transport in a single fracture. Retardation is accounted for.

The variables used in the solution are dimensionless in all cases. The solution is coded using the Laplace domain and numerically inverted using the DeHoog or Talbot algorithms. For a complete derivation of the solutions, refer to the paper entitled "The Analysis of Tracer Experiments Conducted in Divergent Radial Flow Fields" authored by Kent Novakowski and published in WRR 28(12), 1992.

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Department of Civil Engineering
Queen's University
Kingston, ON
K7L 3N6

Version 1.0, November, 2009
Based on RAD2 by Kent Novakowski (1996)

The variables are:

- A = radial flow coefficient, \(=\frac{Q}{2\pi TWOB}\) or \(=\frac{DELH*TR}{LN(RI/RWO)}*TVOB\)
- CD = dimensionless concentration \(C_0/C\) at a point in the aquifer or in an observation well, \([\text{DIM}]\)
- DD = effective diffusion coefficient, \(=DS*TAO\) \([L^2/T]\)
- DM = matrix diffusion coefficient, \(=DD*THETAM\) \([L^2/T]\)
- DS = free-water diffusion coefficient, \([L^2/T]\)
- P = Laplace variable
- Q = volumetric flow rate, \([L^3/T]\)
- R = radial distance, \([L]\)
- RD = dimensionless radius, \(=RW/ALPHAR\) \([\text{DIM}]\)
- RDE = dimensionless radius of injection well, \(=RW/ALPHAR\)
- RI = dimensionless radial distance, \(=RI/ALPHAR\) \([\text{DIM}]\)
- TR = radial transmissivity of aquifer, \([L^2/T]\)
- VE = volume of isolated zone in the observation well, \(=\pi RW^2*XLE\) \([L^3]\)
- VI = volume of isolated zone in the injection well, \(=\pi RW^2*XLI\) \([L^3]\)
- XLE = length of the isolated interval in the injection well, \([L]\)
- XLI = length of the isolated interval in the observation well, \([L]\)
\[ Y = \frac{RDE+1}{4\Phi} \]
\[ YE = \frac{RDE+1}{4\Phi} \]
\[ YR = \frac{RDI+1}{4\Phi} \]

**ALPHAR** = di spersivity, [L]

**BETADI** = dimensionless mixing coefficient for the injection well, \( \frac{(VI*RW)}{(ALPHAR^2*GAMI)} \), [DIM]

**BETADE** = dimensionless mixing coefficient for the observation well, \( \frac{(VE*RI)}{(ALPHAR^2*GAME)} \), [DIM]

**GAME** = cross-sectional area available for flow at the observation well, \( \sqrt{PI*RW*TWOB} \), [L^2]

**GAMI** = cross-sectional area available for flow at the injection well, \( 2\sqrt{PI*RW*TWOB} \), [L^2]

**DELH** = difference in hydraulic head between injection and observation wells/points, [L]

**THETAM** = matrix porosity, [DIM]

**PHI** = \( P + OMEGA*\sqrt{P/PSI} \)

**OMEGA** = \( 2*DM*ALPHAR/(A*TWOB) \)

**TWOB** = fracture aperture, [L]

**GRAV** = gravitational acceleration, [L/T^2]

**RHO** = fluid density, [M/L^3]

**XMU** = fluid viscosity, [L*T^2/M]

**SI MULATION CONTROL SWITCHES:**

**IPS** - code for selection of solution

- **INJECT ON IN INTERVAL TO OBSERVATION POINT:**
  1. Injection interval to observation point - PULSE - MATRIX DIFFUSION
  2. Injection interval to observation point - PULSE - NO MATRIX DIFFUSION

- **INJECT ON IN INTERVAL TO OBSERVATION INTERVAL:**
  3. Injection interval to observation interval - PULSE - MATRIX DIFFUSION
  4. Injection interval to observation interval - PULSE - NO MATRIX DIFFUSION

- **INJECT ON POINT TO OBSERVATION POINT:**
  5. Injection point to observation point - PULSE - MATRIX DIFFUSION
  6. Injection point to observation point - PULSE - NO MATRIX DIFFUSION
  7. Injection point to observation point - CONSTANT SOURCE - MATRIX DIFFUSION
  8. Injection point to observation point - CONSTANT SOURCE - NO MATRIX DIFFUSION

**NEW POINT TO POINT FORMULAS:**

- **IPO** - code for output
  1. Concentration vs. time
  2. Concentration vs. radial distance

- **IST** - code for selection of time output
  1. Real time
  2. Dimensionless time

- **ISD** - code for selection of distance output
  1. Real radial distance
2 - dimensionless radial distance

IRAD - code for radial flow coefficient
  1 - flow-based solution
  2 - head-based solution

ITR - code for calculation of transmissivity
  1 - calculated
  2 - read from input file

ICD - code for selection of output type when IPO=1
  1 - CD vs. TD
  2 - CD vs. TD RDE**2

INV - code for selection of numerical inverter
  1 - DeHoog
  2 - Talbot

IGAM - code for calculation of cross-sectional area
  1 - calculated
  2 - read from input file

IDD - code for calculation of diffusion coefficient of solute in matrix
  1 - calculated
  2 - read from input file

IBD - code for calculation of the mixing coefficients
  1 - calculated
  2 - read from input file

IVOL - code for calculation of well volume
  1 - calculated
  2 - read from input file

ITD - code for calculation of dimensionless time
  1 - calculated
  2 - read from input file

ITS - code for time generation
  1 - log time generation
  2 - linear time generation

IPA - code for peak normalization
  1 - for CD only
  2 - for concentration normalized to peak concentration

******************************************************************************
** USE CONSISTENT UNITS - CURRENT OUTPUT FILES ARE SETUP FOR kilogram-metres-second**
******************************************************************************

******************************************************************************
** DECLARATION OF VARIABLE TYPES:                                           **
******************************************************************************
 implicit real*8 (A-H,O-Z)
dimension CD(901), TDD(901), RDD(901), TIME(901), R(901)
data SI GMV 0./,ANN 1./, N 32/
PI = 4.0*D+0.0, DATAN(1.0*D+0.0)
201
! OPEN FILES:

open(unit=1, file='RTRANS.INP', status='unknown')
open(unit=2, file='RTRANS.OUT', status='unknown')

! READ CONTROL SWITCHES FROM INPUT FILE:

read(1,*)IPS
read(1,*)IPO
read(1,*)IST
read(1,*)ISD
read(1,*)IRAD
read(1,*)ITR
read(1,*)ICD
read(1,*)IV
read(1,*)IGAM
read(1,*)ID
read(1,*)IBD
read(1,*)VC
read(1,*)ITD
read(1,*)TS
read(1,*)PA

! READ THE PROPERTIES OF THE TEST:

read(1,*)ALPHAR
read(1,*)RW
read(1,*)RWO
read(1,*)RI
read(1,*)CAPFAC
read(1,*)RET
read(1,*)DS
read(1,*)TAO
read(1,*)THETAM
read(1,*)TVDB
read(1,*)Q
read(1,*)DELH
read(1,*)TR
read(1,*)VI
read(1,*)XLI
read(1,*)VE
read(1,*)XLE
read(1,*)GAM
read(1,*)GAM
read(1,*)BETADE
read(1,*)BETADC

! READ IN THE DISTANCES OF INTEREST:

read(1,*)NR
read(1,*)RSTART
read(1,*)FR

if (NR .EQ. 1) then
    R(1) = RSTART
else

202
DR=(FR-IRSTART)/NR
DRND=0.0
NR=NR+1
do 16 I=1,NRR
   (I)=IRSTART+DRND
   NR=NR+1
16 continue
do 16 I=1,NRR
   (I)=IRSTART+DRND
   NR=NR+1
16 continue

! READ IN THE TIME RANGE OF INTEREST:
read(1,*)NLT
read(1,*)NT
read(1,*)TSTART
read(1,*)FST
if(NLT.EQ.1)then
   TIME(1)=TSTART
   TMAX=TSTART
else if(TS.EQ.1)then
   TTT=TSTART
   NTT=0
   do 15 I=1,NLT
      do 17 J=1,9
         TD=TTT*float(J)
      enddo
      do 18 K=1,10
         TEMP=TTT*float(K-1)*.1
      enddo
      NTT=NTT+1
      TIME(NTT)=TD+TEMP
      TTT=TTT*10.
   enddo
   TMAX=TIME(NTT)
else
   TMAX=FST
   DT=(FST-TSTART)/NT
   DADD=0.0
   NTT=NT+1
   do 25 I=1,NTT
      TIME(I)=TSTART+DADD
      DADD=DADD+DT
   enddo
25 continue
endif

! READ IN THE PARAMETERS CONTROLLING THE INVERSION:
read(1,*)ERROR
read(1,*)AL
read(1,*)TFACT
read(1,*)NTERM
read(1,*)IOPT
read(1,*)GRAV
read(1,*)RHO
read(1,*)XMU

! CALCULATE DIMENSIONLESS PARAMETERS:

if (IDD .EQ. 1) then
    DD = DS * TAO
end if

DM = DD * THETAM

if (ITR .EQ. 1) then
    TR = RHO * GRAV / (12 * XMU) * (TWOB)**3
else
    A = DELH * TR / (DLOG(RI/RW) * TWOB)
endif

OMEGA = 2 * DM * ALPHAR / (A * TWOB)
PSI = DD / A

if (IVOL .EQ. 1) then
    VI = PI * RW**2 * XLI
    VE = PI * RW**2 * XLE
endif

if (IGAM .EQ. 1) then
    GAMI = 2 * PI * RW * TWOB
    GAME = PI * RWO * TWOB
end if

if (IBD .EQ. 1) then
    BETADI = (VI * RW) / (ALPHAR**2 * GAMI * RET)
    BETADE = (VE * RI) / (ALPHAR**2 * GAME * RET)
endif

! RET1 = face retardation coefficient

AA = TWOB / 2 * RET1 / (THETAM * SQRT(RET * DD))

! Calculate the volume and velocity of the disk at RI/2

VOL = PI * RI**2 * TWOB
VEL = RI * Q / VOL

BETA = RI**3 / (4 * AA**2 * VEL * SQRT(ALPHAR))

! TI ME AND DISTANCE CALCULATI ONS:

if (NLT .EQ. 1) then
    if (ITD .EQ. 1) then
        TD = TME(1) / (ALPHAR**2 / RET)
        TMAX = MAX(A / ALPHAR**2 / RET
    else
        TD = TME(1)
endif

else
  if(I TD. EQ. 1) then
    do 11 I = 1, NTT
  TDD(I) = ME(I) * A * ALPHAR**2 / RET
 11 continue
  TMXX = TMXX / A * ALPHAR**2 / RET
  else
    do 12 I = 1, NTT
  TDD(I) = ME(I)
 12 continue
  endif
endif

if(NR. EQ. 1) then
  RD = R(1) / ALPHAR
else
  do 19 I = 1, NRR
  RDD(I) = R(I) / ALPHAR
  19 continue
endif

! BEGIN EXECUTION: ! ===============
write(*,*) ' Executing........be patient! '
write(*,*) '
if(IPO. EQ. 1) then
  NP = 0
  do 88 I = 1, NTT
  TDT = TDD(I)
  TMXX = TMXX / TDT
  BIGT = TFACT * TMXX
  ATERM = A / (TDT / 2.0 * BIGT)
  if(I INV. EQ. 1) then
    call HOOG2(BIGT, ATERM, TDT, FT, RD, BETADI, BETADE, OMEGA, PSI, RDE, ROI, IPS, I OPT, I Inv)
  else
    ALAMDA = 6. / TDT
    call TALBOT(FT, TDT, ALAMDA, SIGMA, ANU, N, RD, BETADI, BETADE, OMEGA, PSI, RDE, ROI, IPS, I OPT, I Inv)
  endif
  NP = NP + 1
  CD(NP) = FT
     88 continue
else
  NP = 0
  BIGT = TFACT * TMXX
  ATERM = A / (TDT / 2.0 * BIGT)
  do 10 I = 1, NRR
  RDX = RDD(I)
  if(I INV. EQ. 1) then
    call HOOG2(BIGT, ATERM, TDT, FT, RDX, BETADI, BETADE, OMEGA, PSI, RDE, ROI, IPS, I OPT, I Inv)
  else
    ALAMDA = 6. / TDT
    call TALBOT(FT, TDT, ALAMDA, SIGMA, ANU, N, RDX, BETADI, BETADE, OMEGA, PSI, RDE, ROI, IPS, I OPT, I Inv)
  endif
  NP = NP + 1
  CD(NP) = FT
10 continue
endif

else
  endif
endif
206

10 continue
endif

! WRITE THE RESULTS:
! NT=NP

! CONSTRAIN THE OUTPUT:
!
do 444 I=1,NT
 if(CD(I).LT.1.E-5) CD(I)=1.E-5
 if(CD(I).GT.1.) CD(I)=1.0
444 continue

! NORMALIZE TO PEAK CONCENTRATION
!
if(IPA.EQ.2) then
 PEAK=0.0
 do 445 I=1,NT
  if(CD(I).GE.PEAK) PEAK=CD(I)
445 continue
 do 446 I=1,NT
  CD(I)=CD(I)/PEAK
446 continue
endif

! INITIALIZE INFO IN THE OUTPUT FILE:
!
write(2,5)
write(2,9)
write(2,9)

! Injection interval to observation point - PULSE - MTRI X DIFFUSION
if(IP.EQ.1) then
 write(2,5009) IPS
 write(2,5000) ALPHAR
 write(2,5001) RI
 write(2,5002) TWOB*1000000
 write(2,5017) THETAM*100
 if(IRAD.EQ.1) then
  write(2,5003) C"60*1000*1000
  else
  write(2,5004) DELH
  write(2,5005) TR
  write(2,5014) GMAV
  write(2,5015) RHO
  write(2,5016) XMU
  endif
 if(IDD.EQ.1) then
  write(2,5019) DS
  else
  write(2,5021) TAO
  endif
 write(2,5022) DD
endif
write(2,5008) VI*1000
write(2,5007) BETADI
write(2,5018) IINV
write(2,2100) ERROR
! Injection interval to observation point - PULSE - NO MATRIX DIFFUSION
else if(IPS.EQ.2) then
  write(2, 5009) IPS
  write(2, 5000) ALPHAR
  write(2, 5001) R
  write(2, 5002) TWD*1000000
  if(IRAD.EQ.1) then
    write(2, 5003) Q*60*1000*1000
  else
    write(2, 5004) DELH
    write(2, 5005) TR
  endif
  write(2, 5006) GRAV
  write(2, 5007) XMU
  write(2, 5008) VI*1000
  write(2, 5007) BETAD
  write(2, 2100) ERROR
else if(IPS.EQ.3) then
  write(2, 5009) IPS
  write(2, 5000) ALPHAR
  write(2, 5001) R
  write(2, 5002) TWD*1000000
  write(2, 50017) THETAM*100
  if(IRAD.EQ.1) then
    write(2, 5003) Q*60*1000*1000
  else
    write(2, 5004) DELH
    write(2, 5005) TR
  endif
  write(2, 5006) GRAV
write(2,5015) RHO
write(2,5016) XMU
endif
if(DD.EQ.1) then
write(2,5019) DS
write(2,5021) TAO
else
write(2,5022) DO
endif
write(2,5008) VI*1000
write(2,5007) BETAD
write(2,5011) VE*1000
write(2,5010) BETAD
write(2,5018) II*NV
write(2,2100) ERROR
write(2,2200) AL
write(2,2300) TFACT
write(2,2400) NTERM
write(2,5006)
write(2,5023)
write(2,5024) VEL
write(2,5025) AA
write(2,5026) BETA
write(2,5027) VOL
write(2,5028) Q
write(2,5006)
write(2,6005)

! Injection interval to observation interval - PULSE - NO MATRIX DIFFUSION
elseif(IPS.EQ.4) then
write(2,5009) IPS
write(2,5000) ALPHAR
write(2,5001) RI
write(2,5002) TV*1000000
if(IRAD.EQ.1) then
write(2,5003) Q*60*1000*1000
else
write(2,5004) DELH
write(2,5005) TR
write(2,5014) QRA
write(2,5015) RHO
write(2,5016) XMU
endif
write(2,5008) VI*1000
write(2,5007) BETAD
write(2,5011) VE*1000
write(2,5010) BETAD
write(2,5018) II*NV
write(2,2100) ERROR
write(2,2200) AL
write(2,2300) TFACT
write(2,2400) NTERM
write(2,5006)
write(2,5023)
write(2,5024) VEL
write(2,5025) AA
write(2,5026) BETA
write(2,5027) VOL

208
write(2, 5028) Q
write(2, 5006)
write(2, 6007)

! Injection point to observation point - PULSE - MATRIX DIFFUSION
elseif(IPS.EQ.5)then
write(2, 5009) IPS
write(2, 5000) ALPHAR
write(2, 5001) R
write(2, 5002) TWOB*1000000
write(2, 5017) THETAM*100
if(IRAD.EQ.1)then
write(2, 5003) Q*60*1000*1000
else
write(2, 6004) DELH
write(2, 5005) TR
write(2, 5014) GRAV
write(2, 5015) RHO
write(2, 5016) XMU
endif
if(IDD.EQ.1)then
write(2, 5019) DS
write(2, 5021) TAO
else
write(2, 5022) DD
endif
write(2, 5018) IINV
write(2, 2100) ERROR
write(2, 2200) AL
write(2, 2300) TFACT
write(2, 2400) NTERM
write(2, 5006)
write(2, 5023)
write(2, 5024) VEL
write(2, 5025) AA
write(2, 5026) BETA
write(2, 5027) VOL
write(2, 5028) Q
write(2, 5006)
write(2, 6009)

! Injection point to observation point - PULSE - NO MATRIX DIFFUSION
elseif(IPS.EQ.6)then
write(2, 5009) IPS
write(2, 5000) ALPHAR
write(2, 5001) R
write(2, 5002) TWOB*1000000
if(IRAD.EQ.1)then
write(2, 5003) Q*60*1000*1000
else
write(2, 5004) DELH
write(2, 5005) TR
write(2, 5014) GRAV
write(2, 5015) RHO
write(2, 5016) XMU
endif
if(IDD.EQ.1)then
write(2, 5019) DS
if (IPS.EQ.7) then
    write(2,5009) IPS
    write(2,5000) ALPHAR
    write(2,5001) R
    write(2,5002) TWOB*1000000
    write(2,5017) THETAM*100
    if (IRAD.EQ.1) then
        write(2,5003) Q*60*1000
        else
        write(2,5004) DELH
        write(2,5005) TR
        write(2,5014) GRAV
        write(2,5015) RHO
        write(2,5016) XMU
    endif
    if (IDD.EQ.1) then
        write(2,5019) DS
        write(2,5021) TAO
    else
        write(2,5022) DD
    endif
else
    write(2,5006)
    write(2,6010)
endif

! Injection point to observation point - CONSTANT SOURCE - MATRIX DIFFUSION
elseif(IPS.EQ.8) then

! Injection point to observation point - CONSTANT SOURCE - NO MATRIX DIFFUSION
! NEW Injection point to observation point - PULSE - MATRIX DIFFUSION
elseif(IPS.EQ.9)then
write(2,5009) IPS
write(2,5000) ALPHAR
write(2,5001) R
write(2,5002) TVEB*1000000
if(I RAD EQ 1)then
write(2,5003) Q*60*1000*1000
else
write(2,5004) DELH
write(2,5005) TR
write(2,5014) GRAV
write(2,5015) RHO
write(2,5016) XMU
endif
if(IDD.EQ.1)then
write(2,5019) DS
write(2,5021) TAO
else
write(2,5022) DD
endif
write(2,5018) |I| NV
write(2,2100) ERROR
write(2,2200) AL
write(2,2300) TFACT
write(2,2400) NTERM
write(2,5006)
write(2,5023)
write(2,5024) VEL
write(2,5025) AA
write(2,5026) BETA
write(2,5027) VOL
write(2,5028) Q
write(2,5006)
write(2,6012)
else
write(2,5009) IPS
write(2,5000) ALPHAR
write(2,5001) R
write(2,5002) TVEB*1000000
write(2,5017) THEA*M100
if(I RAD EQ 1)then
write(2,5003) Q*60*1000*1000
else
write(2,5004) DELH
write(2,5005) TR
write(2,5014) GRAV
write(2,5015) RHO
write(2,5016) XMU
endif
if(IDD.EQ.1)then
write(2,5019) DS
write(2,5021) TAO
else
write(2,5022) DD
endif
write(2,5018) |I| NV
write(2,2100) ERROR
! NEW Injection point to observation point - PULSE - NO MATRIX DIFFUSION
else if(IPS.EQ.10)then
  write(2,5009) IPS
  write(2,5000) ALPHAR
  write(2,5001) R
  write(2,5002) T<X>1000000
  if(IRAD.EQ.1)then
    write(2,5003) Q*60*1000*1000
  else
    write(2,5004) DELH
    write(2,5005) TR
    write(2,5014) GRAV
    write(2,5015) RHO
    write(2,5016) XMU
  endif
  if(DD.EQ.1)then
    write(2,5019) DS
    write(2,5021) TAO
  else
    write(2,5022) DD
  endif
else if(IPS.EQ.11)then
  write(2,5018) IV
  write(2,2100) ERROR
  write(2,2200) AL
  write(2,2300) TFACT
  write(2,2400) NTERM
  write(2,5009) IPS
  write(2,5000) ALPHAR
  write(2,5001) R
  write(2,5002) T<X>1000000
  write(2,5017) THETAM*100
  if(IRAD.EQ.1)then
    write(2,5003) Q*60*1000*1000
  else
    write(2,5004) DELH
    write(2,5005) TR
    write(2,5014) GRAV
    write(2,5015) RHO
    write(2,5016) XMU
  endif
else
write(2, 5004) DELH
write(2, 5005) TR
write(2, 5014) QRAV
write(2, 5015) RHO
write(2, 5016) XMU
endif
if(IDD.EQ.1) then
write(2, 5019) DS
write(2, 5021) TAO
else
write(2, 5022) DD
endif
write(2, 5018) IIV
write(2, 2100) ERROR
write(2, 2200) AL
write(2, 2300) TFACT
write(2, 2400) NTERM
write(2, 5006)
write(2, 5023)
write(2, 5024) VEL
write(2, 5025) AA
write(2, 5026) BETA
write(2, 5027) VOL
write(2, 5028) Q
write(2, 5006)
write(2, 5010)

! NEW Injection point to observation point - CONSTANT SOURCE - NO MATRIX DIFFUSION
elseif(IPS.EQ.12) then
write(2, 5009) IPS
write(2, 5000) ALPHAR
write(2, 5001) R
write(2, 5002) TV*1000000
endif
write(2, 5003) Q*60*1000*1000
else
write(2, 5004) DELH
write(2, 5005) TR
write(2, 5014) QRAV
write(2, 5015) RHO
write(2, 5016) XMU
endif
if(IDD.EQ.1) then
write(2, 5019) DS
write(2, 5021) TAO
else
write(2, 5022) DD
endif
write(2, 5018) IIV
write(2, 2100) ERROR
write(2, 2200) AL
write(2, 2300) TFACT
write(2, 2400) NTERM
write(2, 5006)
write(2, 5023)
write(2, 5024) VEL
write(2, 5025) AA
! WRITE DATA TO THE OUTPUT FILE:
! =============================
if(IPO.EQ.1)then
  if(ICD.EQ.1)then
     write(2,5006)  write(2,7)
  else
     write(2,2114)
  endif
write(2,9)
write(2,8) (TIME(I),TIME(I)/60,TIME(I)/60/60,TIME(I)/60/60/24,CD(I),TDD(I),I=1,NT)
else
write(2,28)
write(2,9) write(2,8) (R(I),CD(I),RDD(I),I=1,NT)
endif
! END EXECUTION:
! =============
write(*,*)' ' write(*,*)' Completed........thanks for waiting!'
write(*,*)' '
! FORMAT STATEMENTS:
! =================
5   format(/'   RADIAL ADVECTION-DISPERSION WITH DISCONTINUOUS TIME-DEPENDENT BOUNDARY CONDITIONS' /)
7     format('    TIME(s)          TIME(min)          TIME(hour)       TIME(day)           CONC.               TD')
8     format(E12.4,6X,E12.4,6X,E12.4,6X,E12.4,6X,E12.4,1X,F16.4)
9     format('***********************************************************************************************************')
21    format(7I10)
22    format(2E12.5)
24    format(4F12.4,3I5)
28    format('       DI ST.              CONC.             RD')
71    format(/'     Dimensionless radial distance = ',F12.4/)     format(/'     Dimensionless time = ',F12.4/)     format(/'***********************************************************************************************************')
1001  format(E16.7)
1002  format(/'***********************************************************************************************************')
2100  format(3X,'ERROR' = ',E12.5)
2200  format(3X,' AL' = ',F12.5)
2300  format(3X,'TFACT' = ',F12.5)
2400  format(3X,' NTERM' = ',12D)
2114  format('       TIME s' = ',12D)
5000  format(3X,' Dispersion = ',F12.4,' m')
5001  format(3X,'Distance = ',F12.4,' m')
5002  format(3X,'Aperture = ',F12.1,' micron(s)')
5003  format(3X,'Flow rate = ',F12.1,' mL/min')
5004  format(3X,'Head difference = ',F12.4,' m')
5005  format(3X,'Transmissivity = ',E12.4,' m^2/s')
5006  format(/'***********************************************************************************************************')
5007  format(3X,'Inj. Mix. Co. = ',F12.4)
STOP
END PROGRAM RTRANS

!**************************************************************************************
function FS(P,RD,BETADI,BETADE,OMEGA,PSI,RDE,RDI,IPS,IOPT,IINV) !**************************************************************************************
implicit real*8(A-H,O-Z)
complex*16 FS,P,ONE,TWO,THREE,FOUR,COMEGA,CRD,CRDE,CRDI,CPSI,CBETADI,CBETADE,CPHI,CXPHI complex*16 Y,YE,YR,AI,AIP,TERM1,TERM2,TERM3,TERM4,CP
! CONVERT TO DOUBLE COMPLEX VARIABLES: ! ===================================
ONE=dcmplx(1.0D+00)
TWO=dcmplx(2.0D+00) THREE=dcmplx(3.0D+00)
FOUR=dcmplx(4.0D+00)
COMEGA=dcmplx(OMEGA) CRD=dcmplx(RD)
CRDE=dcmplx(RDE) CRDI=dcmplx(RDI) CPSI=dcmplx(PSI)
CBETADI=dcmplx(BETADI) CBETADE=dcmplx(BETADE) CPHI=(P+(COMEGA*SQRT(P/CPSI)))
CXPHI=CPHI**(ONE/THREE)
CP=P**(ONE/THREE)
!**************************************************************************************
!**************************************************************************************

if(IPS.EQ.1) then
! Injection interval to observation point - PULSE - MATRIX DIFFUSION - EQUATION 5:

! Y = CRD + ONE/(FOUR*CPHI)
YE = CRD + ONE/(FOUR*CPHI)
TERM1 = CBETADI / (CBETADI * P + ONE)
TERM2 = (CRD - CRDE) / TWO
TERM3 = AI(CXPHI*Y,IOPT)
TERM4 = ONE/TWO*AI(CXPHI*YE,IOPT) - CXPHI*AIP(CXPHI*YE,IOPT)
FS = TERM1*cdexp(TERM2)*TERM3/TERM4

elseif(IPS.EQ.2) then
! Injection interval to observation point - PULSE - NO MATRIX DIFFUSION - EQUATION 8:

! Y = CRD + ONE/(FOUR*P)
YE = CRD + ONE/(FOUR*P)
TERM1 = CBETADI / (CBETADI * P + ONE)
TERM2 = (CRD - CRDE) / TWO
TERM3 = AI(CP*Y,IOPT)
TERM4 = ONE/TWO*AI(CP*YE,IOPT) - CP*AIP(CP*YE,IOPT)
FS = TERM1*cdexp(TERM2)*TERM3/TERM4

elseif(IPS.EQ.3) then
! Injection interval to observation interval - PULSE - MATRIX DIFFUSION - EQUATION 9:

! YR = CRDI + ONE/(FOUR*CPHI)
YE = CRDE + ONE/(FOUR*CPHI)
TERM1 = CBETADI/((CBETADI*P+ONE)*(CBETADE*P+ONE))
TERM2 = (CRDI - CRDE) / TWO
TERM3 = ONE/TWO*AI(CXPHI*YR,IOPT) - CXPHI*AIP(CXPHI*YR,IOPT)
TERM4 = ONE/TWO*AI(CXPHI*YE,IOPT) - CXPHI*AIP(CXPHI*YE,IOPT)
FS = TERM1*cdexp(TERM2)*TERM3/TERM4

elseif(IPS.EQ.4) then
! Injection interval to observation interval - PULSE - NO MATRIX DIFFUSION - EQUATION 10:

! YR = CRDI + ONE/(FOUR*P)
YE = CRDE + ONE/(FOUR*P)
TERM1 = CBETADI/((CBETADI*P+ONE)*(CBETADE*P+ONE))
TERM2 = (CRDI - CRDE) / TWO
TERM3 = ONE/TWO*AI(CP*YR,IOPT) - CP*AIP(CP*YR,IOPT)
TERM4 = ONE/TWO*AI(CP*YE,IOPT) - CP*AIP(CP*YE,IOPT)
FS = TERM1*cdexp(TERM2)*TERM3/TERM4

elseif(IPS.EQ.5) then
! Injection point to observation point - PULSE - MATRIX DIFFUSION - EQUATION 14:

! Y = CRD + ONE/(FOUR*CPHI)
YE = CRDE + ONE/(FOUR*CPHI)
TERM1 = (CRD - CRDE) / TWO
FS = cdexp(TERM1)*AI(CXPHI*Y,IOPT)/(ONE/TWO*AI(CXPHI*YE,IOPT) - CXPHI*AIP(CXPHI*YE,IOPT))

elseif(IPS.EQ.6) then
! Injection point to observation point - PULSE - NO MATRIX DIFFUSION - EQUATION 15:

! Y = CRD + ONE/(FOUR*P)
YE = CRD + ONE/(FOUR*P)
TERM1 = (CRD - CRDE) / TWO
FS = cdexp(TERM1) * AI(CP*Y, IOPT) / (ONE/TWO * AI(CP*YE, IOPT) - CP * AIP(CP*YE, IOPT))

elseif(IPS.EQ.7) then
! Injection point to observation point - CONSTANT - MATRIX DIFFUSION - EQUATION 12:
Y = CRD + ONE / (FOUR * CPHI)
YE = CRDE + ONE / (FOUR * CPHI)
TERM1 = (CRD - CRDE) / TWO
FS = (ONE/P) * cdexp(TERM1) * AI(CXPHI*Y, IOPT) / (ONE/TWO * AI(CXPHI*YE, IOPT) - CXPHI * AIP(CXPHI*YE, IOPT))
endif return
end function FS
SUBROUTINE FOR NUMERICAL INVERSION OF LAPLACE TRANSFORMS

IMPLEMENTED BY: C.J. NEVILLE
SEPTEMBER 1989

NOTES: 1. THIS IS A DOUBLE PRECISION VERSION
2. THIS VERSION IS DESIGNED TO INVERT ANALYTICAL LAPLACE
TRANSFORMED EXPRESSIONS

DECLARATION OF VARIABLES

DIMENSION D(0:40), WORK(0:40)

DOUBLE PRECISION T, BIGT, ATERM, F, PI, FACTOR, ARGI, RESULT

PI = 3.14159265358979323846264338327950D+00
ZERO = DCMPLX(0.0D+00, 0.0D+00)
ONE = DCMPLX(1.0D+00, 0.0D+00)
TWO = DCMPLX(2.0D+00, 0.0D+00)

M2 = 2 * NTERM

IF (M2 .LT. 2) THEN
   WRITE(6, 100)
   RETURN
END IF

M2 = (M2 / 2) * 2

Z = DCMPLX(DCOS(T * FACTOR), DSIN(T * FACTOR))

A = FS(DCMPLX(ATERM, ARGI), RD, BETADI, BETADE, OMEGA, PSI, RDE, RD, IPS, IOPT, IINV)

D(0) = A
WORK(0) = ZERO
WORK(1) = A

DO 10 J = 2, M2
   A = FS(DCMPLX(D(0), RD, BETADI, BETADE, OMEGA, PSI, RDE, RD, IPS, IOPT, IINV)
   WORK(J) = WORK(J-1)
   A = WORK(J) - A
   D(J) = A
10 CONTINUE

CALCULATE THE PADE TABLE

ARGD = DCMPLX(ATERM, O. 0D+00)
ACLD = FS(ARGD, RD, BETADI, BETADE, OMEGA, PSI, RDE, RD, IPS, IOPT, IINV) / TWO

ARGI = FACTOR
A = FS(DCMPLX(ATERM, ARGI), RD, BETADI, BETADE, OMEGA, PSI, RDE, RD, IPS, IOPT, IINV)

CALCULATE THE PADE TABLE ENTRY

D(0) = A
WORK(0) = ZERO
WORK(1) = A

DO 10 J = 2, M2
   A = WORK(J) - A
   D(J) = A
10 CONTINUE

CALCULATE SUCCESSIVE DIAGONALS OF THE TABLE

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INITIALIZE CALCULATION OF THE DIAGONAL

OLD2=WORK(0)
OLD1=WORK(1)
ARGI=ARGI+FACTOR

A=FS(DCMPLX(ATERM,ARGI),RD,BETADI,BETADE,OMEGA,PSI,RDE,RDI,IPS,IOPT,IINV)

CALCULATE NEXT TERM AND SUM OF POWER SERIES

WORK(0)=ZERO
WORK(1)=A/AOLD
AOLD=A

CALCULATE DIAGONAL USING THE RHOMBUS RULES

DO 20 I=2,J
OLD3=OLD2
OLD2=OLD1
OLD1=WORK(I)

IF((I/2)*2.EQ.I) THEN
  WORK(I)=OLD3+(WORK(I-1)-OLD2)
ELSE
  WORK(I)=OLD3*(WORK(I-1)/OLD2)
END IF 20

SAVE CONTINUED FRACTION COEFFICIENTS

D(J)=-WORK(J)

DO 10 J=0,M2
A=AOLD2+D(J)*Z*AOLD2
AOLD2=AOLD1
AOLD1=A

B=BOLD2+D(J)*Z*BOLD2
BOLD2=BOLD1
BOLD1=B

10 CONTINUE

EVALUATE CONTINUED FRACTION

INITIALIZE RECURRANCE RELATIONS

ACLD2=ACLD1
ACLD1=ACLD0
BOLD2=ONE
BOLD1=ONE+(D(1)*Z)

USE RECURRANCE RELATIONS

DO 30 J=2,M2
A=ACLD1*ACLD1+ACLD2
ACLD2=ACLD1
ACLD1=A
B=BOLD1*BOLD1+BOLD2
BOLD2=BOLD1
BOLD1=B

30 CONTINUE
RESULT OF QUOTIENT-DIFFERENCE ALGORITHM

RESULT=DBLE(A/B)

CALCULATE REQUIRED APPROXIMATE INVERSE

F=DEXP(ATERM*T)*RESULT/BIGT       RETURN

FUNCTION AI(Z,IOPT)

!***********************************************************************
! THIS FUNCTION SUBROUTINE COMPUTES THE AIRY FUNCTION AI(Z) !
!
! A SCALING OPTION IS AVAILABLE FOR LARGE COMPLEX ARGUMENTS: !
! IF IOPT=1, THE RESULT IS NOT SCALED. !
! IF IOPT=2, THE RESULT IS THE FUNCTION VALUE MULTIPLIED !
! BY EXP(U), WHERE U=(2./3.)*(Z**1.5). !
!
! Z=K+iY
!
!***********************************************************************

IMPLICIT REAL*8 (A-H,O-Z)
COMPLEX*16 AI,Z,ZN,P,A,B,SQRTZ,U,W       DATA C1,C2,PI/.3550280538878D0,.2588194037928D0, 3.141592653590D0/

! CALL TRAPS(0,100,100)
PID4=PI/4.d0       PIRT2=DSQRT(PI)*2.d0
TWTHRD=2.d0/3.d0
!
IF (CDABS(Z).GT.4.8d0) GOTO 100 !-------COMPUTE AI(Z) FOR -4.8 < Z < 4.8

SQRTZ=CDSQRT(Z)


AI=C1*A-C2*B

IF (IOPT.EQ.2) GOTO 30       RETURN

30    U=TWTHRD*Z*SQRTZ
    AI=CDEXP(U)*(C1*A-C2*B)       RETURN

!-------COMPUTE AI(Z) FOR |Z| > 4.8, (X.GT.0)

100   CONTINUE       IF(DBLE(Z).LT.0.d0) GOTO 200

SQRTZ=CDSQRT(Z)
!
!-------- COMPUTE AI(Z) FOR -4.8 < Z < 4.8

SORTZ=DSQRT(Z)

LIST=0
!
!-------- COMPUTER AI(Z) FOR |Z| > 4.8, (X.GT.0)

200   CONTINUE

P=1.d0/U

AI = C1*A*Z**B
!
!------- COMPUTE AI(Z) FOR |Z| > 4.8, (X.GT.0)

100   CONTINUE
FUNCTION AIP(Z,IOPT)
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AIP = C1*A - C2*B

IF (IOPT.EQ.2) GOTO 30       RETURN

30    U = TWTHRD*Z*SQRTZ

AIP = CDEXP(U)*COMPLEX(C1*A-C2*B)       RETURN

!-------COMPUTE AIP(Z) FOR |Z| .GT. 4.8, (X.GT.0)

100   CONTINUE       IF (DBLE(Z).LT.0.d0) GOTO 200

SQRTZ = CDSQRT(Z)

U = TWTHRD*Z*SQRTZ

P = 1.d0/U

A = P*( 0.9204799924129d-01+P*(-3.210493584649d+00+P*( 1.28072930874d+01+P*(-5.750830351391d+01+P*( 2.870332371092d+01+P*(-1.576357303373d+03+P* (9.446354823095d+03)))))))


AIP = -(CDCOS(W)*A+CDSIN(W)*B)*CDSQRT(SQRTZ/PI)

RETURN

130   AIP = -A/PIRT2*COMPLEX(COS(W)*A+SIN(W)*B)*CDSQRT(SQRTZ)

RETURN

200   ZN = Z

SORTZ = CDSQRT(ZN)

U = VVRHD2*ZSORTZ

W = PI/4

P = 1.d0/(U**2)

A = P*( 4.388503086420d-02+P*(-6.26216349203d-02+P*( 3.082537649011d-01+P*(-3.210493584649d+00+P*( 5.750830351391d+01+P*(-1.576357303373d+03+P* (6.135706666385d+04)))))))

B = (1.d0/U)*(-9.72222222222d-02+P*( 4.46354823095d+03+P*(-4.289524004000d+04))))

IF (IOPT.EQ.2) GOTO 230

AIP = -(CDCOS(W)*A+CDSIN(W)*B)*CDSQRT(SORTZ/PI)

RETURN

230   AIP = CDEXP(U)*(CDCOS(W)*A+CDSIN(W)*B)*CDSQRT(SORTZ/PI)

RETURN

END

!*****************************************************************************************************************************************************
SUBROUTINE TALBOT(FT,T,ALAMDA,SIGMA,ANU,N,RD,BETADI,BETADE,OMEGA,PSI,RDE,RDI,IPS,IOPT,IINV)
!*****************************************************************************************************************************************************
!****** THIS ROUTINE INVERTS THE LAPLACE TRANSFORM FS(S) NUMERICALLY
!       TO GIVE FT(T).
!       FS(S) IS A COMPLEX*8 FUNCTION OF ITS COMPLEX*8 ARGUMENT S. !       FOR MOST APPLICATIONS IT IS RECOMMENDED THAT:
!       SIGMA=0.0, ANU=1.0, ALAMDA=6.0/T, N=32
!******************************************************************
IMPLICIT DOUBLE PRECISION(A-H,O-Z)

DOUBLE COMPLEX S(1024),DS(1024),ZZ,FS,SUM,B1,B2,V2,ARG1

DOUBLE COMPLEX CON1,CON2,CLAMDA,CNU,CSIGMA,ARG2

!*****************************************************************************************************************************************************

SUBROUTINE TALBOT(FT,T,ALAMDA,SIGMA,ANU,N,RD,BETADI,BETADE,OMEGA,PSI,RDE,RDI,IPS,IOPT,IINV)

IMPLICIT DOUBLE PRECISION(A-H,O-Z)

DOUBLE COMPLEX S(1024),DS(1024),ZZ,FS,SUM,B1,B2,V2,ARG1

DOUBLE COMPLEX CON1,CON2,CLAMDA,CNU,CSIGMA,ARG2

END
DATA Z/0.0/, PI/3.141592654/
CON1=CMPLX(0.5,0.0)
CON2=CMPLX(2.0,0.0)
CLAMDA=CMPLX(ALAMDA,Z)
CNU=CMPLX(ANU,Z)
CSIGMA=CMPLX(SIGMA,Z)
PIBYN=PI/FLOAT(N)
TAU=ALAMDA*T
ZZ=CMPLX(Z,Z)
NM1=N-1

DO 10 K=1,NM1
    THETA=FLOAT(K)*PIBYN
    ALPHA=THETA/TAN(THETA)
    S(K)=CMPLX(ALPHA,ANU*THETA)
    DS(K)=CMPLX(ANU,THETA+ALPHA*(ALPHA-1)/THETA)*CON1
10    CONTINUE

PSI=TAU*ANU*PIBYN
CP=2.0*COS(PSI)
SP=Sin(PSI)
B=ZZ
B1=B

DO 20 KA=1,NM1
    K=N-KA
    RS=TAU*REAL(S(K))
    RSMAX=DMAX1(RS,-50.0D0)
    RSMEXP=EXP(RSMAX)
    V2=CMPLX(RSMEXP,Z)
    B2=B
    B1=B
    ARG1=CLAMDA*S(K)+CSIGMA
    B=CMPLX(CP,Z)*B1-B2+V2*DS(K)*FS(ARG1,RD,BETADI,BETADE,OMEGA,PSI,RDE,RDI,IPS,I OPT,I INV)
20    CONTINUE

ARG2=CLAMDA+CSIGMA+ZZ
SUM=CMPLX(EXP(TAU),Z)*CNU*FS(ARG2,RD,BETADI,BETADE,OMEGA,PSI,RDE,RDI,IPS,I OPT,I INV)*CON1+CMPLX(CP,Z)*B-CON2*(B1-B*CMPLX(Z,SP))
FT=ALAMDA*EXP(SIGMA*T)*REAL(SUM)/FLOAT(N)
RETURN
END

FUNCTION BI(Z,IOPT)
!***********************************************************************
! THIS FUNCTION SUBROUTINE COMPUTES THE AIRY FUNCTION BI(Z) !
! A SCALING OPTION IS AVAILABLE FOR LARGE COMPLEX ARGUMENTS: !
! IF IOPT=1, THE RESULT IS NOT SCALING. !
! IF IOPT=2, THE RESULT IS THE FUNCTION VALUE MULTIPLIED BY !
! EXP(-U), WHERE U=(2./3.)*(Z**1.5) !
! Z=X+iY !
!***********************************************************************
FUNCTI ON BI (Z, I OPT)
...
IMPLICIT REAL*8 (A-H,O-Z)
COMPLEX*16 BI,Z,ZN,P,A,B,SQRTZ,U,V,W,TEMP
DATA D1,D2,PI/.6149266274460d0,.448283573538d0, 3.141592653590d0/
CALL TRAPS(0,100,100)
PI=4.*PI/3.d0
PI=3.141592653590d0
PI=PI/4.d0
PI=PI/3.d0
PI=DSQRT(PI)
XLN2=DLOG(2.d0)
SQRT2=DSQRT(2.d0)
V=DCMPLX(0.d0,PI/3)

IF (CDABS(Z).GT.4.8d0) GOTO 100

SQRTZ=CDSQRT(Z)
P=Z**3

B =(P*( 8.3333333333d-02+P*( 1.98412698412d-03+P*( 2.04585537919d-03+P*( 5.8216720846053d-12+B))))))

BI=D1*A+D2*B
IF (IOPT.EQ.2) GOTO 30

U=TWTHRD*Z*SQRTZ
BI=CDEXP(-U)*(D1*A+D2*B)      RETURN

IF (CDABS(Z).LT.0.d0) GOTO 200

ARCTZ=DATAN(DIMAG(Z)/DBLE(Z))
IF(DABS(ARCTZ).GT.0.1d0) GOTO 300

SQRTZ=CDSQRT(Z)
U=TWTHRD*Z*SQRTZ
P=1.d0/U

BI=A/PIRT/CDSQRT(SQRTZ)
RETURN

IF (IOPT.EQ.2) GOTO 130

BI=A/CDEXP(U/PI RT/CDSORT(SQRTZ)
RETURN

IF (CDABS(Z).GT.4.8) GOTO 300

Z=Z**2

RETURN

IF (IOPT.EQ.2) GOTO 130

BI=\text{CDEXP}(U/PI RT/CDSORT(SQRTZ)
RETURN

IF (CDABS(Z).GT.4.8) GOTO 300

Z=Z**2

RETURN

224
FUNCTION BIP(Z, IOPT)
!
! THIS FUNCTION SUBROUTINE COMPUTES BIP(Z), THE FIRST DERIVATIVE OF THE AIRY FUNCTION BI(Z).
!
! A SCALING OPTION IS AVAILABLE FOR LARGE COMPLEX ARGUMENTS:
! IF IOPT=1, THE RESULT IS NOT SCALED.
! IF IOPT=2, THE RESULT IS THE FUNCTION VALUE MULTIPLIED BY \( e^{-U} \), WHERE \( U = \frac{2}{3} |Z|^{1.5} \).
!
! Z=+X+iY
!
 !******************************************************************************
!
DATA D1,D2,PI/.6149266274460d0,.4482883573538d0,3.141592653590d0/
!
CALL TRAPS(0,100,100) PID4=PI/4.d0
!
PID3=PI/3.d0 PIRT=SQRT(PI)
!
!
IF(IOPT.EQ.2) GOTO 230
!
BI = CDCEXP( W*I + CDCEXP( W*I + W*B ) / CDSORT( PI*I*SORT2 ) )
RETURN
!
230
!
U=TVHRD*Z*CDSQRT( Z )
BI = CDCEXP(-U) *( CDCEXP( W*I + W*B ) / CDSORT( PI*I*SORT2 ) )

!-------COMPUTE BI(Z) FOR Z > GT. 4.8, (X > GT. 0, Y LARGE POS.; II= 1)
! OR FOR Z > GT. 4.8, (X > GT. 0, Y LARGE NEG.; II= -1)
!
300 CONTINUE
!
II = I
!
IF (DIMAG(Z).LT.0.d0) II = -1
!
ZN=Z*CDEXP(-V*I)
SOR2=CDSORT(ZN)
U=TVHRD*Z*CDSQRT( Z )
P=1.d0/(U**2)
!
A= 1.d0*( -3.713348756432d-02+P*( 5.764919041267d-02+P*(-2.915913992307d-01+P*( 3.079453030173d+00+P*(-5.562278536591d+01+P*( 1.533169432013d+03+P*(-5.98925135687d+04+P*( 3.148257417867d+06))))))))
B= 1.d0/(U**2)
!
W=U+PID4
XX=DBLE(W)
YY=IM(XX)
!
W=DCMPLX(XX,YY)
!
TEMP=SQRT2/PIRT/CDSQRT(SORT2)*(CDCEXP(W*I)+W*B)
TEMP=CDCEXP(II*V/2.0)+TEMP
!
IF(IOPT.EQ.2) THEN
!
U=TVHRD*Z*CDSQRT( Z )
BI = CDCEXP(-U)*TEMP
ELSE
BI = TEMP
ENDIF
!
RETURN
END
\[ SQRT2 = SQRT(2.0) \]
\[ XLN2 = LOG(2.0) \]
\[ V = CMPLX(0.0, 0.0) \]
\[ TWTHRD = 2.0/3.0 \]

! -------- COMPUTE BI(P(Z)) FOR -4.0 < Z < 4.0

\[ SQRTZ = SQRT(Z) \]
\[ CDABS = |Z| \]
\[ CDEXP = e^{-U} \]
\[ CSQRT = \sqrt{Z} \]
\[ CEXP = e^{U} \]
\[ CDSD = SD \]
\[ CDIM = IM \]
\[ CDIMAG = IM \]
\[ PI = 3.1415926535897932384626433832795 \]

IF (CDABS(Z).GT.4.8) GOTO 100

!------- COMPUTE BI(P(Z)) FOR |Z| .GT. 4.8, (X.GT.0, |Y| SMALL)

\[ U = TWTHRD*Z*SQRTZ \]
\[ BIP = CDEXP(-U)*(A*P2 + B*P3) \]

IF (IOPT.EQ.2) GOTO 30
RETURN

50 CONTINUE

IF (DI0LIE(Z)).LT.0.0) GOTO 200

ARCTZ = ATAN(DIMAG(Z)/DBLE(Z))
IF (ABS(ARCTZ).GT.0.1E0) GOTO 300

!------- COMPUTE BI(P(Z)) FOR |Z| .GT. 4.8, (X<0)

\[ U = TWTHRD*Z*SQRTZ \]
\[ W = U + PI \]
\[ A = 1.0/(U**2) \]
\]

IF (IOPT.EQ.2) GOTO 230
RETURN

100 CONTINUE

IF (DI0LIE(Z)).LT.0.0) GOTO 200

ARCTZ = ATAN(DIMAG(Z)/DBLE(Z))
IF (ABS(ARCTZ).GT.0.1E0) GOTO 300

!------- COMPUTE BI(P(Z)) FOR |Z| .GT. 4.8, (X, Y SMALL)

\[ SQRT2 = SQRT(Z) \]
\[ V = VM*2.0*SQRT2 \]
\[ W = VM*2.0*SQRT2 \]
\[ A = (1.0/U**2) \]
\]

IF (IOPT.EQ.2) GOTO 230
RETURN

200 CONTINUE

IF (DI0LIE(Z)).LT.0.0) GOTO 200

ARCTZ = ATAN(DIMAG(Z)/DBLE(Z))
IF (ABS(ARCTZ).GT.0.1E0) GOTO 300

!------- COMPUTE BI(P(Z)) FOR |Z| .GT. 4.8, (X, Y SMALL)

\[ U = VM*2.0*SQRT2 \]
\[ W = VM*2.0*SQRT2 \]
\[ A = (1.0/U**2) \]
\]

IF (IOPT.EQ.2) GOTO 230
RETURN

226
BIP = CDEXP(-U) * (CDSIN(W) * A - CDCOS(W) * B) * CDSQRT(SQRTZ / PI)
RETURN

! ------ COMPUTE BIP(Z) FOR Z .GT. 4.8, (X.GT.0, Y LARGE POS.; II = 1)
!                   OR FOR Z .GT. 4.8, (X.GT.0, Y LARGE NEG.; II = -1)
CONTINUE
II = 1
IF (DIMAG(Z).LT.0.d0) II = -1
ZN = Z * CDEXP(-V*II)
SQRTZ = CDSQRT(ZN)
U = TWTHRD*ZN*SQRTZ
P = 1.d0 / (U**2)
Aium = 4.4047999924129d-01**2 ( - 204799924129d-01**2 + 1280729308074d-01**2)
Bium = 9.246283078989d-01**2 + 4.246283078989d-01**2 + 1241058960273d-01**2 + 2.870332371092d-02**2 + 9.446354823095d-03**2 + 4.289524004000d-05)

TEMP = SQRT2 / PI * CDSQRT(SQRTZ) * (CDCOS(W) * A - CDSIN(W) * B)
IF (IOPT.EQ.2) THEN
   U = TWTHRD*Z*CDSQRT(Z)
   BIP = CDEXP(-U)*TEMP
ELSE
   BIP = TEMP
ENDIF
RETURN
END
Example Input File:

8                       IPS: SELECTS SOLUTIONS; SEE MAIN PROG.
1                       IPO: 1 FOR CONC - TIME; 2 FOR CONC - DIST
1                       IST: 1 FOR REAL TIME; 2 FOR DIM. TIME
1                       ISD: 1 FOR REAL DIST.; 2 FOR DIM. DIST.
1                       ITR: 1 FOR CALC TR; 2 FOR READ DIRECTLY
1                       IC: 1 FOR CD VS TD; 2 FOR CD VS TD/RD**2
1                       IIV: 1 FOR DEHOOG; 2 FOR TALBOT
1                       IGM: 1 FOR CALC GAM, GAME; 2 FOR READ DIRECTLY
1                       ID: 1 FOR CALC DD; 2 FOR READ DIRECTLY

1                       IB: 1 FOR CALC BETAI, BETAE; 2 FOR READ DIRECTLY
1                       IV: 1 FOR CALC VE, VI; 2 FOR READ DIRECTLY
1                       ITS: 1 FOR LOG TIME GENERATION; 2 FOR LINEAR
1                       IPA: 1 FOR CD ONLY; 2 FOR PEAK NORMAL

0.05                   ALPHAR: DISPERSIVITY, L
1.0e-5                      RW: RADIUS OF INJECTION WELL, L
1.0e-5                     RWO: RADIUS OF OBSERVATION WELL, L
5.0                        RI: RADIAL DIST. BETWEEN INJECTION AND OBSERVATION, L
1.0                    CAPFAC: CAPTURE FACTOR, DIM.
1.0e-10                    DS: FREE WATER DIFFUSION COEFF., L**2/T
0.72                      TAO: MATRIX TORTUOSITY, DIM.
0.0                        DD: DIFFUSION COEFFICIENT OF SOLUTE IN MATRIX, L**2/T

0.01                   THETA: POROSITY OF MATRIX, DIM.

5.00e-4                  TWOB: FRACTURE APERTURE, L
8.3333333e-5                Q: FLOW RATE, L**3/T !5L/min /1000/60 = 8.333E-5 m**3/s

0.0                   DELH: HEAD DIFFERENCE, L
0.0                    TR: TRANSMISSIVITY, L**2/T
0.0                      VI: VOLUME OF ISOLATED INJECTION INTERVAL, L**3
0.5                     XL: LENGTH OF ISOLATED INJECTION INTERVAL, L
0.0                      VE: VOLUME OF ISOLATED OBSERVATION INTERVAL, L**3
0.5                     XLE: LENGTH OF ISOLATED OBSERVATION INTERVAL, L

0.0                     GAM: CROSS-SECTIONAL AREA INLET RESERVOIR, L**2
0.0                      GAME: CROSS-SECTIONAL AREA EFF. RESERVOIR, L**2
0.0                     BETAI: DIM. MIXING COEFF., INLET
0.0                     BETAE: DIM. MIXING COEFF., OUTLET
1                       NR: NUMBER OF DISTANCE POINTS MINUS ONE
5.0                     RSTART: START DISTANCE NOTE: must match with RI
5.0                     FSRT: START DISTANCE NOTE: must match with RI
8                       NLT: NUMBER OF LOG CYCLES TIME TO A MAX OF 9
800                     NT: NUMBER OF TIME POINTS (LINEAR TIME GENERATION)
100.0                   TSTART: START OF TIME (FOR FIRST LOG CYCLE)
864000                   TST: STOP TIME (FOR LINEAR TIME GENERATION)

1.000E-6                    ERROR:
0.000000                   ALPHA:
0.7993                   TFACT:
10                       IOPT: SCALING CODE FOR AIRY FUNCTIONS
9.80665                  GRAV: GRAVITATIONAL ACCELERATION [m/s**2]
1000.0                   RHO: FLUID DENSITY [kg/m**3]
1.124e-3                  XMU: FLUID VISCOSITY [m*s**2/kg]
Example Output File:

RADIAL ADVECTION-DISPERSION WITH DISCONTINUOUS
TIME-DEPENDENT BOUNDARY CONDITIONS

Solution = 8
Dispersivity = 0.0500 m
Distance = 5.0000 m
Aperture = 500.0 microns
Flow rate = 5000.0 mL/min
Solver = 1=DeHoog, 2=Talbot
ERROR = 0.10000E-05
AL = 0.00000
TFACT = 0.79930
NTERM = 10

DI SPERSIVE-DIFFUSIVE SCENARIO
Velocity = 0.1061E-01 m/s
A = 2946.2783
BETA = 0.6069E-04 <1=dispersive, >1=diffusive
VOL = 0.3927E-01 m^3
Q = 0.8333E-04 m^3/s

Injection point to observation point - CONSTANT SOURCE - NO MATRIX DIFFUSION

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Appendix D
Example HydroGeoSphere Input Files (Chapter 3 Supplement)
GROK Input File:

Radial flow and transport in a axisymmetric domain

Single fracture

TRANSPORT SOLUTION - STEADY STATE

end title

!---------------------------grid

generate blocks interactive
grade x
  0, 1000, 0.01, 1.05, 1000
  1, 1, 1, 1, 1
  5, 5, 1, 1, 1
  10, 10, 1, 1, 1
  25, 25, 1, 1, 1
  50, 50, 1, 1, 1
  75, 75, 1, 1, 1
  100, 100, 1, 1, 1
grade y
  0, 1, 1, 1, 1
grade z
  0.25, 0.5, 0.0002, 2, 0.25
  0.25, 0.0, 0.0002, 2, 0.25
end generate blocks interactive

end

!---------------------------simulation

units: kilogram-metre-day

do transport

axisymmetric coordinates

!---------------------------porous media

use domain type porous media

properties file sp.mprops

clear chosen zones
choose zones all
read properties matrix

!---------------------------flow

clear chosen nodes
choose nodes all
initial head 0

clear chosen nodes
choose nodes x plane

1000

1E-5

specified head
flow solver convergence criteria
1E-10

flow solver maximum iterations
1000000

!---------------------------well
make well node
pump1
0, 0, 0.25
1, 0.288
!200mL/min /1000 /1000 =2E-4 m^2/min * 1440 min/day = 0.288 m^2/day
1E-5
0.0

make well node
pump2
0, 1. 0.25
1, 0.288
!200mL/min /1000 /1000 =2E-4 m^2/min * 1440 min/day = 0.288 m^2/day
1E-5
0.0

!-------------------------------transport species
solute
free solution diffusion coefficient
8.64e-6
!1. E-10 m^2/s*86400 = 8.64e-6 m^2/day
end solute

transport solver convergence criteria
1E-15

transport time weighting
1

!---------------------------fracture
use domain type
fracture
properties file
sp.fprops

clear chosen faces
choose faces z plane
0.25
1E-5

new zone
1
clear chosen zones
choose zone number
1
read properties
200

!impermeable matrix

!---------------------------output times
minimum timestep
1E-1000
output times
10
end

!---------------------------controls
concentration control
0.01

!---------------------------output
make observation point
obs x = 0
0, 0, 0.25

make observation point
obs x = 1
1, 0, 0.25

make observation point
obs x = 5
5, 0, 0.25

make observation point
obs x = 10
10, 0, 0.25

make observation point
obs x = 25
25, 0, 0.25

make observation point
obs x = 50
50, 0, 0.25

make observation point
obs x = 75
75, 0, 0.25

make observation point
obs x = 100
100, 0, 0.25

make observation point
obs x = 1000
1000, 0, 0.25

! K I L L switch
!clear chosen nodes
!choose node
!10, 0, 0.25

!flux output nodes from chosen

!detection threshold concentration
!0.999

!flag observation nodes if exceed detection threshold concentration
!stop run if flux output nodes exceed detection threshold concentration
MPROPS Input File:

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**FPROPS Input File:**

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aperture
200.E-6

longitudinal dispersivity
1.0

transverse dispersivity
0.0

dend material
Array Sizes Input File (modified from auto-generated file):

channel flow: 1d elements
    50000
channel flow: material zones
    20
channel flow bc: zero-depth gradient segments
    5000
dual flow bc: flux faces
    10000
dual flow bc: flux function panels
    10
dual flow bc: flux nodes
    10000
dual flow bc: flux zones
    10
dual flow bc: head function panels
    100
dual flow bc: head nodes
    10000
dual: material zones
    20
flow: material zones
    20
flow bc: drain-type flux nodes
    2
flow bc: evaporation faces
    10000
flow bc: evaporation nodes
    10000
flow bc: evaporation zones
    10
flow bc: evaporation function panels
    10
flow bc: flux nodes
    10000
flow bc: flux faces
    10000
flow bc: flux zones
    10
flow bc: flux function panels
    10
flow bc: free drainage nodes
    1000
flow bc: head nodes
    10000
flow bc: head function panels
    100
flow bc: river-type flux nodes
    2
flow bc: specified nodal flowrate
    501
flow bc: specified nodal flowrate function panels
    100
flow bc: hydrostatic node columns
    100
heat transfer permafrost: thawing table
    50
heat transfer permafrost: freezing table
    50
heat transfer permafrost: thawing-freezing table
    50
heat transfer permafrost: temperature function panels
    300
fractures: 2d elements
    100000
fractures: zones
    300
general: list
    300
mesh: node connections
    100
mesh: node sheets in z for layered grids
    50
mesh: x grid lines (rectangular) 10000
mesh: y grid lines (rectangular) 1000
mesh: z grid lines (rectangular) 6000
mesh: number of layers 100
mesh: number of sublayers per layer 100
observation wells: nodes 501
output: flux volume nodes 1000
output: flux volumes 10
output: nodes 100
output: times 1000
permafrost: elements 10000
permafrost: function panels 100
seepage face: 3d elements intersecting 1000
seepage face: nodes 1000
solution: target times 3000
surface flow: 2d elements 50000
surface flow: boundary segments 5000
surface flow: hydrographs 20
surface flow: hydrograph nodes 100
surface flow: material zones 20
surface flow bc: critical depth segments 5000
surface flow bc: zero-depth gradient segments 5000
tile drains: 1d elements 10000
tile drains: 3d elements intersecting 10000
tile drains: concentration function panels 100
tile drains: nodes 1000
transport: species 5
transport: species kinetic reactions 2
transport bc: concentration nodes 10000
transport bc: concentration function panels 100
transport bc: flux nodes 10000
transport bc: flux function panels 100
transport bc: immiscible phase dissolution nodes 1000
transport bc: third-type concentration faces 10000
transport bc: third-type concentration function panels 100
transport bc: zero-order source function panels 100
transport bc: first-order source function panels 100
wells: 1d elements
wells: 2d fracture elements intersecting
wells: 3d elements intersecting
wells: flux function panels
tiles: flux function panels
wells: injection concentration function panels
wells: nodes
stress: stressed nodes
stress: stress function panels
end
Appendix E

Contour and Geological Maps (Chapter 5 Supplement)
Figure E1: Contour map and surface water features around the Site. Note: elevations are in units of feet above mean sea-level. Reference: Wynne-Edwards (1967).
Figure E2: Bedrock outcrops around the Site. Reference: Wynne-Edwards (1967).
Figure E3: Undifferentiated bedrock outcrops around the Site. Approximately 19.8 of the 106.1 km² of land surface shown is exposed rock (~18.7%). Reference: Wynne-Edwards (1967).
Appendix F
Detailed Methods (Chapter 5 Supplement)
Hydraulic Testing

Hydraulic testing was conducted in bedrock wells to locate significant fracture features and determine their hydraulic properties. Slug (P1 to P3, P7 to P8) or constant-head (P4 to P6) tests were conducted on contiguous straddle-packer intervals. The length of the isolated section varied between 1.325 m (P1 to P3), 1.1 m (P4 to P6), and 1.19 m (P7 to P8). Slug tests were analyzed using the Hvorslev (1951) and Van der Kamp (1976) methods. Constant-head tests were interpreted using the Thiem solution.

Multi-level Completion

The boreholes were completed as multi-level piezometers designed to isolate transmissive features identified during the hydraulic testing. Up to three intervals were constructed in each well using polyvinylchloride (PVC) screen and riser, bentonite, and well sand (#2). Bentonite was placed above the top of the shallow interval in the annular space between the risers and the casing and extended up into the casing to eliminate potential problems with water short-circuiting into the well via an incomplete casing seal, and to prevent the water in the shallow interval from coming in contact with the steel casing. This method of multi-level completion allowed for the creation of 23 sampling locations. However, P8-D was not water-bearing upon completion and subsidence occurred in P3-S part way through the study leaving both abandoned.

Groundwater Sampling

Groundwater samples were collected using a dedicated polyethylene tube with a foot valve or a submersible environmental pump. Each interval was purged until the stabilization of the field parameters (temperature, pH, electrical conductivity, and dissolved oxygen) prior to the collection of the sample. Chemical analytes included major ions and nutrients (ammonia, chloride,
dissolved organic carbon (DOC), nitrate-N, nitrite-N, and total phosphorus). Groundwater samples were also collected for isotopic analysis ($\delta^{18}$O and $\delta^2$H). Both chemical and isotope samples were collected in clean high density polyethylene (HPDE) bottles. Microbiological analytes included *E. coli*, total coliform, fecal coliform, and fecal streptococci. The samples were collected in pre-sterilized bottles provided by the commercial laboratory. All samples were stored in coolers in the field and then refrigerated in the laboratory until analysis.

**Analytical Methods**

Chemical analysis was performed at the Analytical Services Unit (ASU) at Queen’s University, Kingston, ON, Canada. This laboratory is accredited by CALA (Canadian Association for Laboratory Accreditation Inc.) to the standards of ISO/IEC 17025. Nitrate-N, nitrite-N, and chloride were analyzed using a Dionex DX300 ion chromatograph system with autosampler, eluent degas system, computer interface, and gradient module. The detection limit for each analyze was 0.05 mg/L (ppm). Ammonia and total phosphorus were analyzed colorimetrically using a Seal Analytical Flow Analyzer with XY-Z autosampler. The detection limit for both analytes was 0.1 mg/L. Aliquots for DOC analysis were filtered using 0.45 micron filter paper and a vacuum system. The analytical instrument was a Shimadzu TOC-V CPN that measures non-purgeable organic carbon. A series of standards and blanks were included in all runs for quality control. The analytical methods for each parameter are based on those referenced in the Standard Methods for the Examination of Water and Wastewater (Clesceri et al. 2005).

Stable isotopic analyses were performed at the Queen’s Facility for Isotope Research (QFIR) at Queen’s University, Kingston, ON, Canada. Oxygen isotope ratios ($\delta^{18}$O) were measured using a GasBench II interfaced with a Thermo Finnigan DELTAplusXP continuous flow stable isotope
ratio mass spectrometer (IRMS). Hydrogen isotope ratios ($\delta^2$H) were measured using a Thermo H/Device interfaced with a Finnigan MAT 252 IRMS. Isotope values are reported in units of per mil ($\%$) relative to Vienna Standard Mean Ocean Water (VSMOW). The analytical error was approximately $\pm 1\%$ and $\pm 0.1\%$ for oxygen and hydrogen, respectively. A series of standards and blanks were included in each run.

Bacterial analysis was conducted at Caduceon Laboratories in Kingston, ON, Canada. The laboratory is a member of CALA and fully accredited for the analysis of E. coli, total coliform, and fecal streptococci. The membrane filtration methods SM 9222 B (E. coli and total coliform), SM 9222 D (fecal coliform), and SM 9230 C (fecal streptococci) from Clesceri et al. (2005) were used. Results were reported in counts per 100 millilitres (cts/100 mL).
Table F1: Target pharmaceuticals and personal care products (PPCPs).

<table>
<thead>
<tr>
<th>Compound</th>
<th>Common Use</th>
<th>Example Trade Name</th>
<th>CAS Number</th>
<th>Chemical Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chlorotetracycline</td>
<td>Antibacterial</td>
<td></td>
<td>57-62-5</td>
<td>C_{22}H_{23}ClN_{2}O_{8}</td>
</tr>
<tr>
<td>Clarithromycin</td>
<td>Antibacterial</td>
<td>Clarpen</td>
<td>81103-11-9</td>
<td>C_{36}H_{50}NO_{12}</td>
</tr>
<tr>
<td>Oxolinic acid</td>
<td>Antibacterial</td>
<td></td>
<td>14698-29-4</td>
<td>C_{13}H_{18}NO_{8}</td>
</tr>
<tr>
<td>Oxytetracycline</td>
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<td></td>
<td>79-57-2</td>
<td>C_{10}H_{12}N_{2}O_{4}</td>
</tr>
<tr>
<td>Sulfacetamide</td>
<td>Antibacterial, acne treatment</td>
<td>Rosalin</td>
<td>144-80-9</td>
<td>C_{6}H_{11}N_{2}O_{5}S</td>
</tr>
<tr>
<td>Sulfachloropyridazine</td>
<td>Antibacterial</td>
<td></td>
<td>80-32-0</td>
<td>C_{10}H_{14}ClN_{2}O_{4}</td>
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<tr>
<td>Sulfadiazine</td>
<td>Antibacterial</td>
<td></td>
<td>68-35-9</td>
<td>C_{6}H_{11}N_{2}O_{5}S</td>
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<tr>
<td>Sulfadimethoxine</td>
<td>Antibacterial, veterinary use</td>
<td>Rofenaid</td>
<td>122-11-2</td>
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<td>Sulfaguanidine</td>
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<td>57-67-0</td>
<td>C_{6}H_{12}N_{2}O_{5}S</td>
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<tr>
<td>Sulfamerazine</td>
<td>Antibacterial</td>
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<td>127-79-7</td>
<td>C_{15}H_{24}N_{4}O_{5}S</td>
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<td>Sulfamethazine (sulfadimidin)</td>
<td>Antibacterial, veterinary use</td>
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<td>57-68-1</td>
<td>C_{15}H_{22}N_{2}O_{4}S</td>
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<tr>
<td>Sulfamethoxazole</td>
<td>Antibacterial, antiprotozoal</td>
<td></td>
<td>723-46-6</td>
<td>C_{8}H_{12}N_{4}O_{5}S</td>
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<tr>
<td>Sulfapyridine</td>
<td>Antibacterial</td>
<td>M&amp;B 693</td>
<td>000144-83-2</td>
<td>C_{15}H_{24}N_{2}O_{5}S</td>
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<tr>
<td>Sulfathiazole</td>
<td>Antibacterial</td>
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<td>71-14-0</td>
<td>C_{15}H_{21}N_{2}O_{5}S</td>
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<td>Sulfisoxazole</td>
<td>Antibacterial, antiprotozoal</td>
<td>Aoxin</td>
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<td>Tetracycline</td>
<td>Antibacterial</td>
<td>Sumycin</td>
<td>64-75-5</td>
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<tr>
<td>Triclosan</td>
<td>Antibacterial agent in toothpaste and shampoo</td>
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<td>3380-34-5</td>
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<td>Trimethoprim</td>
<td>Antibacterial</td>
<td>Proloprim</td>
<td>738-70-5</td>
<td>C_{15}H_{20}N_{4}O_{5}S</td>
</tr>
</tbody>
</table>

Chest Pain, Hypertension and Blood Circulation

| Metoprolol tartrate       | Chest pain, hypertension                        | Lopressor          | 56392-17-7  | C_{19}H_{31}NO_{9}   |
| Pentoxifylline            | Blood circulation, dementia                      | Pentox             | 6493-05-6   | C_{16}H_{22}N_{3}O_{3} |
| Propranolol               | Chest pain, hypertension                         | Inderal            | 318-98-9    | C_{16}H_{21}N_{2}O_{6} |

Cholesterol Reducers

| Bezafibrate               | Cholesterol reducer                              | Bezelip            | 41859-67-0  | C_{19}H_{29}CINO_{4} |
| Clofibrate                | Cholesterol reducer                              | Atromid-S          | 637-07-0    | C_{12}H_{14}ClO_{3}  |
| Fenofibrate               | Cholesterol reducer                              | Fenoglide          | 49562-28-9  | C_{20}H_{22}ClO_{4}  |
| Gemfibrozil               | Cholesterol reducer                              | Lopid              | 25812-30-0  | C_{17}H_{20}O_{3}    |

Food-related

| Caffeine                  | Stimulant                                        |                    | 58-08-2     | C_{6}H_{10}N_{4}O_{2} |

Pain Killers, Fever Reducers and Anti-inflammatories

<p>| Acetaminophen             | Painkiller, reduces fever                        | Tylenol            | 103-90-2    | C_{6}H_{12}NO_{2}    |
| Diclofenac                | Painkiller                                      | Cambia             | 15307-79-6  | C_{14}H_{10}CINO_{4}Na_{2} |
| Fenoprofen                | Painkiller, anti-inflammatory                    |                    | 29679-58-1  | C_{15}H_{20}O_{4}    |
| Ibuprofen                 | Painkiller, anti-inflammatory                    | Advil              | 15687-27-1  | C_{13}H_{18}O_{2}    |
| Indomethacin              | Painkiller                                      | Indocin            | 53-86-1     | C_{13}H_{12}CINO_{4} |</p>
<table>
<thead>
<tr>
<th>Compound</th>
<th>Common Use</th>
<th>Example Trade Name</th>
<th>CAS Number</th>
<th>Chemical Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ketoprofen</td>
<td>Painkiller, anti-inflammatory, reduces fever</td>
<td>Orudis</td>
<td>22071-15-4</td>
<td>C_{16}H_{14}O_{3}</td>
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<td>Naproxen</td>
<td>Painkiller, anti-inflammatory</td>
<td>Aleve</td>
<td>22204-53-1</td>
<td>C_{16}H_{14}O_{3}</td>
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<tr>
<td>Phenazone</td>
<td>Painkiller, reduces fever</td>
<td></td>
<td>60-80-0</td>
<td>C_{11}H_{12}N_{2}O</td>
</tr>
<tr>
<td>Propyphenazone</td>
<td>Painkiller, reduces fever</td>
<td></td>
<td>479-92-5</td>
<td>C_{14}H_{15}N_{2}O</td>
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<tr>
<td>Salicylic acid</td>
<td>Painkiller</td>
<td>Asprin</td>
<td>50-78-2</td>
<td>C_{9}H_{8}O_{4}</td>
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<td><strong>Psychiatric and Anticonvulsants</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Amitriptyline HCl</td>
<td>Antidepressant, painkiller</td>
<td>Tryptizol</td>
<td>549-18-8</td>
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<tr>
<td>Carbamazepine</td>
<td>Anticonvulsant, antimanic, antipsychotic</td>
<td></td>
<td>298-46-4</td>
<td>C_{13}H_{12}N_{2}O</td>
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<tr>
<td>Fluoxetine HCl</td>
<td>Antidepressant, antiobsessional</td>
<td>Prozac</td>
<td>59333-67-4</td>
<td>C_{13}H_{16}ClF_{3}NO</td>
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<td>Primidone</td>
<td>Anticonvulsant</td>
<td>Mysoline</td>
<td>125-33-7</td>
<td>C_{12}H_{14}N_{2}O_{2}</td>
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</table>

**Notes:**
1 May not include all uses and treatments
2 May not include all trade names
Table F2: Analytical method detection limits (MDL) for the target pharmaceuticals and personal care products (PPCPs). The MDL may differ between analysis dates or laboratories for the same compound.

<table>
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<tr>
<th>Compound</th>
<th>February 2007 (ng/L)</th>
<th>September 2008 (ng/L)</th>
<th>May 2009 (ng/L)</th>
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<td><strong>Antibiotics</strong></td>
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<td>Chlorotetracycline</td>
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</tr>
<tr>
<td>Clarithromycin</td>
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</tr>
<tr>
<td>Oxolinic acid</td>
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<td></td>
</tr>
<tr>
<td>Oxytetracycline</td>
<td>21.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sulfacetamide</td>
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<tr>
<td>Sulfachloropyridazine</td>
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<td>Sulfamethazine (sulfadimidine)</td>
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<td>Sulfapyridine</td>
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<td>Sulfisoxazole</td>
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<td>Trimethoprim</td>
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<td><strong>Chest Pain, Hypertension and Blood Circulation</strong></td>
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<td>Clofibrate</td>
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<td>Fenofibrate</td>
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<td>Acetaminophen</td>
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<td>5.00</td>
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<td>Compound</td>
<td>February 2007 (ng/L)</td>
<td>September 2008 (ng/L)</td>
<td>May 2009 (ng/L)</td>
</tr>
<tr>
<td>---------------------------</td>
<td>----------------------</td>
<td>-----------------------</td>
<td>-----------------</td>
</tr>
<tr>
<td>Indomethacin</td>
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<td>Propyphenazone</td>
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<td>Salicylic acid</td>
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**Psychiatric and Anticonvulsants**

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<tr>
<td>Amtriptyline HCl</td>
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</tr>
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<td>Carbamazepine</td>
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<tr>
<td>Primidone</td>
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<td>3.73</td>
</tr>
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</table>
Appendix G
Overburden Analysis (Chapter 5 Supplement)
Figure G1: Overburden augering locations. The location number, depth to refusal (mbgs, written in red) and depth to the water table (mbgs, written in blue) are shown.
Table G1: Field descriptions and USCS designation of overburden samples. SM = silty sand, SC = clayey sand.

<table>
<thead>
<tr>
<th>Unit #</th>
<th>Description</th>
<th>Unified Soil Classification System Designation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unit 1</td>
<td>Clumpy, dark-brown, contains organics, topsoil</td>
<td>SM to SC</td>
</tr>
<tr>
<td>Unit 2</td>
<td>Light brown, sandy, sticky, slurry</td>
<td>SM to SC</td>
</tr>
<tr>
<td>Unit 3</td>
<td>Medium-brown, less clumpy, top soil and sand</td>
<td>SM to SC</td>
</tr>
<tr>
<td>Unit 4</td>
<td>Green to medium-brown, sandy</td>
<td>SM to SC</td>
</tr>
<tr>
<td>Unit 5</td>
<td>Medium brown, similar to Unit 3, but finer</td>
<td>SM to SC</td>
</tr>
<tr>
<td>Unit 6</td>
<td>Like Unit 2, but clumpier</td>
<td>SM to SC</td>
</tr>
<tr>
<td>Unit 7</td>
<td>Like unit 1, but more clay and larger clumps</td>
<td>SM to SC</td>
</tr>
<tr>
<td>Unit 8</td>
<td>Medium brown, similar to Unit 1, sandy and more clay</td>
<td>SM to SC</td>
</tr>
<tr>
<td>Unit 9</td>
<td>Medium brown, similar to Unit 1, but smaller clumps</td>
<td>SM to SC</td>
</tr>
<tr>
<td>Unit 10</td>
<td>Medium brown, sandy soil, minor clay</td>
<td>SM to SC</td>
</tr>
</tbody>
</table>

Table G2: Depth profile of overburden samples using unit numbers determined in Table G1.

<table>
<thead>
<tr>
<th>Depth Interval (ftlbs)</th>
<th>Sample Location #</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>3</td>
</tr>
<tr>
<td>0-5</td>
<td>1</td>
</tr>
<tr>
<td>5-10</td>
<td>2</td>
</tr>
<tr>
<td>10-15</td>
<td>4</td>
</tr>
<tr>
<td>15-20</td>
<td></td>
</tr>
</tbody>
</table>

Table G3: Cumulative percent weight retained in overburden material sieve analysis.

<table>
<thead>
<tr>
<th>ISO Sieve Size (ASTM)</th>
<th>Unit 1</th>
<th>Unit 2</th>
<th>Unit 3</th>
<th>Unit 4</th>
<th>Unit 5</th>
<th>Unit 6</th>
<th>Unit 7</th>
<th>Unit 8</th>
<th>Unit 9</th>
<th>Unit 10</th>
</tr>
</thead>
<tbody>
<tr>
<td>19 mm (3/4&quot;)</td>
<td>1.7</td>
<td>3.9</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>2.1</td>
<td>3.0</td>
<td>0.0</td>
<td>0.0</td>
<td>3.7</td>
</tr>
<tr>
<td>4.75 mm (No. 4)</td>
<td>6.9</td>
<td>11.2</td>
<td>4.1</td>
<td>1.0</td>
<td>2.2</td>
<td>8.0</td>
<td>4.3</td>
<td>9.9</td>
<td>4.9</td>
<td>6.4</td>
</tr>
<tr>
<td>2 mm (No. 10)</td>
<td>14.6</td>
<td>15.5</td>
<td>11.5</td>
<td>2.9</td>
<td>6.0</td>
<td>23.3</td>
<td>7.8</td>
<td>5.0</td>
<td>10.7</td>
<td>13.6</td>
</tr>
<tr>
<td>1 mm (No. 18)</td>
<td>28.8</td>
<td>20.3</td>
<td>16.6</td>
<td>6.0</td>
<td>9.2</td>
<td>27.4</td>
<td>11.9</td>
<td>10.3</td>
<td>19.0</td>
<td>18.7</td>
</tr>
<tr>
<td>0.5 mm (No. 35)</td>
<td>40.7</td>
<td>26.6</td>
<td>25.1</td>
<td>14.8</td>
<td>16.3</td>
<td>37.7</td>
<td>23.8</td>
<td>24.3</td>
<td>37.8</td>
<td>22.7</td>
</tr>
<tr>
<td>0.25 mm (No. 60)</td>
<td>57.2</td>
<td>40.4</td>
<td>40.7</td>
<td>35.1</td>
<td>34.2</td>
<td>53.2</td>
<td>41.8</td>
<td>43.0</td>
<td>55.7</td>
<td>43.9</td>
</tr>
<tr>
<td>0.15 mm (No. 100)</td>
<td>68.2</td>
<td>62.9</td>
<td>60.4</td>
<td>53.1</td>
<td>51.6</td>
<td>65.0</td>
<td>56.7</td>
<td>57.4</td>
<td>67.5</td>
<td>60.1</td>
</tr>
<tr>
<td>0.075 mm (No. 200)</td>
<td>80.9</td>
<td>78.8</td>
<td>82.5</td>
<td>72.8</td>
<td>71.9</td>
<td>78.5</td>
<td>74.0</td>
<td>74.7</td>
<td>80.2</td>
<td>75.7</td>
</tr>
<tr>
<td>Pan</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>% &lt; No. 4</td>
<td>91.4</td>
<td>84.9</td>
<td>95.9</td>
<td>99</td>
<td>97.5</td>
<td>99.9</td>
<td>92.9</td>
<td>99.1</td>
<td>95.1</td>
<td>89.9</td>
</tr>
<tr>
<td>% &lt; No. 200</td>
<td>19.1</td>
<td>21.2</td>
<td>17.5</td>
<td>27.2</td>
<td>28.1</td>
<td>21.5</td>
<td>26.0</td>
<td>25.3</td>
<td>19.8</td>
<td>24.3</td>
</tr>
</tbody>
</table>
Appendix H
Monitoring Well Schematics (Chapter 5 Supplement)
MONITORING WELL: P4

Coring Date: August 25, 2007
Easting: 435177.24 m
Northing: 4900070.60 m
Coring True Elevation: 130.069 m
Coring Length: 1.127 m (3.7 ft)
Coring Bit Size: 3 in
Bit number: 4
Total penetration: 110.026 m
Wet Depth: 58.6 m
Hydraulic Testing Date: August 25, 2006
Hydraulic Testing Interval: 4 ft
Total Transmissivity: 1.497E-1 m/s
Multi-Level Completion Date: September 2, 2008
P-4-C top of sand pack: 28.644 m, 113.256 m, and 3.950 m screen length: 6.069 m (20 ft)
P-4-C top of sand pack: 28.644 m, 113.256 m, and 3.950 m screen length: 6.069 m (20 ft)
P-4-C top of sand pack: 28.644 m, 113.256 m, and 3.950 m screen length: 6.069 m (20 ft)

LEGEND
ELEVATION
Discontinuities
Borehole Camera Observations

Log Transmissivity (mL/s)
Sampling Zones

Hydraulic Head (mst)

SYMBOLS
Casing
Water-bearing zone identified by asterisk
Horizontal or sub-horizontal feature observed with borehole camera
Vertical or sub-vertical feature observed with borehole camera
Precipice p.1 (multiple fractures in close proximity)

REFERENCES
4. Precipice p.1 (multiple fractures in close proximity)

HYDRAULIC HEAD DATA
Daily average (September 25 to May 22, 2008)
One-day average (August 25 to September 22, 2008)
Appendix I

Geologic Cross-sections (Chapter 5 Supplement)
Cross-section: A-A'

LEGEND

SURFICIAL GEOLOGY
Ground moraine: sandy till, less than 0.5 m thick regionally

PALEOZOIC GEOLOGY
Lower Ordovician
Marsh Formation: interbedded quartz sandstone, sandy dolostone and dolostone

Cambro-Ordovician
Nepean Formation: fine- to coarse-grained quartz sandstone, partially calcareous in upper part

PRECAMBRIAN GEOLOGY
Weathered unconformity: may represent a preserved regolith or paleosol formed prior to deposition of Precambrian units, or may be due to groundwater leaching
Coarse-grained leucocratic red monzonite, syenite, quartz monzonite, and granodiorite
Crystalline limestone and dolomite, siliceous limestone, skarn; includes fragments of white pegmatite, rusty gneiss and diorite

SYMBOLS
Monitoring well or residential drinking water well
Well screen
Contact
Inferred contact
Water-producing feature or recommended pump location

*identification number is from the RNCA database, not the MOE water well record number;
**recommended pumping rate determined by drilling, typically done by short-term pumping tests
Appendix J

Hydraulic Gradient and Flow Direction (Chapter 5 Supplement)
Figure J1: Groundwater gradients and flow directions using the three- and four-point graphical method.
Table J1: Hydraulic gradient and flow direction calculation parameters and results using the three- and four-point graphical method.

<table>
<thead>
<tr>
<th>Interval</th>
<th>Water Level (masl)</th>
<th>Gradient ((\Delta h))</th>
<th>Flow Direction</th>
</tr>
</thead>
<tbody>
<tr>
<td>P1-M</td>
<td>139.65</td>
<td>0.077 (~1m/13m)</td>
<td>325° (~NW)</td>
</tr>
<tr>
<td>P2-S</td>
<td>127.03</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P7-M</td>
<td>139.37</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P1-M</td>
<td>139.65</td>
<td>0.078 (~1m/13m)</td>
<td>325° (~NW)</td>
</tr>
<tr>
<td>P2-S</td>
<td>127.03</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P5-S</td>
<td>128.33</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P1-M</td>
<td>139.65</td>
<td>0.036 (~1m/28m)</td>
<td>358° (N)</td>
</tr>
<tr>
<td>P3-S</td>
<td>124.90</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P6-M</td>
<td>138.80</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P3-S</td>
<td>124.90</td>
<td>0.022 (~1m/45m)</td>
<td>336° (~NNW)</td>
</tr>
<tr>
<td>P6-M</td>
<td>138.80</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P8-M</td>
<td>128.79</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P1-M</td>
<td>139.65</td>
<td>0.078 (~1m/13m)</td>
<td>319° (NW)</td>
</tr>
<tr>
<td>P2-S</td>
<td>127.03</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P3-S</td>
<td>124.90</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P1-M</td>
<td>139.65</td>
<td>0.043 (~1m/23m)</td>
<td>357° (N)</td>
</tr>
<tr>
<td>P5-S</td>
<td>128.33</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P6-M</td>
<td>138.80</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P1-M</td>
<td>139.65</td>
<td>0.028 (~1m/36m)</td>
<td>349° (~N)</td>
</tr>
<tr>
<td>P3-S</td>
<td>124.90</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P6-M</td>
<td>138.80</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P8-M</td>
<td>128.79</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Appendix K

Water Level and Precipitation Data (Chapter 5 Supplement)
Six Months

One Month

One Day

294
Six Months

One Month

One Day
Six Months

One Month

One Day
Six Months

One Month

One Day
Six Months

One Month

One Day

pressure transducer above water level
Six Months

One Month

One Day
Six Months

One Month

One Day
Six Months

One Month

One Day

310
Six Months

One Month

One Day
Appendix L
Stable Isotopes (Chapter 5 Supplement)
Figure A5-8-1: Isotopic composition of groundwater collected from multi-level monitoring wells plotted with respect to the: a) monitoring well sampled, b) monitoring well interval sampled, c) sampling date, and d) rock type the interval is completed in. The global meteoric water line (GMWL) from Craig (1961) and the local meteoric water line for Ottawa (LMWL) from Birks et al. (1987) dataset are provided for reference.
Figure A5-8-2: Long-term data for isotopes in precipitation collected at the Ottawa station from Birks et al. (2003). The horizontal red lines denote amount-weighted mean annual values (1973-1994; 1999-2002). The gray bars give the range in isotopic values of groundwater samples collected during 2007 and 2008 from monitoring wells at the Site.
Appendix M

Nutrients (Chapter 5 Supplement)
Table M1: Nitrite (NO\textsubscript{2}-N mg/L). The current Ontario drinking water standard is 1 mg/L. Results greater than or equal to the method detection limit are highlighted.

| Date       | P1-S | P1-M | P1-D | P2-S | P2-M | P2-D | P3-S | P3-M | P3-D | P4-S | P4-D | P5-S | P5-M | P5-D | P6-S | P6-M | P6-D | P7-S | P7-M | P7-D | P8-S | P8-M |
|------------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 22-Feb-07  | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.06 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 |
| 04-Apr-07  | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 |
| 23-May-07  | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 |
| 19-Jul-07  | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 |
| 10-Sep-07  | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 |
| 14-Nov-07  | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 | ND / 0.1 |
| 07-Jan-08  | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 |
| 21-Feb-08  | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 |
| 07-Apr-08  | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 |
| 27-May-08  | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.2 | ND / 0.2 | ND / 0.2 | ND / 0.2 | ND / 0.2 | ND / 0.2 | ND / 0.2 | ND / 0.2 | ND / 0.2 | ND / 0.2 | ND / 0.2 | ND / 0.2 | ND / 0.2 | ND / 0.2 | ND / 0.2 | ND / 0.2 | ND / 0.2 | ND / 0.2 | ND / 0.2 |
| 02-Jul-08  | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 | ND / 0.05 |

Notes:
ND / ## = not detected, method detection limit given
Blank cells indicate a sample was not collected
| Date       | P1-S | P1-M | P1-D | P2-S | P2-M | P3-S | P4-S | P5-S | P6-S | P6-M | P6-D | P7-S | P7-M | P7-D | P8-S | P8-M |
|------------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 07-Jan-08  | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | 0.2 | 0.2 | 0.1 | ND/0.05 | 0.1 | 0.2 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 |
| 21-Feb-08  | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | 0.2 | 0.2 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 |
| 07-Apr-08  | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | 0.2 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 |
| 27-May-08  | ND/0.1 | ND/0.05 | ND/0.1 | ND/0.1 | ND/0.1 | 0.2 | 0.2 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 |
| 04-Sep-08  | 0.1 | 0.1 | ND/0.1 | ND/0.1 | ND/0.1 | 0.3 | 0.2 | 0.1 | 0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | ND/0.1 | 0.2 |

Notes:
ND/## = not detected, method detection limit given
Blank cells indicate a sample was not collected

---

<table>
<thead>
<tr>
<th>Date</th>
<th>P1-S</th>
<th>P1-M</th>
<th>P1-D</th>
<th>P2-S</th>
<th>P2-M</th>
<th>P3-S</th>
<th>P3-M</th>
<th>P4-S</th>
<th>P4-M</th>
<th>P5-S</th>
<th>P5-M</th>
<th>P6-S</th>
<th>P6-M</th>
<th>P6-D</th>
<th>P7-S</th>
<th>P7-M</th>
<th>P7-D</th>
<th>P8-S</th>
<th>P8-M</th>
</tr>
</thead>
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<td>ND/0.01</td>
<td>ND/0.01</td>
<td>ND/0.01</td>
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<td>ND/0.01</td>
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<td>ND/0.01</td>
<td>ND/0.01</td>
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</tr>
<tr>
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<td>ND/0.01</td>
<td>ND/0.01</td>
<td>ND/0.01</td>
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<td>07-Apr-08</td>
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</tr>
</tbody>
</table>

Notes:
ND/## = not detected, method detection limit given
Blank cells indicate a sample was not collected
### Table M4: Dissolved organic carbon (mg/L).

| date       | P1-S | P1-M | P1-D | P2-S | P2-M | P2-D | P3-S | P3-M | P3-D | P4-S | P4-D | P5-S | P5-M | P5-D | P6-S | P6-M | P6-D | P7-S | P7-M | P7-D | P8-S | P8-M |
|------------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 21-Feb-08  | 1.69 | 1.41 | 2.33 | 0.86 | 1.10 | 1.83 | 2.38 | 0.95 | 1.45 | 1.21 | 2.39 | 1.36 | 2.07 | 0.72 | 1.37 | 1.09 |

**Notes:**
- ND / # = not detected, method detection limit given
- Blank cells indicate a sample was not collected
Appendix N

Field Parameters, Sulphate, and Fluoride (Chapter 5 Supplement)
Table N1: Temperature (°C).
6.3

8.1

7.4

4.2

7.3

28‐Mar‐07

9.5

9.2

9.3

8.9

9.5 10.0

9.6 10.7 10.4

9.9

9.6 10.3 10.1

04‐Apr‐07

9.5

9.3

9.3

8.9

03‐May‐07

9.7

9.6

9.6

9.0 10.0
9.4

19‐Jul‐07 10.0

6.7
9.0

6.8

8.2

8.0 temperature data from this collection date not included in the statistics

22‐Feb‐07

9.1 10.5 10.8 10.4

9.9

9.9

14‐Nov‐07

9.9

9.6

9.6 10.8 10.0

07‐Jan‐08

9.5

9.3

9.6 10.3 10.3 10.1 10.8 10.7 10.4

9.7

9.3 11.0 10.0 10.4

9.8

9.9

9.4

21‐Feb‐08

9.5

9.3

9.2

9.5

9.2 10.7

9.4

9.7

9.4

07‐Apr‐08 10.2

9.9 11.0 11.4 11.1 10.6
9.9 11.4 11.0 10.8 10.1 10.0 11.5

10.0

9.7

9.8 10.0

10.5 10.2 10.1
9.7

9.6

8.9

9.9 10.0

10.7 10.8

9.9 10.1

9.6

27‐May‐08

9.5

9.7

9.5

8.8

9.9 10.2

10.4 10.2 10.3

10.5 11.3 10.7

9.8 10.1

9.8

02‐Jul‐08

9.5

9.4

9.4

8.9

9.0 10.2

10.8 10.7 10.5 10.1 10.4 10.6 10.4

9.8 10.2

9.9 10.1 10.1

04‐Sep‐08 10.3 10.2 10.1 10.2 10.2 10.0
07‐May‐09 10.4 10.0 10.5

10.7 10.8 10.0

9.3 10.7 10.3

9.8 10.3 10.8

9.8 10.5 11.2 12.2 10.1 10.2 10.4 12.1 10.5 10.7 12.1 10.5

11.0 10.4 10.3 10.2 11.8

9.7 10.1 10.9

9.8 11.3 10.2

9.5

Table N2: Electrical conductivity (μS/cm).
22‐Feb‐07

449

491

365

558

750

419

822

812

775

28‐Mar‐07

691

508

390

631

819

392

916

839

805

04‐Apr‐07

625

519

403

672

849

393 1230

860

827

03‐May‐07

528

516

404

686

871

399 1060

976

848

893 1159

19‐Jul‐07

501

515

406

709

836

418

944

14‐Nov‐07

666

453

375

785

711

368

826

909

833

428

421 1246

07‐Jan‐08

720

447

416

740

815

382

746

868

865

424

427 1379

901

945

495

352

945

21‐Feb‐08

672

412

460

835

801

785

987

849

425

424 1341

886

950

349

349

344

817

866

388

1471

932

347

352

347

27‐May‐08

583

599

485

977 1093

483

1139 1045

529

1895 1118 1235

433

433

428

02‐Jul‐08

562

514

408

927

903

403

892

887

450

444 1723

983 1165

372

373

370

933

493

404

543

520

04‐Sep‐08

513

513

408

907

864

402

869

872

438

436 1768 1130 1832

369

364

370

866

470

406

557

508

07‐May‐09

674

677

577 1209 1182

533

1123 1126

583

591 2557

474

475

475 1043

592

516

722

07‐Apr‐08

369

347

Table N3: pH.
22‐Feb‐07

6.9

6.8

6.9

7.1

7.0

7.3

7.3

7.0

7.0

28‐Mar‐07

6.7

6.8

6.9

7.0

7.0

7.6

7.5

6.9

6.8

04‐Apr‐07

6.9

6.9

7.0

7.0

7.0

7.6

7.0

6.9

6.9

03‐May‐07

7.1

6.9

7.1

7.1

7.1

7.7

7.3

7.1

7.0

19‐Jul‐07

7.1

6.9

7.1

7.1

7.1

7.8

7.7

7.1

7.0

14‐Nov‐07

6.4

6.4

6.6

6.7

7.3

7.1

6.7

6.6

6.6

6.7

6.7

6.8

6.7

6.7

07‐Jan‐08

7.0

6.8

7.2

7.0

7.2

7.6

7.6

7.1

7.1

7.3

7.2

7.1

8.1

7.1

7.1

7.4

7.3

21‐Feb‐08

7.0

7.1

7.0

6.8

6.9

7.5

7.1

7.1

7.2

7.2

7.1

7.1

7.2

7.2

7.2

7.2

07‐Apr‐08

7.0

6.9

7.1

7.8

7.1

7.1

7.3

7.4

7.5

27‐May‐08

7.0

7.1

7.1

7.8

7.0

7.0

7.2

7.2

7.3

6.9

7.0

6.7

6.8

7.1

7.0

02‐Jul‐08

6.9

6.9

7.0

6.9

7.0

7.7

6.9

7.0

7.1

7.1

6.9

7.0

7.0

7.2

7.2

7.2

6.6

7.0

6.9

6.8

7.1

04‐Sep‐08

7.1

7.1

7.2

7.1

7.2

7.8

7.1

7.2

7.3

7.3

7.1

7.2

7.2

7.4

7.4

7.4

6.8

7.1

7.2

6.9

7.2

07‐May‐09

7.2

7.2

7.3

7.1

7.2

8.0

7.3

7.2

7.4

7.4

7.2

6.6

7.0

6.3

7.1

7.2

7.3

6.8

321


Table N4: Dissolved oxygen (mg/L).

|       | P1-S | P1-M | P1-D | P2-S | P2-M | P2-D | P3-S | P3-M | P3-D | P4-S | P4-M | P4-D | P5-S | P5-M | P5-D | P6-S | P6-M | P6-D | P7-S | P7-M | P7-D | P8-S | P8-M |
|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 22-Feb-07 | 29.5 | 30.8 | 29.3 | 48.0 | 45.8 | 101.7 | 78.9 | 57.2 | 75.1 |
| 04-Apr-07 | 18.6 | 3.3  | 28.2 | 48.9 | 41.3 | 47.3  | 54.7 | 44.0 |      |
| 07-Jan-08 | 21.8 | 29.3 | 29.3 | 49.9 | 44.3 | 52.8 | 44.9 | 55.3 | 47.6 | 27.0 | 28.6 | 89.2 | 51.6 | 58.6 | 25.1 | 25.6 | 25.2 |
| 21-Feb-08 | 19.7 | 29.6 | 28.9 | 49.8 | 41.9 | 53.1  |      | 151.1 | 49.4 | 27.1 | 27.8 | 93.5 | 49.7 | 77.8 | 25.7 | 16.1 | 25.6 |
| 07-Apr-08 | 46.0 | 38.2 | 51.0 |      |      |      |      | 88.3 | 49.8 | 69.0 | 23.4 | 23.7 | 23.4 |      |      |      |      |      |
| 27-May-08 | 24.6 | 30.7 | 27.1 | 48.1 | 18.5 | 52.4  | 60.3 | 48.1 | 26.1 | 26.0 | 79.9 | 49.0 | 55.5 | 25.3 | 24.6 | 24.4 |      |      |      |      |      |      |
| 02-Jul-08 | 29.7 | 32.4 | 26.8 | 45.6 | 38.0 | 50.1  | 49.3 | 46.6 | 36.0 | 25.9 | 84.3 | 48.0 | 81.3 | 25.4 | 24.1 | 25.1 | 22.0 | 23.8 | 25.9 | 56.8 | 42.6 |

Table N5: Sulphate (mg/L).

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<th>P1-M</th>
<th>P1-D</th>
<th>P2-S</th>
<th>P2-M</th>
<th>P2-D</th>
<th>P3-S</th>
<th>P3-M</th>
<th>P3-D</th>
<th>P4-S</th>
<th>P4-M</th>
<th>P4-D</th>
<th>P5-S</th>
<th>P5-M</th>
<th>P5-D</th>
<th>P6-S</th>
<th>P6-M</th>
<th>P6-D</th>
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<th>P7-M</th>
<th>P7-D</th>
<th>P8-S</th>
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Table N6: Fluoride (mg/L).

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<th>P5-D</th>
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