DESIGN OF EXPERIMENTS IN A THREE DIMENSIONAL SYNTHETIC AQUIFER FOR EVALUATION OF WIRELESS SENSOR NETWORK TECHNOLOGIES APPLIED TO REAL-TIME MODEL CALIBRATION AND PLUME MANAGEMENT

by

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ABSTRACT

The monitoring of subsurface contaminant plumes is typically conducted by the collection of aqueous samples from monitoring wells. The samples are then analyzed in a laboratory to determine contaminant concentrations. This method often proves to be time consuming and cost prohibitive. Limited samples are taken providing data sets with low spatial and temporal resolution. The continual improvements in sensors and wireless sensor network (WSN) technologies is opening up new opportunities for the development of efficient and cost effective methods of monitoring the subsurface environment.

The purpose of this study is to develop a large three dimensional synthetic aquifer to act as a laboratory test bed for the evaluation of WSN technologies. A series of experiments were then designed to create complex tracer plume configurations within the synthetic aquifer. A network of electrical conductivity sensors was employed to monitor the plume migration. The sensor data was then used to develop a transport model calibration methodology which uses temporal method of moments to quantify breakthrough curve global characteristics.

Moments of break through curves were used to calculate the center of mass transport times and dispersivities. These characteristics proved to be effective observations for the calibration of MT3DMS transport models, providing estimates for the input parameters of longitudinal and transverse grid-scale dispersivity and aquifer porosity.
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CHAPTER 1
INTRODUCTION

The present chapter discusses the overall topic addressed in this thesis document. The motivation and current industry issues are addressed followed by the research objectives and an outline of the thesis manuscript.

1.1 Motivation

The quality and availability of water as a natural resource is an issue of ever increasing global significance. The present work concerns the quality of water in the subsurface, generally termed groundwater. Significant interactions between groundwater, surface water, and atmospheric water are such that a serious groundwater contamination issue can readily become a regional or even global environmental concern. From an economic perspective, groundwater is a significant source of potable water throughout the world and provides industry and agriculture a local source of this essential resource. As groundwater is so pervasive a resource to human activity, monitoring and maintaining its quality is a primary goal in the water and environmental industries.

Human activity that relies on groundwater supplies is also responsible for most contaminants of concern impacting groundwater quality. Just a few anthropogenic sources of groundwater contamination include: application of fertilizers and pesticides, industrial spills, leaking tanks and storage facilities, and sewage leaks or dumping. The health and environmental concerns generated by these pollutants in groundwater sources necessitate locating, identifying, and ultimately remediating the contaminated site.

Characterization and monitoring of the subsurface environment is vital to a successful contaminated site remediation. The spatial distribution of contaminants and their corresponding concentration levels are highly valuable information that has historically proven to be expensive and time consuming to obtain. Equally important is the extent of propagation and direction of travel of contaminants. Obtaining knowledge
of a site’s current characterization often proves difficult and expensive, add to this the uncertainty associated with soil and geologic properties and the prediction of the future state of the site becomes daunting. Sophisticated numerical modeling is a tool typically employed to make such predictions; however considerable knowledge of the site’s characteristics is still required to build a realistic and well calibrated predictive model (Hill and Tiedeman, 2007).

Traditional methods used to characterize a subsurface contamination site involve acquiring physical samples from wells and boreholes. Physical aspects of the site can be obtained from the wells and boreholes, such as water level and geologic make up of the underlying strata. Chemical and biologic properties are obtained by sending water samples to laboratories that specialize in water quality analysis. Additional monitoring wells frequently need to be installed when characterizing a site by traditional means. To adequately identify the spatial distribution of the contaminant plume many wells may be required resulting in a significant investment in time, manpower, and capital. Various methods of automatic data sampling and collection are in common use, however the expense still leads to a site characterization that is spatially and temporally lacking in information. It has been noted by researchers in the groundwater modeling calibration field that in practice model calibrations frequently lack sufficient site observations to adequately calibrate a model (Poeter & Hill, 1997, Carrera, et al., 2005).

The latest sampling methods use a combination of traditional sampling procedures along with data logging sensors. It is desired to continue to improve subsurface sensor technology and data communication to the point that networks of near-autonomous sensors will be the primary source of site characterization data. These sensor networks provide real-time data collection and in-situ monitoring while reducing the required manpower. Detection of a contaminant will occur much quicker and the temporal distribution of the data will allow for the determination of contaminant velocity and direction of travel. (Trubilowicz, Cai, and Weiler, 2009, Hart and Martinez, 2006)

Sensors can be grouped according to the type of data they are designed to collect, the three primary categories are physical, chemical, and biological (Goldman, et al., 2007). Sensors classified for measurement of physical properties quantify flow, temperature, pressure head, and moisture content. Chemical sensors measure pH, dissolved oxygen,
electrical conductivity, etc. Biologic sensors measure microbial populations. Often a sensor will measure one characteristic for the purpose of determining a corollary value, such as measuring electrical conductivity to determine ionic concentration. Two immersing classes of chemical sensors are ion selective, and chemiresistors (Ho et al., 2001, Ho et al., 2002) which directly measure the concentration of a given chemical species. The high level of maintenance required and lack of robustness has prevented these sensor types from being employed in long-term site characterizations (Ramanathan et al., 2006).

Sensors in use to date are typically read from a hand-held meter or are connected to a datalogger. A hand-held reader only provides data when an individual connects to the sensor in the field. Sensors connected to a datalogger can sample large amounts of data while unattended for a long period of time but require physical wiring from the sensor to the logger and an excitation power supply. The wires and connections can be problematic in a field-site environment, requiring maintenance and periodic data downloads. Remote, dangerous, or environmentally sensitive sites may preclude regular human interaction with a sensor or datalogger. To overcome these issues wireless sensors, which communicate data via radio transmission are being investigated (Hart and Martinez, 2006).

The use of wireless sensors has become prevalent in numerous disciplines over the past 10 years. A typical application employs a sensor connected to a mote, which is a data acquisition board that also contains a radio sending unit, antenna and power source. Such wireless sensors have been providing real-time data to the military, environmental scientists, and traffic controllers (Akyildiz et al., 2002).

Hydrogeologic applications of wireless sensors present several feasibility issues. The subsurface environment can be quite damaging to electronic equipment and to enable adequate radio communication the sending unit must be above the ground surface. Rocky or uneven terrain can further impede proper wireless data transmission. To make wireless subsurface monitoring feasible, the use of motes has been employed. A mote is a mini-computer with a radio sending unit and onboard memory. The mote is placed at or above ground level while one or more sensors are plugged into the mote and placed in the subsurface environment. The motes control and power the sensor while
communicating with a central computer and other motes in the network. The motes are programmed with their own control and logic software and so can be used to make autonomous decisions about the sensor’s and network’s operations. If an area of the contamination site is showing no contaminant present, then the mote can shut down sensing to conserve power. Further, dynamic control of the network can be enabled where the motes, by communicating with each other, can detect contaminant plume direction of travel and wake up dormant sections of the network as the plume approaches. A central computer collects all sensor data and controls mote and sensor operations. Updates to the mote software can also be transmitted wirelessly from the central computer.

A goal of employing such sensor networks is to increase the level of temporal and spatial resolution of field data in a cost effective manner by reducing the laboratory and manpower overhead currently required in field sampling. The increased availability of site characterization data leading to improved calibrations of computational models and more reliable predictive tools. Present day methods of model calibration take a single time snapshot of field data or a limited time average across a short data acquisition period. Integration of wireless sensor networks with inverse modeling calibration methodologies will enable dynamic calibrations that change and update as the contaminant and site environmental conditions change. This is a significant step forward in predictive capability. The development of such dynamic calibration capability and the underlying wireless sensor network technology is the subject of ongoing research at the Colorado School of Mines Center for Experimental Study of Subsurface Environmental Processes (CSM-CESEP). The present thesis focuses on a subset of this overall research project by conducting a series of intermediate, lab-scale experimental and computational studies to develop sensor and network operation protocols.

1.2 Project objectives and scope of research

One of the long term goals for WSN technology is the development of an autonomous sensor network which collects groundwater contamination data and is
wirelessly linked to numerical models which predict future contaminant migration. In support of this overall goal, this investigation has several objectives which are:

- Develop a large three dimensional, laboratory-scale synthetic aquifer which is to be used a test bed for development of WSN technologies.
- Design experiments which create complex plume configurations from an ionic tracer.
- Employ a network of electrical conductivity sensors to track plume movement.
- Develop a methodology which uses the sensor data to calibrate numerical models designed to simulate plume transport through the synthetic aquifer.

All of this will be done with an overall emphasis on creating data sets and techniques which lend themselves to automated methods of data collection and model calibration.

1.3 Thesis Outline

This thesis is comprised of 7 chapters. Chapter 1 provides an introduction to this investigation and states the objectives of the thesis. Chapter 2 provides background information on groundwater flow and solute transport theory, followed by an overview of numerical modeling and calibration technology. WSN and sampling technology is then reviewed followed by the research goals and supporting tasks. Chapter 3 presents the design and construction of the synthetic aquifer test facility and associated instrumentation. Chapter 4 discusses the use of numerical modeling to simulate the physical test facility. Chapter 5 describes the experiments conducted in the synthetic aquifer and the data collected by the network of sensors. Chapter 6 discusses transport model calibration. Chapter 7 provides concluding remarks and recommendations for further work.
CHAPTER 2
LITERATURE REVIEW AND BACKGROUND

To begin the present study, and throughout its development, the relevant literature was reviewed to gain insight and ascertain the current trends in groundwater sensing and wireless sensor network applications. Subsurface flow and transport modeling theory and methods were also reviewed.

2.1 Introduction

Anthropogenic processes are applying ever increasing stresses on sources of potable water. The International Association of Hydrogeologists estimates that groundwater provides 97% of the earth’s fresh water resources (IAH, 2007). While a recent United States Geologic Survey study determined that Volatile Organic Compounds (VOCs) contaminated 90% of urban groundwater aquifers in the United States (Hamilton et al. 2004). To determine the extent of groundwater contamination; make informed decisions about contaminant fate and transport processes; and monitor remediation efforts, considerable effort is put into aquifer characterization. Informative data on the contaminants present, their physical properties, and their spatial distribution is critical to this aquifer characterization.

Traditional characterization and monitoring methods at the aquifer (or field) scale as well as the experimental (or lab) scale have involved the extraction of an aqueous sample at a specific location and point in time. The sample was typically “sent to the lab” for analysis. This process of physical site sampling is expensive and manpower intensive. It also provides data with quite low spatial and temporal resolution, often resulting in an incomplete characterization of the site under investigation.

Technological improvements in the fields of sensors, power sources, distributed computer communication, and data storage are all combining in the emerging technology of Wireless Sensor Networks (WSN). WSNs are comprised of wireless communication
nodes capable of controlling one or multiple sensors and transmitting data and instructions to a central command computer or other nodes. Fields such as environmental bio-complexity mapping have achieved significant improvements in spatial and temporal data resolution by employing WSN technology (Akyildiz et al., 2002). In the field of hydrology, WSNs can be connected to sensors which detect contaminant concentration, head, or other physical properties of interest. Ultimately the goal is to have a robust, energy efficient WSN in the field which requires little operational maintenance and provides real-time data for site characterization, dynamic model calibration, and improved decision making.

2.2 Contaminant Transport Modeling

The modeling of fluid flow through a porous medium typically begins with the Darcy’s Law relationship. Darcy’s Law can be expressed as a phenomenologically derived constitutive equation

\[ q = -K \nabla h \]  \hspace{1cm} (2.1)

where:

- \( q \) = fluid flux averaged across the porous media (LT\(^{-1}\))
- \( K \) = hydraulic conductivity tensor (LT\(^{-1}\))
- \( h \) = hydraulic head (L)

Darcy’s Law proposes that in a fluid filled porous medium, which is assumed to be a continuum, the fluid flux is proportional to the spatial gradient of the hydraulic head. The proportionality term is the hydraulic conductivity and is a characteristic of the porous media. Combining Darcy’s Law with a continuum based conservation of mass equation results in an equation governing transient flow in an anisotropic medium, referred to here as the groundwater flow equation.
In this form of the equation the coordinate axes are aligned with the principle axes of anisotropy and $K_{xx}$, $K_{yy}$, and $K_{zz}$ are the corresponding axis aligned components of the hydraulic conductivity tensor. Additionally:

- $W$ = source or sink volumetric flux per unit volume (T$^{-1}$)
- $S_s$ = porous media specific storage (L$^{-1}$).

The solution to Equation 2.2 gives the field hydraulic potential. The fluid flux field is then determined by inputting the hydraulic potential into Darcy’s Law, Equation 2.1.

Fluid flux, also known as Darcy Velocity is averaged across the porous media. At the pore scale, heterogeneities in the porous media result in a tortuous flow path and a locally diffuse flow pattern. The modeling of transport of a solute contained within the overall fluid-porous media domain must take this tortuosity effect into account along with diffusion due to concentration gradients. The Advection-Dispersion Equation (ADE) governs the flow of a solute by accounting for transport due to advection along with the bulk fluid, chemical diffusion due to a concentration gradient, and mechanical dispersion due to variations in pore scale velocity. For a single species solute, whose primary direction of travel is aligned with the x-coordinate direction, the ADE can be expressed as:

\[
\frac{\partial}{\partial x} \left( K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_{yy} \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_{zz} \frac{\partial h}{\partial z} \right) - W = S_s \frac{\partial h}{\partial t} \tag{2.2}
\]

\[
\left[ \frac{\partial}{\partial x} \left( D_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( D_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( D_z \frac{\partial C}{\partial z} \right) \right] - \left[ \frac{\partial}{\partial x} (v_x C) + \frac{\partial}{\partial y} (v_y C) + \frac{\partial}{\partial z} (v_z C) \right] + q_s C_s + \sum R_n = \frac{\partial C}{\partial t} \tag{2.3}
\]

where:

- $D_x$, $D_y$, $D_z$ = hydrodynamic dispersion coefficient (L$^2$T$^{-1}$)
- $C$ = solute concentration (ML$^{-3}$)
- $v_x$, $v_y$, $v_z$ = seepage velocity or pore water velocity (LT$^{-1}$)
- $q_s$ = volumetric flow rate per unit aquifer volume for sources (positive) and sinks (negative) (T$^{-1}$)
• $C_s =$ solute concentration of the source or sink flux (ML$^3$)
• $\sum R_n =$ chemical reaction rate term (ML$^3$T$^{-1}$)

For a conservative solute, which is what will be used in the present study, the chemical reaction term will be zero. The hydrodynamic dispersion coefficient ($D$) is a function of mechanical dispersion and effective molecular diffusion. It can be expressed as:

$$D_i = \alpha_i v_i + D^*$$

(2.4)

where:
• $i$ represents the coordinate axes
• $\alpha =$ (dynamic) dispersivity (L)
• $D^* =$ effective molecular diffusion due to a concentration gradient (L$^2$T$^{-1}$).

Seepage velocity is related to the Darcy Velocity through the relationship

$$v_{x,y,z} = \frac{q_{x,y,z}}{\theta}$$

(2.5)

where $\theta$ represents the volumetric porosity of the porous media.

There are only a limited number of closed form analytical solutions to Equations 2.2 and 2.3 which apply to very specific physical conditions or approximations. For this reason numerical solution schemes are generally applied.

2.3 Numerical Groundwater Modeling Tools

To solve the groundwater flow and transport equations (Equations 2.2 and 2.3) for the most general class of physical conditions, numerical solvers have been developed. The typical numerical algorithm of these solvers will discretize the solution domain, and thereby the governing partial differential equations, and iterate the resulting equation sets
until an acceptable level of convergence is achieved. MODFLOW (McDonald and Harbaugh, 1998; Harbaugh et al., 2000) and MT3DMS (Zheng and Wang, 1999) are both solvers which employ this discretization and iteration solution methodology. They each employ finite difference numerical schemes and are widely used in industry and academic research and therefore were used in this investigation.

MODFLOW-2000 (Harbaugh et al., 2000) was developed by the United States Geological Survey for the solution of the groundwater flow equation. It is applicable to steady state or transient flow in layered, anisotropic, heterogeneous, three-dimensional domains. The head potential and fluid velocity profiles calculated by MODFLOW can be used as input values to a solute transport code such as MT3DMS.

MT3DMS is a solute transport code designed to solve the Advection Dispersion Equation. It can simulate solute plumes made up of multiple constituents and accounts for chemical reactions.

2.4 Groundwater Model Calibration

Calibration of a groundwater model refers to the process of adjusting the model’s physical parameters or boundary conditions so that the simulated results are in agreement with known measured observations taken from the system being modeled. The initial, un-calibrated model is referred to as the “forward model.” The determination of this set of parameters is known as solving the inverse problem and so model calibration is often called inverse modeling. The objective of inverse modeling is to determine hydrogeologic parameters of the system from field or laboratory measured heads, flows, contaminant concentrations, etc. Whereas forward modeling is used to calculate heads and flows given known parameters (Hill and Tiedeman, 2007).

Trial-and-error calibration procedures have been employed by practitioners since the introduction of numerical modeling techniques. In recent years, automated calibration methods have gained in popularity (Poeter and Hill, 1997). Automated procedures have the obvious advantage of speed, but they also provide a level of mathematical and statistical rigor required for the solution of a complex system with many variables.
Nonlinear least-squares regression is the most widely employed method for determining an optimal set of parameters in subsurface flow inverse modeling. In this procedure the model calculated values are compared to the physically measured values. The difference between the two values is squared and then weighted based upon the uncertainty of the measured observations, resulting in a multi-dimensional objective function. Nonlinear least-squared regression is then applied to determine the set of parameters which will minimize this objective function. Readily available codes which use nonlinear least-squared regression include MODFLOW-2000 (Harbaugh et al., 2000), PEST (Doherty, 2000), and UCODE (Poeter and Hill, 1999). As discussed previously, MODFLOW-2000 solves the groundwater flow equation, but the software package also includes modules for parameter estimation solution of the inverse model problem. The inverse modeling capability of MODFLOW-2000 is integral to its solution of the groundwater flow equation and therefore has no capability to solve general inverse modeling problems. PEST and UCODE are universal inverse modeling codes which can be used with any forward model that uses ASCII text files for input and output and has command-line execution capability (Hill and Tiedeman, 2007). Each of these codes calculates parameters which minimize a weighted least-squares objective function as their method of inverse modeling. The weighted least-squares objective function, sometimes referred to as the sum of squares weighted residual (SSWR), can be expressed as (Poeter et al., 2005):

\[ SSWR(b) = \sum_{i=1}^{N} \omega_i \left[ h_{obs,i} - h'_i(b) \right]^2 \]  \hspace{1cm} (2.6)

where:
- \( N \) = number of observations
- \( b \) = vector of estimated parameter values
- \( h_{obs,i} \) = the \( i^{th} \) observation
- \( h'_i(b) \) = the simulated equivalent of the \( i^{th} \) observation
- \( \omega_i \) = weight of the \( i^{th} \) observation.
The optimal set of parameters is the one which minimizes the sum of squares weighted residual objective function. The majority, if not all, calibration methods which seek to estimate model parameters attempt to minimize an objective function. Carrera et al. (2005) argues that they only differ in the details of their respective computational schemes.

Calibration of subsurface flow and transport models is often hampered by low sensitivity of the measured state variables, such as head or concentration, to aquifer parameters. To increase the sensitivity of observed data to parameters, discreet measurements of the state variables can be transformed into global characteristic terms. Method of moments transformations have been used by Woodbury and Rubin (2000) to transform discreet concentration data into total solute mass in an attempt to increase parameter sensitivity. Temporal moments are often used to provide a global characterization of breakthrough curve data because of their ability to describe the central tendency of a probability distribution, such as a time series breakthrough curve. The first four moments are frequently used because they correspond to total mass, mean value, variance, and skewness respectively (Govindaraju and Das, 2007).

Regularization is another methodology employed in the model calibration process. Regularization allows the introduction of constraints on parameter spatial variability. These constraints are frequently based on prior information from the site being modeled or geostatistical observations. In this way heterogeneity can be introduced to the model in a controlled manner to ensure the objective function is minimized. Through the use of regularization models can be “over-parameterized” that is, the number of parameters being solved for can be larger than the number of state variable observations; a situation that would result in an ill posed problem if regularization was not used (Doherty, 2000, Hill and Tiedeman, 2007).

In this investigation the inversion code known as UCODE-2005 was employed for model calibration purposes. UCODE-2005 (Poeter and Hill, 1999; Poeter et al., 2005) is a universal inverse modeling package that uses a modified Gauss-Newton method to determine the minimum value of the least-squares objective function. In addition to solving the inverse model problem, UCODE-2005 provides numerous statistical
measures of the given model and its parameters, providing information on simulation confidence, data bias, and parameter correlation.

The use of groundwater modeling in this study has been in two main capacities. First, models were created to investigate possible experimental configurations and aid in the design of laboratory facilities. Second, inverse models were created to estimate physical parameters based on observations obtained in laboratory tracer experiments.

2.5 Traditional Groundwater Sampling Methods

Groundwater sampling has traditionally been accomplished by extracting a sample volume of water from a monitoring well. The sample may have rudimentary analysis done on site or will be sent to a laboratory facility for detailed chemical analysis. Many methods for extracting a sample of water and ensuring it is representative of the surrounding aquifer exist. However, investigations by Puls and Paul, (1997) demonstrate that sampled groundwater does not necessarily represent the level of contamination at the sampled site. Their work shows that the accuracy of well sampled groundwater is dependent upon purge volume prior to sampling, extraction method, and sampling time. Further, the data can be subject to misinterpretation either by human analysts or automated instruments (Swallow et al., 1988). Sampling through pumping or bailing methods in a monitoring well is also highly disruptive to the local flow field, and can chemically alter the sample.

The costs associated with drilling monitoring wells, taking samples, and performing laboratory analysis applies pressure to minimize field sampling efforts. This often results in quite low data resolution, both spatially and temporally; leading to less than ideal characterization of the subsurface environment and inaccurate plume delineation.

Advances in sensors, micro-electronics, and digital data storage have dramatically altered groundwater sampling methods in the last two decades (Hart and Martinez, 2007). Temporal data resolution is greatly increased through the use of unmanned sensors connected to dataloggers. At the same time the use of sensor technology can lead to
manpower and laboratory cost reductions that can be redirected to increasing the number of sampling locations and thereby improve spatial data resolution.

### 2.6 Sensor Network Use in Subsurface Hydrology

The integration of computer science and electrical component technologies has in recent years produced an array of powerful sensor networks. These networks can accommodate a wide assortment of sensor types providing data and information in fields as diverse as military science, civil engineering, traffic control, ecology, and earth sciences to name just a few. Advances in data storage and wireless communication has allowed for the collecting of large data sets from networks that cover large geographical areas. The development of wireless senor networks (WSN) is of particular interest in the field of hydrology for the purpose of characterizing groundwater and contaminant migration. Porta (2007) provides an extensive review of the current trends in sensor and wireless network technology. It can be noted from the work of Porta (2007) and Barnhart (2007) that the majority of WSN studies focus on data collection and do not address how the data should best be used.

Wireless sensor networks are comprised of expandable networks of mini-computers called motes. The motes are capable of wireless communication and data transmission with each other and a master control computer. They also control one or more sensors. Motes are typically powered by batteries with the possible addition of a solar cell. Assuming the WSN is using robust sensors, the power limitations of the motes drives maintenance intervals. The greatest amount of power consumption in motes comes from the radio frequency wireless transmission; therefore minimization of transmission is a priority in network protocols (Akyildiz et al., 2002). This however, may be in direct conflict with the need for frequent and timely data acquisition. This indicates the need for application specific control of a WSN. In the case of contaminant plume migration, the integration of a WSN, transport model, and real-time automatic calibration would be mutually beneficial. It would provide improvements in site characterization, model validation and predictions, and feedback control of the WSN itself. The dynamically
calibrated model would make predictions of contaminant velocity and direction of travel, allowing the WSN to turn-off nodes in inactive regions and wake-up nodes that lie in the plume’s path.

### 2.7 Research Goals

It is pertinent to point out that the present study is an integral part of an over-arching investigation which is attempting to re-conceptualize contaminant transport modeling given the rapidly advancing technologies of sensors and WSNs. The work of Porta (2007), which was a precursor to this investigation, was hampered by failures in sensors that were imbedded in a laboratory scale sand tank. It was recommended that future studies use well emplacement of sensors to allow for sensor maintenance and replacement when necessary. Also, to better explore the WSN’s communication potential, a recommendation was made that a large, lab-scale, three-dimensional test facility be developed. This “synthetic aquifer” test bed would allow for the creation of complex two or three dimensional contaminant plumes in a controlled laboratory environment. It would also provide a test bed for development of WSN technology. Finally, the synthetic aquifer would facilitate proof of concept validation of an integrated system which: employs a WSN to autonomously collect solute transport data, screen the data for anomalies, and conduct real-time automatic calibration of contaminant transport models.

New applications in sensors and wireless networks are continually becoming available as underlying technologies become more efficient and robust. As yet, the full potential of applying WSN technology in the field of subsurface hydrology has considerable opportunity for development. One area to be explored is the direct integration of sensor data into groundwater and contaminant transport models. The ability to perform this integration in a wireless, automated manner will be a considerable advancement in technology, allowing for improved site characterization and plume tracking at costs that should be lower than conventional means. In support of this vision of an integrated system, the present study will accomplish the following goals:
• Design and construct a large lab-scale synthetic aquifer capable of acting as a
  WSN research and development test bed. The synthetic aquifer should have
  control mechanisms enabling the creation of complex plume geometries.
• Develop a methodology for transport model calibration employing macro-
  scale dispersivity and plume transport time as the objective function
  observation metrics.

The following tasks are proposed to achieve these goals:
  Task 1) Conduct detailed design and construction of the synthetic aquifer facility.
  Task 2) Perform numerical modeling of synthetic aquifer design proposals.
  Develop operation curves to categorize flow properties based on aquifer fill material.
  Task 3) Develop a custom sensor configuration based on the expected plume characteristics. Ascertain calibration coefficients for each sensor.
  Task 4) Investigate potential experimental plume configurations through the use of numerical models.
  Task 5) Conduct laboratory testing of aquifer flow and tracer plume transport.
  Task 6) Calculate temporal moments and macro-scale longitudinal dispersivity from time series sensor data.
  Task 7) Determine the grid-scale dispersivity and effective porosity through inverse modeling.

Each of these tasks and their outcomes will be discussed further in subsequent sections of this document. They should not be viewed as sequential actions but rather as concurrent interdependent tasks.
CHAPTER 3
SYNTHETIC AQUIFER TEST FACILITY

The first three tasks supporting the goals of this work are concerned with the design and construction of a large lab-scale synthetic aquifer and the operation of sensors to track tracer movement through the synthetic aquifer.

3.1 Introduction

One of the recommendations of Porta, et al., (2009) was for the development of a significantly larger test facility than what was available in the Colorado School of Mines Center for Experimental Study of Subsurface Environmental Processes (CSM-CESEP) at the time. CSM-CESEP is the University research center which supported the work of both Porta, and the present investigation. A three-dimensional test bed with capabilities for transverse plume migration was called for and the use of wells for sensor emplacement was also recommended.

This large lab-scale subsurface flow test facility would come to be referred to as the CESEP synthetic aquifer. This chapter discusses the synthetic aquifer as a laboratory test facility and test bed for investigating WSN applications. Sensors and other data collection methods will also be addressed. Finally the experimental methods used will be presented along with the lessons learned during the course of creating and utilizing the synthetic aquifer facility.

3.2 Materials and Equipment

In this section, the physical equipment used for the purpose of lab-scale experimentation during the course of this study will be described.
3.2.1 Synthetic Aquifer Tank

Previous WSN studies conducted in the CSM-CESEP facility pointed to the need for a large, laboratory-scale test bed to conduct two or three dimensional solute transport experiments. The size, and corresponding weight, envisioned for this facility were well beyond standard two dimensional vertical wall laboratory sand tanks. It was desired that the synthetic aquifer have a large planview area allowing for significant longitudinal travel distance and transverse migration. Physical limitations of laboratory floor space and the ability to work on and around the synthetic aquifer were also important factors influencing the design of the facility.

Figure 3.1 is a photograph of the synthetic aquifer in operation. The overall waterproof “tank” section is 8 feet (2.4 meters) wide by 16 feet (4.9 meters) long and can be filled to a depth of 22.5 inches (0.57 meters).

Figure 3.1: The CSM-CESEP Synthetic Aquifer facility. Overall tank dimensions are 8x16 feet with a maximum fill depth of 22.5 inches.
The outer structure of the tank was built from commercial construction grade lumber that was treated with a water sealant. The floor structure is constructed of 2x8 inch dimensional joists spaced at 12 inches on center. The joists are supported by three steel platform rails sitting on the laboratory concrete floor. One steel platform rail is permanently affixed to the concrete floor and so the synthetic aquifer had to be constructed around this platform. Two additional steel rails were placed on the lab floor and leveled to the permanent rail’s height. Figure 3.2 shows the underside of the tank. The steel rails can be seen with the 2x8 inch support joists running perpendicular to them.

![Figure 3.2: The underside of the synthetic aquifer tank, the steel platform rails are seen in black.](image)

The side wall structure is constructed of 2x6 inch lumber with 4x4 inch posts at the four corners. All lumber joints are fastened with course thread deck screws, lag bolts, or lag screws. The floor joists are lag bolted to the 16 foot length walls to provide lateral support. The 8 foot length walls are supported by a steel stanchion bolted into the concrete lab floor and a cross beam of laminated 2x4’s (inch). Figure 3.3a shows the
joist-wall structural joint on the 16 foot wall, and Figure 3.3b shows the stanchion support of the 8 foot wall.

Figure 3.3: a) lag bolting the 16 foot wall structure to the floor joists provides lateral support. b) steel stanchion and 2x4 cross beam which provides lateral support to the 8 foot walls. Two platform rails can be seen extending from under the tank.

The tank floor is constructed from ¾ inch (19 mm) marine grade plywood that was sealed and waterproofed prior to installation. It is two layers of plywood thick. The first layer was placed length wise with the second layer running 90 degrees to the first so that no plywood joints overlap and create a weak spot in the span.

The tank side walls are constructed of a single layer of the same marine plywood. The floor to wall plywood joints are reinforce with aluminum “L” angle, which can be seen in Figure 3.3a. Outward bowing of the 16 foot wall under hydrostatic loading is prevented by 2x6 inch stringers tying the walls together along the concrete floor, and stainless steel wire cables along the tank’s top cap.

The inside of the tank is made watertight by a laminated layer of 3mm thick flexible PVC sheeting. All corners and seams were reinforced then heat and chemically welded.
The tank was cycled through several fills with water to stress the structure and ensure no leaks.

This section has described the construction of the main watertight tank. Once the tank is filled with a porous media, fitted with wells, and hydrostatic flow control is applied it then can be considered the complete synthetic aquifer system.

3.2.2 Porous Media and Well Field

To create a porous media “synthetic aquifer” the tank was filled with laboratory grade silica sand purchased from the Unimin Corporation in Idaho. Unimin sands have been well characterized and used extensively in CSM-CESEP research (Fernandez-Garcia et al., 2004, Moreno-Barbero and Illangasekare, 2006). For this investigation #70 sieve size sand was used to create a homogeneous isentropic porous field. Table 3.1 lists the column derived parameter values for #70 sand.

<table>
<thead>
<tr>
<th>Table 3.1: Properties of #70 Sieve Sand</th>
</tr>
</thead>
<tbody>
<tr>
<td>From Limsuwat and Sakaki, 2007 (not published)</td>
</tr>
<tr>
<td>Bulk Density (gm/cm³)</td>
</tr>
<tr>
<td>-----------------------</td>
</tr>
<tr>
<td>1.54</td>
</tr>
</tbody>
</table>

As the tank design developed, it was decided to pack the synthetic aquifer with a homogeneous isotropic porous media. It was believed that, given adequate hydraulic flow control, a homogeneous media would be sufficient for the purpose of evaluating WSN technologies. A homogeneous packing was also chosen based on logistics reasons. The volume and mass of the synthetic aquifer would have required a considerable investment in time and manpower to pack as a heterogeneous aquifer. The depth of the tank would allow for the creation of a three dimensional subsurface environment, however it was reasoned that two dimensional flow and plume configurations would be
adequate for WSN investigations and all tracer flows would fully penetrate the depth of the synthetic aquifer.

A wet fill sand packing technique was used to fill the tank. This entails filling the tank with water to a depth of several inches and slowly and evenly filling with sand. Ponded water several inches above the sand height is maintained throughout the packing process. Dry sand was sifted into the water as best as possible to try and eliminate any trapped air during the tank packing. Once the desired sand depth was achieved, the water level remained ponded above the sand height for several days. During this time the sand was manually churned and re-leveled to eliminate air trapped in the pores. The selection of the target sand depth will be discussed further in section 4.2. To limit evaporation, the sand field was covered with polyethylene sheeting.

Following the recommendation of Porta (2007), wells were designed to be placed in the porous media field. The wells were laid out in the tank prior to being packed with sand. The wells were constructed of 1-¼ inch inside diameter schedule 40 PVC pipe which can accommodate insertion of a Decagon Devices, Inc. 5TE sensor (refer to section 3.2.4). Figure 3.4 demonstrates the construction of the wells. Each well has a PVC end cap which is affixed to the tank floor.

![Figure 3.4: Construction of a synthetic aquifer well.](image)

The wells were intended to fully penetrate the aquifer depth, so a screened section was created by drilling 3/8 inch holes in the PVC pipe and covering the wall with a fine stainless steel wire mesh. The mesh density is 145x145 wires per square inch with a pore opening size of 0.0022 inches. Small diameter holes were also drilled into the end caps.
to provide for inflow and drainage during leak testing of the tank. The wells were affixed
to the tank floor with silicone adhesive and fixed at their top to the wire ropes which span
the transverse direction of the tank.

44 wells penetrate the aquifer field in 8 down gradient rows. The well distribution
and naming convention can be seen in Figure 3.5. In the transverse direction, the odd
numbered rows have 5 wells and the even numbered rows have 6 wells, creating a
staggered distribution pattern. This distribution maximized the planview coverage of the
aquifer field under the constraints of a limited number of available sensors. A staggered
pattern was chosen to ensure that if a plume passed between two wells in one row, it
would be intercepted by a well in the next row. The left side of this schematic represents
the up gradient, or source side, of the synthetic aquifer with the flow moving from left to
right. The wells are identified by the letter W followed by a two digit code. The first
digit of this code is the well’s transverse position; the second digit represents the row
number. Transverse well numbers increase from left to right when looking in the down
gradient direction. For example, well W11 is the first transverse well in row number 1
and well W68 is the 6th well in row number 8. “S” identifies the centerline location of
source reservoirs, “D” identifies the centerline location of drain reservoirs, and “C”
represents the aquifer corners. Flow is from left to right in this figure.

3.2.3 Fluid Flow Control

The synthetic aquifer facility was designed to represent an unconfined aquifer. In
order to create complex plume transport patterns in the aquifer, it was desired to have a
high degree of control over the subsurface flow velocity and direction. To accomplish
this, a series of seven reservoirs were constructed at both the supply and drain side of the
sand field. The outer transverse boundaries of the synthetic aquifer are bound by the
inner tank wall and so, are no flow boundaries forcing tangential flow in the near-wall
vicinity.
The supply, or high hydraulic head, reservoirs are identified by the label S1 – S7. Similarly the drain, or low hydraulic head, reservoirs are labeled D1-D7 as seen in Figure 3.5. The reservoirs were constructed from 12 inch ID, schedule 40 PVC pipe. The pipe was supplied in a 20 foot length with an expansion flange at one end. The flange was removed and the pipe was cut into 2 foot axial length sections. Each 2 foot section was then cut down the pipe diameter creating a half-cylinder section. Figure 3.6 shows one 2 foot pipe section and several of the half-cylinder pieces. A ½ inch hose barb was attached to each half-cylinder reservoir section near the bottom and allowing for hand clearance for hose attachment. Seven reservoir sections were connected at each end of the tank as seen in Figure 3.7 below. The end and center reservoirs (S1, S4, S7 and D1, D4, D7) each required some modification at the bottom to ensure they fit flush to the tank floor. Cut-outs were made in each of these reservoirs to allow for the centerline seam and corner reinforcements in the tanks water-tight liner. Using 7 reservoirs spaced across the tank’s transverse direction left an approximately 5.5 inch blank space on either side of the reservoir bank. This blank space was filled in with a flat PVC spacer.
Figure 3.6: Photo of the 12 inch ID PVC pipe sections used to create the supply and drain reservoirs. On the left is a 2 foot section. On the left are several of the pieces resulting from splitting the pipe down the diameter.

Figure 3.7: Assembly of the 7 reservoirs which provide hydraulic control for the synthetic aquifer. This photo shows the drain side bank of reservoirs being constructed.
The reservoir to reservoir attachment points were affixed with waterproof PVC epoxy cement then sealed with silicone adhesive. The reservoir to tank interfaces were waterproofed with both silicone adhesive and marine grade glue. The forward (aquifer facing) seams between each reservoir were reinforced with a flat PVC strip. The back side of each reservoir interface was reinforced with a section of ½ inch ID PVC pipe chemically cemented in place and overlaid with PVC epoxy. ½ inch PVC pipe pieces were attached to the back side apex of each reservoir near the top and bottom to provide support against the hydrostatic load of the synthetic aquifer and provide working clearance behind the reservoirs. These features can be seen in Figure 3.8.

To provide increased hydraulic control, each reservoir was fitted with an operable gate. The gates were constructed of ¼ inch PVC sheet with EPDM rubber gasket material glued to the sides and bottom. The gates were held in place by PVC U-channel that was glued to the walls and bottom of each reservoir. A test model of the reservoir gate system was built for leak testing of the concept. Figure 3.9 displays this test model.

**Figure 3.8:** Reservoir construction. Small diameter PVC pipe is glued to the back-side seam between reservoirs creating a more rigid and water-tight seam. PVC pipe standoffs provide support for the entire reservoir bank against hydrostatic loads. Hose barbs for water supply lines can also be seen.
Figure 3.9: Reservoir shut-off gate test model. Picture a) demonstrates a reservoir with the gate removed. The PVC U-channel guides remain in place. Picture b) shows the reservoir closed to through flow with the gate in place.

The reservoir gates provide only on or off flow control, but it was thought that 7 supply and 7 drain gates would enable the creation of unique flow and tracer plume configurations.

Two layers of stainless steel mesh were attached to the front of the reservoirs to provide a porous boundary between the water field reservoirs and the synthetic aquifer sand. The mesh layer can be seen in Figure 3.10. The first layer is comprised of T316 stainless steel wire with a mesh rating of 12 mesh per inch. This layer provided strength but could not retain the aquifer sand. The second layer is comprised of T316 stainless steel cloth rated at 145 mesh per inch and is the same material as that used on the wells. The fine mesh layer was wrapped around all of the edges of the course 1st layer with the fine mesh facing the reservoirs. The mesh wall was sealed to the tank floor, and all of the reservoir edges. Figure 3.10 was taken while leak testing the “synthetic aquifer” section of the tank. In this photo, all walls and reservoirs are in place. The well field was filled with tap water and once water tightness was confirmed wet packing of the sand began. With the reservoirs in place the final longitudinal length of the synthetic aquifer is 429.26 cm.
Figure 3.10: Synthetic aquifer leak testing just prior to filling with sand. The reservoir’s wire mesh porous boundary is highlighted in red.

Water level in the reservoirs is maintained through the use of a spill constant head device, one each for supply and drain sides of the synthetic aquifer. The center ring of this device is plumbed with 8 flexible tubing lines. Seven of these tubes connect to the reservoir hose barbs, while the 8th line is used as a manometer tube to compare water head levels between the supply and drain sides. The drain side manometer tube runs under the length of the tank and is mounted near the supply side manometer tube. Figure 3.11 demonstrates the supply side spill constant head device and the two manometer tubes for checking the head difference between the two reservoir banks. Each spill constant head device is mounted on a slider mechanism so that water head height can be changed by sliding the entire mechanism up or down. A faucet spigot provides a steady flow of water to the supply side constant head device. As long as a flow rate greater than the overall synthetic aquifer flow rate is maintained, then the head level will remain constant. The supply overflow spills into the outer ring of the device and is returned to a supply tank. The drain-side spill constant head device operates in a similar fashion except that flow is from the bottom up and drain flow spills out of the inner ring and out to a waste drain.
As can be seen in Figure 3.11, $\frac{1}{2}$ inch ID tubing runs from the constant head device up and over the tank outer wall and then connect to the reservoirs. No holes exist in the main tank so that it remains watertight, however to do this, supply tubing has to be run above the height of the constant head devices. The disadvantage of this is that gas builds up in the tubing and will block off water flow if not degassed regularly. Degassing ports were added to each reservoir supply line and is depicted in Figure 3.12. Degassing is accomplished by attaching a 60 ml syringe to the valve at the top of the port and drawing out the gas. During the course of experimentation, it was found that opening a degas valve would effectively close off the associated reservoir to flow. Individual reservoir flow control by means of these valves was easier to implement than the use of the shut-off gates and so later experiments took advantage of this and did not use the gate system.
Figure 3.12: Degas ports as used on each reservoir tube. Gas accumulates in the vertical tube and is drawn off with a syringe.

Water is provided to the synthetic aquifer by a storage tank located nearby. The storage tank is filled by running tap water through two 5 micron filters. Commercial bleach is then added at a concentration of 250 ml/l tap water to prevent microbial growth. The water from the storage tank is then pumped through an ultraviolet light filter and a 3rd 5 micron filter as it passes to the supply constant head device. The pump draws from the bottom of the storage tank and splits the flow so that some goes to the constant head device and the rest is returned to the top of the storage tank to ensure constant mixing in the tank. Overflow from the supply side constant head device flows to a float activated condensation pump which drains back into the storage tank. Figure 3.13 shows the storage tank and the pump and filter plumbing used to supply water to the synthetic aquifer.
3.2.4 Conservative Tracer Plume

This investigation intended to track tracer plume migration through the use of electrical conductivity sensors. A conservative tracer was desired, and given the large volume of water that would exit a synthetic aquifer of this size, it was also advantageous to use a tracer which could safely be disposed of in a public waste drain in small amounts. Ionic salts as a tracer material generally met these requirements, and so sodium bromide (NaBr) was selected.

Prior to ordering sensors and during the synthetic aquifer design and construction phase, an investigation into tracer electrical conductivity and density effects was conducted. A high electrical conductivity resolution was desired to ensure a tracer plume could be adequately detected. It was noted that the filtered tap water supplied to the
A synthetic aquifer had a significant measurable electrical conductivity which was further increased by the addition of anti-microbial bleach. The background conductivity of the tap water was quite variable over time. During the time frame of early February to mid-March, 2009 the supply water conductivity was measured to be in the range of 4.40 – 4.50 dS/m, while in late June 2009, the conductivity was measured to be 1.90 dS/m. It is believed this drop in tap water conductivity is due to snowpack melt runoff because the local municipal water utility is supplied from surface water sources. It was not known at first if this change in background conductivity was due to sensor drift or a natural effect. The EC sensors were repeatedly checked to ensure they were not the source of the conductivity drift. Once it was determined that the ambient water supply was the cause, a linear drift subtraction method was created as part of the experimental data processing procedure. This method is discussed in further detail in Chapter 5.

Creating a plume with a large ionic aqueous concentration to ensure a significant electrical conductivity over the background aquifer water’s conductivity is not necessarily a viable option for subsurface tracer testing. Adding a tracer which has a density that differs from the background aquifer water’s density will tend to generate density driven migration. In the case of a sodium bromide tracer, density driven sinking of the tracer as it moves through the subsurface is a probable effect that should be avoided. Therefore the selection of a tracer concentration to be employed during synthetic aquifer experimentation needed to balance electrical conductivity detectability, and density driven sinking.

The molar conductivity of strong electrolytes in a low concentration solution is governed by Kohlrausch’s Law, which can be expressed as (Wright 2007):

$$\Lambda_m = \Lambda^0_m - K\sqrt{c}$$

(3.1)

where:

- $\Lambda_m$ = the molar conductivity (S L$^2$ mol$^{-1}$)
- $\Lambda^0_m$ = the limiting molar conductivity for an infinitely dilute solution (S*L$^2$ mol$^{-1}$)
- $K$ = an electrolyte dependent, empirical coefficient
Values from the Kohlrausch’s Law equation can be rearranged to give electrical conductivity as a function of aqueous concentration. Results for several strong electrolytes are presented in Figure 3.14 along with the values obtained by Porta (2007) for sodium bromide. Porta’s values track fairly well to the theoretical values except they are offset by a positive conductivity of approximately 27.8 mS/m which is most likely due to background water conductivity. Porta’s data is also seen to have a slightly larger slope than the theoretical sodium bromide curve. This is likely due to the fact that Kohlrausch’s law is applicable to low concentration electrolyte solutions and becomes less accurate with increasing concentrations.

**Figure 3.14:** Electrical conductivity of strong electrolytes in aqueous solution as a function of concentration. Theoretical values for NaBr, NaCl, KCl, and values from Porta (2007).
The data from Figure 3.14 was useful in determining the range of conductivity to be expected from tracer plume experimentation, and thereby provide an operational range for electrical conductivity sensor specification.

The prediction of the onset of density driven instabilities in a homogeneous, isotropic subsurface media was presented by Oostrom, et al., (1992). This work indicated that density instabilities could be characterized by the following unit less ratio:

\[ \alpha = \frac{K \left( \frac{\rho_s - \rho_w}{\rho_w} \right)}{q} \]  

(3.2)

where:

- \( K \) = the hydraulic conductivity (LT\(^{-1}\))
- \( \rho_s \) = the solute or tracer density (ML\(^{-3}\))
- \( \rho_w \) = ambient groundwater density (ML\(^{-3}\))
- \( q \) = the Darcy velocity (LT\(^{-1}\)).

Subsurface flows with an \( \alpha \) greater than the critical value of 0.3 were found to exhibit density instabilities, while flows with an \( \alpha \) term less than 0.3 tended to maintain stability. Based upon this criteria, the maximum aqueous concentration of sodium bromide tracer used in synthetic aquifer experimentation should be selected so that the \( \alpha \) ratio remains well below the critical value of 0.3.

A maximum allowable sodium bromide tracer concentration was determined based upon uncalibrated sand properties and synthetic aquifer flow rates estimated from a DuPuit approximation solution of the groundwater flow equation (equation 2.2). The parameters used to calculate the Darcy velocity for the aquifer were:

<table>
<thead>
<tr>
<th>Inlet head ((h_{inlet}))</th>
<th>Outlet head ((h_{outlet}))</th>
<th>Hydraulic conductivity ((K))</th>
<th>Aquifer length ((L))</th>
</tr>
</thead>
<tbody>
<tr>
<td>36.83 (cm)</td>
<td>27.94 (cm)</td>
<td>0.0141 (cm/s)</td>
<td>429.54 (cm)</td>
</tr>
</tbody>
</table>
For a one-dimensional, steady-state flow in an unconfined aquifer such as our experimental facility, the DuPuit solution has the form.

\[ \bar{q} = K \left[ \frac{h_{inlet}^2 - h_{outlet}^2}{2 \times (Length)} \right] \]  

(3.3)

Where \( \bar{q} \) is the flux per unit width of the synthetic aquifer. The maximum tracer concentration should occur at the aquifer inlet, so to obtain the Darcy velocity, \( \bar{q} \) is divided by the inlet head. For the above conditions, \( \bar{q} = 9.45 \times 10^{-3} \) cm/s and the Darcy velocity \( q = 2.566 \times 10^{-4} \) cm/s. Plugging these values into Equation 3.2 with an assumed critical \( \alpha \) value of 0.3 and water density \( \rho_w = 0.9983 \) kg/L results in a maximum allowable tracer density of \( \rho_s = 1.00375 \) kg/L. This tracer density equates to a maximum aqueous concentration of 7136 mg/L before the onset of density sinking effects.

Sodium bromide tracer experiments conducted by Porta (2007) used a maximum tracer concentration of 200 mg/L in a heterogeneous media tank. It was desired to have a greater tracer conductivity range than seen in Porta’s work to provide greater sensor response range, while still remaining well below the critical point of density instability. A target tracer concentration of 1000 mg/L was ultimately chosen which is 5 times greater than Porta’s value while remaining 7 times less than the critical density value.

### 3.3 Measurement Methods and Experimental Procedures

Having completed the design and construction of a new large, lab-scale synthetic aquifer test facility, several tasks needed to be accomplished to ensure the test bed was operating as expected and that meaningful data could be collected.
3.3.1 Electrical Conductivity Sensors and Data Acquisition

The Decagon Devices Inc. 5TE sensor was selected for this investigation. The Decagon 5TE sensor is designed to measure soil moisture, subsurface temperature, and bulk electrical conductivity. These sensors are constructed for robust operation in harsh subsurface environments. The inclusion of a temperature reading allows the sensor to fully temperature compensate the electrical conductivity measurements. Circuitry internal to the sensor processes the measured data and provides a calibrated, digital response. For this work, sensor excitation and data acquisition was accomplished by plugging the 5TE sensors into Decagon Devices model EM50 dataloggers.

The Decagon Devices 5TE sensor is seen in Figure 3.15 (Decagon Devices, 2009). Electrical conductivity is measured through the use of the two stainless steel screws seen in the photo. This sensor is intended for use in partially saturated soil environments, but is fully functional in an all solution well environment as used in this investigation. Volumetric soil moisture readings from the sensor were not used in this investigation as sensor placement was always below the water level in a well. For most readings, the sensor was dropped into a well until it touched the bottom. Some experiments were conducted with sensors stacked at several well depths to investigate if density sinking of the tracer plume was occurring. These findings will be discussed further in a latter section.

Figure 3.15: Decagon Devices Inc. 5TE Soil moisture, temperature, and electrical conductivity sensor. Photo from Decagon Devices online product specification page: http://www.decagon.com/soil_moisture/5te/index.php?pg=specs.
Operational specifications for the 5TE sensor are provided by Decagon Devices as: (Decagon Devices, 2009)

- Dimensions: 10 x 3.2 x 0.7 cm
- Probe Length: 5.2 cm
- Dielectric Measurement Frequency: 70 MHz
- Measurement Time: 150 ms
- Power: 3.6 – 15 VDC, 0.3 mA quiescent, 10mA during 150 ms measurement

Electrical Conductivity
- Accuracy: ±1% from 0-7 dS/m
- Resolution: 0.01 dS/m from 0-7 dS/m, 0.05 dS/m from 7-23 dS/m
- Range: 0 – 23 dS/m (bulk)

Temperature
- Accuracy: ±1°C
- Resolution: 0.1°C
- Range: 40°C to +50°C

Because the maximum tracer concentration would be limited to 1000 mg/L of aqueous sodium bromide, the 5TE sensors were ordered from Decagon with a custom internal calibration which truncated the response range leaving only the bottom 10% to cover the output span. This enabled the measurement accuracy to be increased by an order of magnitude over the standard model. The values listed above are for the custom sensors.

The 5TE sensors were connected to Decagon Devices EM50 dataloggers to complete the data acquisition system. Each EM50 is capable of connecting to 5 5TE sensors and is powered by 5 AA-sized batteries. The EM50 datalogger has 1Mb of onboard memory and is capable of storing 36,000 scans with 5 sensors connected (Decagon Devices, 2009).
Data from the dataloggers was downloaded to a notebook computer, usually on a daily basis, by means of an RS232 to USB converter cable. The EM50 data is stored in columnar format and is capable of being downloaded in a Microsoft Excel file format for data processing. A sample rate of one scan every 30 minutes was used throughout this investigation.

### 3.3.2 Well Head Pressure Monitoring

To measure well head pressure, a down-well pressure instrument was developed from an off-the-shelf differential pressure transducer. This transducer purchased from Omega Engineering Inc. (model PX26-001DX) is a low cost, wet/wet sensor with a range of ±6895 Pa (±1 psi). To make it capable of functioning as a down-well sensor, it was fitted with an atmospheric vent tube and had all electrical connections sealed in a waterproof epoxy. The sensor was attached to a brass rod for placement in to the synthetic aquifer wells. Figure 3.16 depicts the down-well sensor and its process meter and controller, model DP25B also purchased from Omega Engineering Inc. This system is capable of providing measurement resolution of 1mm of water depth.

![Figure 3.16: Down-well pressure head measurement system. Circled in red is an Omega Engineering Inc. PX26 differential pressure sensor as it comes from the manufacturer.](image)
The process meter and controller was programmed with calibration data provided by the pressure transducer vendor to provide head data in units of millimeters. It was believed that encasing the transducer in epoxy may have altered the piezoelectric response, and therefore the manufacturer’s calibration values. To ensure accurate water level values would be acquired, the head pressure system was calibrated each time well pressure measurements were taken. Calibration was conducted by creating a water tight cylinder out of clear acrylic material. Water level index marks were placed on the cylinder and these gauge measurements were calibrated to the water level measurements obtained from the down-hole system. It was found that a linear calibration curve was required to adjust the measured values to the gauge values.

Well pressure head measurements were taken while the synthetic aquifer was flooded with several inches of still water above the sand level. The measured head values from each well were expected to be equal under this condition; however it was found that several wells produced water level values that were several millimeters below the other well’s values. It is believed there are two causes of this offset; first the tank floor seam running down the centerline of the aquifer may have raised the centerline wells, second improper fitting of the well body to the PVC end cap may have caused an offset. Centerline wells proved to have a consistent 2 mm offset and all water level measurements from these wells were adjusted by 2 mm. Any other offset which proved to be consistent and repeatable were noted and these well’s readings were adjusted accordingly.

3.3.3 Outflow Rate

The outflow rate from the synthetic aquifer was measured by collecting the outflow from the drain side constant head device in a 5 gallon bucket, recording the fill time and measuring the mass of outflow water collected. From this data and assuming a constant water density referenced to 20°C, a volumetric flow rate can be calculated. The water temperature in the constant head device and or the drain side reservoirs was simultaneously collected. The outflow rates were then temperature corrected to a
standard of 20°C to account for changes in fluid viscosity as ambient laboratory
temperature changed.

3.3.4 Steady State Operation

To ensure the synthetic aquifer had achieved a steady state flow condition, outflow
was monitored to ensure a steady outflow rate was maintained for at least 4 days, which
corresponds to approximately 0.95 pore volumes at the baseline flow configuration.
Once 4 days of stable outflow was confirmed, a pressure mapping of all 44 wells and 14
reservoirs was conducted. If the pressure mapping proved to be stable over a two day
period in addition to the stable outflow rate, then the synthetic aquifer flow pattern was
deemed to be at steady state and tracer introduction could proceed. This procedure to
ensure steady state operation was conducted whenever a change was made to the inflow
or outflow reservoirs or constant head devices.

3.3.5 Electrical Conductivity Sensor Calibration

Monitoring of the sodium bromide electrolyte tracer was to be carried out by
measuring the electrical conductivity of the water traveling through the synthetic aquifer.
Therefore the Decagon 5TE electrical conductivity sensors needed to be calibrated to
tracer concentration. Thirty-eight (38) total sensors were available for this investigation
and each one was calibrated to provide unique fitting parameters relating the sensor’s
measured electrical conductivity to a sodium bromide aqueous concentration. Six (6)
dilution sets were created using Millipore™ laboratory-grade water as the base solution.
Each dilution set began as a unique 10,000 mg/L NaBr concentrate. Each of these
concentrated solutions was then diluted to create calibration standards of 100, 500, and
1000 mg/L NaBr. An initial calibration set of 20, 100, 250, 500, 1000, and 2000 mg/L
NaBr was used to calibrate the first 6 electrical conductivity (EC) sensors and determine
if a linear relationship existed between measured conductivity and NaBr aqueous
concentration. Figure 3.17 is a plot of the results from this initial calibration study. It shows that a linear calibration scheme is appropriate to relate measured conductivity to expected NaBr concentration. It also pointed to the fact that each sensor has its own calibration slope and zero offset intercept, therefore requiring a unique calibration be conducted for each sensor.

![Initial STE EC Sensor Calibration](image)

**Figure 3.17:** Initial calibration of first 5 EC sensors.

Having confirmed that a linear calibration process is applicable, each sensor was calibrated in the 100, 500, 1000 mg/L dilutions to obtain a calibration slope and intercept value. The sensors calibration data was acquired by directly connecting each sensor to a datalogger and then to a notebook computer for real-time sampling. Five (5) data samples were collected at each NaBr concentration. The square of the Pearson product-moment correlation coefficient ($R^2$) was calculated for each calibration curve fit. For all 38 sensors the minimum $R^2$ value obtained was 0.991, further indicating that a linear calibration relationship exists for all sensors used.
The Decagon EM50 dataloggers are capable of reading 5 sensors each; therefore 8 dataloggers were required for all 38 sensors. Another sensor calibration exercise was conducted with the same dilution set and 4 sensors to determine if measured electrical conductivity was independent of the datalogger. Three randomly selected dataloggers were used for this study.

Table 3.2: Results of Datalogger Independence Study

<table>
<thead>
<tr>
<th>Datalogger ID</th>
<th>NaBr Concentration (mg/L)</th>
<th>EC2</th>
<th>EC3</th>
<th>EC4</th>
<th>EC5</th>
</tr>
</thead>
<tbody>
<tr>
<td>EM3931</td>
<td>100</td>
<td>1.26</td>
<td>1.28</td>
<td>1.22</td>
<td>1.29</td>
</tr>
<tr>
<td></td>
<td>500</td>
<td>6.05</td>
<td>5.82</td>
<td>6.07</td>
<td>5.94</td>
</tr>
<tr>
<td></td>
<td>1000</td>
<td>11.36</td>
<td>10.98</td>
<td>12.31</td>
<td>10.90</td>
</tr>
<tr>
<td>EM6403</td>
<td>100</td>
<td>1.25</td>
<td>1.28</td>
<td>1.22</td>
<td>1.28</td>
</tr>
<tr>
<td></td>
<td>500</td>
<td>5.86</td>
<td>5.82</td>
<td>6.10</td>
<td>5.91</td>
</tr>
<tr>
<td></td>
<td>1000</td>
<td>11.41</td>
<td>10.86</td>
<td>12.40</td>
<td>10.91</td>
</tr>
<tr>
<td>EM6411</td>
<td>100</td>
<td>1.24</td>
<td>1.26</td>
<td>1.22</td>
<td>1.28</td>
</tr>
<tr>
<td></td>
<td>500</td>
<td>5.93</td>
<td>5.84</td>
<td>6.10</td>
<td>5.88</td>
</tr>
<tr>
<td></td>
<td>1000</td>
<td>11.26</td>
<td>10.83</td>
<td>12.31</td>
<td>10.85</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>R²</th>
<th>0.999</th>
<th>0.999</th>
<th>1.000</th>
<th>0.998</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normalized st.dev. @ 100mg/L</td>
<td>0.007</td>
<td>0.008</td>
<td>0.001</td>
<td>0.004</td>
</tr>
<tr>
<td>Normalized st.dev. @ 500mg/L</td>
<td>0.016</td>
<td>0.002</td>
<td>0.003</td>
<td>0.005</td>
</tr>
<tr>
<td>Normalized st.dev. @ 1000mg/L</td>
<td>0.007</td>
<td>0.008</td>
<td>0.004</td>
<td>0.003</td>
</tr>
</tbody>
</table>

Measured electrical conductivity was deemed adequately independent of the datalogger used; results are seen in Table 3.2. Standard deviation of the measured electrical conductivity at each concentration point was taken across the 3 dataloggers tested. This

44
standard deviation value was then normalized by the average value of electrical conductivity measured by the 3 dataloggers. The Pearson coefficient ($R^2$) value is also listed in Table 3.2 showing that a good linear fit is achieved across the 3 dataloggers.

To ensure the dilution sets were accurate to the target concentration values of 100, 500, and 1000 mg/L, a grab sample was taken from each and analyzed with a Dionex DX-600 Ion Chromatograph. Ion chromatography (IC) quantifies ion concentrations by using an ion exchange resin to separate different ions present within a solution sample, and then quantify them individually with a detector. The bromide ion concentrations from the chromatography analysis were used to calculate an upper and lower value range at a 95% confidence interval for each target concentration value. The results are presented in Table 3.3, and show that the calibration dilution standards were quite accurate.

### Table 3.3: 95% Confidence Interval Range for NaBr Dilution Sets

<table>
<thead>
<tr>
<th>Target Concentration (mg/L)</th>
<th>Lower Limit (mg/L)</th>
<th>Upper Limit (mg/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>99.6</td>
<td>100.4</td>
</tr>
<tr>
<td>500</td>
<td>499.1</td>
<td>500.2</td>
</tr>
<tr>
<td>1000</td>
<td>998.1</td>
<td>1001.9</td>
</tr>
</tbody>
</table>

To eliminate concerns that the EC sensors and their calibration may be affected by the synthetic aquifer wells and sand, calibrations were done on a few sensors to investigate this possible issue. The sensors were immersed in 100, 500, and 1000 mg/L aqueous solutions from the 5th calibration standard set. First the sensors were emplaced in an extra PVC well which did not have a stainless steel mesh cover. Next the sensors were emplaced in another well which did have a stainless steel mesh cover. Finally the sensors were emplaced in a stainless steel mesh covered well that was surrounded by synthetic aquifer sand. All three of these bench experiments resulted in the same calibration curve as the base sensor calibration. Therefore it was concluded that the presence of the PVC, stainless steel mesh, and aquifer sand did not impart a charge effect which would affect the EC sensor readings.
CHAPTER 4
NUMERICAL MODELING OF PHYSICAL SYSTEM

The following chapter provides an overview of how numerical simulation codes were employed to aid in the design of the synthetic aquifer and help develop physical test configurations of relevance to WSN technology development.

4.1 Introduction

Numerical modeling of the synthetic aquifer was an integral part of this investigation from the beginning. Subsurface head and flow analysis was conducted using the simulation software MODFLOW-2000 and tracer transport was modeled using the code MT3DMS. Inverse modeling and calibration of the flow models was conducted using UCODE-2005, calibration of the transport models is addressed in Chapter 5.

Having constructed the tank, it was then necessary to advance it into a synthetic aquifer capable of creating plumes relevant to WSN technology development. Numerical modeling was used to investigate any actions prior to employing them on the physical synthetic aquifer. The tasks of:

- packing the synthetic aquifer
- performing flow experiments of several configurations to check aquifer operation
- compare flow models to experimental flow measurements
- calibrate flow models based on experimental observations
- create complex plume configurations which test WSN and real-time model calibration capabilities

are discussed throughout this chapter along with the lessons learned during the process.
4.2 Synthetic Aquifer Sand Packing and Initial Calibration

Prior to packing the experimental tank with aquifer sand a study was conducted to investigate the effects of aquifer depth and hydraulic gradient. The results of this study were used to establish the sand depth and difference in hydraulic head between the supply and drain side reservoirs in the synthetic aquifer. This modeling used uncalibrated parameters for the sand as listed in Table 3.1, and only solved for hydraulic head and flow using MODFLOW-2000. The reservoirs were modeled as a constant head value along the entire transverse width of the aquifer and no wells were included. A computational cell size of 1.27 cm x 1.27 cm (0.5 inch x 0.5 inch) was used resulting in a grid domain size of 193 cells in the transverse direction and 339 cells in the longitudinal direction and 1 cell layer thick. The sand was assumed to be fully homogeneous and isotropic.

A matrix of simulations was created where the aquifer thickness was varied from 10.16 cm to 40.64 cm in 5.08 cm increments (4 – 16 inches in 2 inch increments), while the change in hydraulic head across the length of the aquifer varied in increments of 2.54, 3.81, 6.35, 8.89, and 10.16 cm (1, 1.5, 2.5, 3.5, and 4 inches). Figure 4.1 plots the resulting aquifer discharge calculated from these simulations in units of liters per day. Each curve represents results at a constant head drop value. The condition of a 10.16 cm aquifer depth with a corresponding 10.16 cm head drop across the aquifer represents an untenable physical test situation and therefore was not modeled.

Figure 4.2 displays the travel time it would take for a packet of water to move through the synthetic aquifer from the supply side reservoir boundary to the drain side reservoir boundary. Having an estimate of aquifer travel time was essential from a project management point of view. Experiments needed to be completed in a reasonable amount of time while allowing time for stabilization of the flow field in between experiments. An experiment duration time of approximately 10 days was deemed acceptable, and therefore based on the data seen in Figure 4.2, an aquifer depth of 36.83 cm was selected along with a hydraulic head drop of approximately 9.9 cm from supply to drain reservoirs.
Figure 4.1: MODFLOW simulation of synthetic aquifer discharge with varying hydraulic gradients and aquifer thicknesses.

Figure 4.2: Synthetic aquifer travel times based on MODFLOW analysis at varying hydraulic gradients and aquifer thicknesses.
For all the conditions modeled, the maximum value of Reynolds number based upon the mean particle diameter for #70 sand was $8.313 \times 10^{-4}$, well below a value of 1.0; therefore it could be assumed that the synthetic aquifer flow will be laminar and that Darcy’s Law and the DuPuit Approximation are applicable. An empirical relationship due to Neuman and Zhang (1990) was used to estimate the synthetic aquifer’s apparent dispersivity.

\[ \alpha_m = 0.0175 (L_s)^{1.46} \]  

(4.1)

Using the total aquifer length for $L_s$, results in an apparent dispersivity value of $\alpha_m = 122.13$ cm. Ignoring chemical diffusion, the Peclet number can then be estimated by equation 4.2.

\[ P_e = \frac{L_s}{\alpha_m} \]  

(4.2)

Resulting in a full length synthetic aquifer Peclet number of 3.515, indicating transport by both advection and dispersion will be significant.

Once the synthetic aquifer was completed and ready for its first operational condition, it was set up so that the supply side water level was a few millimeters below the top of the sand and the drain side head was 9.9 cm below the supply side. All reservoirs were open. The aquifer was allowed to come to steady state conditions and upon achieving this, head pressure readings were taken in all of the wells and reservoirs along with the volumetric outflow rate. The MODFLOW model was updated to represent each bank of reservoirs as closely to the physical aquifer as possible. A 2 cell wide (2.54 cm) no-flow wall existed between each reservoir and the spacers at either end of the reservoir rows was modeled as a no-flow wall boundary. Wells were represented as a 3x3 matrix of cells. Throughout this study the well’s hydraulic conductivity was established as a parameter defined to be equal to 1000 times the sand field hydraulic conductivity. The first and last longitudinal cells were established as an inlet and outlet zone respectively. By doing this the inlet and outlet would have their own unique
hydraulic conductivity value associated with them. This was done to allow for any effects of the reservoir screen.

UCODE coupled to MODFLOW was employed to calibrate the updated model. The measured reservoir head values were inputted as constant head boundary conditions, while the hydraulic conductivity of the inlet, outlet, and bulk sand field were the parameters to be optimized by the inverse modeling. The 44 well heads and the outflow rate were used as observation data in the calibration. The results of the calibration modeling are seen in Table 4.1. It is noted that the calibrated value for the bulk sand field is approximately double the published value for #70 sand, indicating the synthetic aquifer is not optimally compressed. The published value for #70 sand was obtained from column experiments which achieve a high degree of uniform sand compaction. The synthetic aquifer packing has likely led to greater sand compaction with depth due to the mass of the overburden. Also of note is that the inlet and outlet zones have a significantly reduced hydraulic conductivity indicating that the stainless steel mesh is acting as an additional resistance to flow and should be accounted for when modeling an experimental sand tank.

<table>
<thead>
<tr>
<th>Parameter Zone</th>
<th>Hydraulic Conductivity (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>#70 Sand (column values)</td>
<td>1.41x10^{-2}</td>
</tr>
<tr>
<td>Calibrated Bulk Sand Field</td>
<td>2.80x10^{-2}</td>
</tr>
<tr>
<td>Inlet</td>
<td>9.56x10^{-4}</td>
</tr>
<tr>
<td>Outlet</td>
<td>5.66x10^{-3}</td>
</tr>
<tr>
<td>Wells (1000*Bulk Sand)</td>
<td>28.03</td>
</tr>
</tbody>
</table>

Because the inverse modeling indicated that the aquifer sand pack compression was less than ideal the sand porosity was recalculated. Packing the aquifer with sand to a depth of 36.83 cm required 124 bags of #70 sand which have a nominal mass of 45.36 kg. The total volume of the synthetic aquifer can be calculated and dividing the packed sand
mass by the total volume gives the aquifer bulk density. The porosity of the aquifer can then be estimated from the following equation.

\[
\phi = 1 - \frac{\rho_b}{\rho_p}
\]

where:
- \(\phi\) = porosity (-)
- \(\rho_b\) = bulk density (ML\(^{-3}\))
- \(\rho_p\) = particle density (ML\(^{-3}\))

Assuming a particle density for silica sand of 2.634 g/cm\(^3\) the porosity and overall mass of the saturated aquifer can be calculated. Table 4.2 summarizes these calculated values.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk density (g/cm(^3))</td>
<td>1.459</td>
</tr>
<tr>
<td>Particle density (g/cm(^3))</td>
<td>2.634</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.446</td>
</tr>
<tr>
<td>Sand mass (kg)</td>
<td>5,624.5</td>
</tr>
<tr>
<td>Pore water mass (kg)</td>
<td>1,712.0</td>
</tr>
<tr>
<td>Total aquifer mass (kg)</td>
<td>7,336.5</td>
</tr>
<tr>
<td>Total aquifer weight (tons)</td>
<td>8.09</td>
</tr>
</tbody>
</table>

Note from Table 3.1 the column experiment porosity value for #70 sand is equal to 0.418, while the synthetic aquifer estimate is 0.446 further indicating a less than optimal sand compaction within the aquifer.
4.3 Complex Flow Patterns

The synthetic aquifer inlet and outlet reservoir systems were developed with the expectation that complex flow patterns could be created in the laboratory. These complex flows are characterized by plume transport which varies in speed and direction of travel as it moves through the synthetic aquifer domain. Plumes which split into multi-modal lobes and then recombine into a single mode were also desired. Plume transport characteristics such as these are relevant to contaminant plumes seen in the field where subsurface heterogeneities or sorption processes can result in similar transport behaviors. As the synthetic aquifer is comprised of a homogeneous media, hydraulic control or non-porous obstructions were used to create these complex flow patterns.

Numerical modeling was used to investigate complex flow capability. Flow configurations were develop numerically by modeling the reservoirs of the synthetic aquifer as being open or closed to flow. Subsurface flow configurations of interest would then be recreated in the physical synthetic aquifer facility. Numerous configurations were modeled, however only the ones that were run experimentally in the synthetic aquifer will be discussed.

4.3.1 Baseline Uniform Flow

The first flow configuration attempted both numerically and physically was as described in section 4.2. This configuration is referred to as the Baseline case and was created by having all reservoirs open to flow with a 9.9 cm drop in hydraulic head from the inlet to the outlet reservoirs. The calibrated aquifer hydraulic conductivities as listed in Table 4.1 were used to characterize the model. A color contour map of head pressure results from the MODFLOW model is seen in Figure 4.3. Well locations along with the centerline location of supply and drain reservoirs are also seen in this plot. A small head drop is seen at the supply corners, while a slight head increase is observed at the drain corners. This effect is due to the spacer walls at each transverse end of the reservoirs.
Figure 4.3: Head pressure contour plot of baseline flow configuration, results from a MODFLOW simulation.

For comparison, Figure 4.4 plots the experimentally measured head values taken from the synthetic aquifer centerline wells against the numerically modeled heads at the same locations. For each of the wells shown the difference between modeled and measured heads is either 1 or 2 millimeters. For all 44 wells in the synthetic aquifer, the average difference between modeled and measured heads is 1.3 millimeters with a maximum difference of 5 millimeters occurring at well W66.

For comparison to an analytical solution, apart from wall effects near the transverse boundaries, this flow configuration can be represented as a 1-dimensional unconfined aquifer with no recharge as analytically modeled by the classic DuPuit equation (Equation 3.3). Using the measured pressure heads and aquifer outflow rate, a DuPuit solution can be applied to determine the hydraulic conductivity of the synthetic aquifer. Table 4.3 lists the results obtained by applying the DuPuit equation across the entire aquifer from supply to drain reservoirs as well as across each row of wells. The mean head pressure across rows of wells or reservoirs was used for this solution. The hydraulic conductivity obtained from the numerical calibration process is also listed for comparison.
Figure 4.4: Centerline well heads for baseline flow configuration, comparison of measured to modeled values.

Table 4.3: Hydraulic conductivity calculated from DuPuit equation

<table>
<thead>
<tr>
<th>Head drop interval</th>
<th>Δ Pressure (cm)</th>
<th>Hydraulic conductivity (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>supply to well row 1</td>
<td>1.04</td>
<td>0.0184</td>
</tr>
<tr>
<td>well row 1 to well row 2</td>
<td>1.05</td>
<td>0.0268</td>
</tr>
<tr>
<td>well row 2 to well row 3</td>
<td>1.02</td>
<td>0.0279</td>
</tr>
<tr>
<td>well row 3 to well row 4</td>
<td>1.08</td>
<td>0.0278</td>
</tr>
<tr>
<td>well row 4 to well row 5</td>
<td>1.08</td>
<td>0.0287</td>
</tr>
<tr>
<td>well row 5 to well row 6</td>
<td>1.39</td>
<td>0.0226</td>
</tr>
<tr>
<td>well row 6 to well row 7</td>
<td>0.68</td>
<td>0.0490</td>
</tr>
<tr>
<td>well row 7 to well row 8</td>
<td>1.28</td>
<td>0.0270</td>
</tr>
<tr>
<td>well row 8 to drain</td>
<td>1.25</td>
<td>0.0231</td>
</tr>
<tr>
<td>average across all intervals</td>
<td>1.10</td>
<td>0.0279</td>
</tr>
<tr>
<td>supply to drain</td>
<td>9.87</td>
<td>0.0267</td>
</tr>
<tr>
<td>model calibration result</td>
<td>9.87</td>
<td>0.0280</td>
</tr>
</tbody>
</table>
There is a 4.75% difference between the hydraulic conductivity calculated by applying the DuPuit solution across the synthetic aquifer supply to drain (0.0267 cm/s) and the numerically calibrated hydraulic conductivity (0.0280 cm/s). While the column derived hydraulic conductivity value for #70 sand (0.0141 cm/s) is nearly exactly half the calibrated value.

4.3.2 Diagonal Flow

A subsurface flow which travels in a diagonal pattern across the synthetic aquifer was desired to demonstrate the capabilities of the test facility. A cross aquifer flow profile was created by leaving all 7 supply reservoirs open while closing all but the #7 drain reservoir. The resulting flow pattern, as seen from tracer transport modeling, can be described more as a curvilinear arc than a diagonal. This will be discussed in more detail in section 4.4.

A pressure head contour plot of the diagonal flow configuration, as simulated by MODLOW, is seen in Figure 4.5. A comparison of modeled to experimentally measured heads along the AA and BB transects seen in Figure 4.5 is plotted in Figure 4.6. The difference between modeled and measured values is more pronounced for the diagonal flow compared to the baseline flow. The average absolute difference between measured and modeled heads was 5.1 mm with a maximum difference of 8 mm occurring at wells W11 and W48. The measured centerline wells along transect AA show a distinct reduction in head-drop slope at wells near the closed drain reservoirs, while the BB transect measured values indicate a reverse trend with a change in slope near the supply reservoirs.
Figure 4.5: Head pressure contour plot of diagonal flow configuration, results from a MODFLOW simulation.

Figure 4.6: Heads for diagonal flow configuration, comparison of measured to modeled values along the AA and BB transects seen in Figure 4.5.
A third flow configuration was modeled which contained areas of non-porous inclusions. This configuration was intended to create a bi-modal plume which would split and recombine as it traversed the length of the synthetic aquifer. The experimental creation of a bi-modal plume was desired in order to simulate multi-lobed plumes observed at contaminated sites. It was also sought in order to provide an experimental data set for future WSN protocol development where wireless nodes will autonomously determine if a plume is splitting or recombining. The configuration was created by opening all of the supply and drain reservoirs as in the baseline configuration and adding 4 rectangular zones of very low hydraulic conductivity ($K = 1.0 \times 10^{-20}$ cm/s) as seen in Figure 4.7.

![Figure 4.7](image)

**Figure 4.7**: Schematic drawing of the synthetic aquifer demonstrating the location of the non-porous zones. Compass axes added for directional reference.

The three shorter rectangles each measure 26.67 cm in the aquifer longitudinal direction, and 36.83 cm in the transverse direction. The longer rectangle has the same longitudinal length and measures 116.84 cm in the transverse direction. In the physical synthetic
aquifer, the non-porous zones were created by inserting boxes constructed from PVC sheeting. The boxes were watertight sealed and had open tops for backfilling with aquifer sand and water so as to counteract buoyancy forces from the aquifer. The bottoms of the PVC boxes were fitted with gasket material to provide a watertight seal with the floor of the synthetic aquifer. The boxes extended well above the height of the aquifer sand. Figure 4.8 shows two of the smaller PVC boxes prior to installation and Figure 4.9 is a photo of the synthetic aquifer after installation of the non-porous PVC boxes. This photo was taken after installation of the wireless motes. It should be noted that all data acquisition presented in this work was conducted with sensors connected to dataloggers. The motes were installed as part of ongoing research efforts into wireless sensor network applications, modeling, and protocol development.

Figure 4.8: Two of the smaller PVC non-porous boxes prior to installation in the synthetic aquifer.
A head pressure contour plot based on the MODFLOW numerical model of the synthetic aquifer with non-porous zones is seen in Figure 4.10. Again a comparison of modeled to experimentally measured heads along the AA and BB transects seen in Figure 4.10 is plotted in Figure 4.11. The largest difference between experimental and modeled heads occurs at well W33 which lies on the aquifer centerline just in front of the long non-porous obstruction. The measured head in well W33 was 1.4 cm lower than the simulated value, indicating that the experimental flow split is asymmetric.

A corresponding head pressure contour plot for the physical synthetic aquifer, as developed by kriging the measured heads is seen in Figure 4.12. The equipotential lines seen here provide further evidence that the long non-porous obstruction generates an asymmetric flow pattern skewed more towards the southern end of the synthetic aquifer.
Figure 4.10: Head pressure contour plot of flow configuration with non-porous inclusions, results from a MODFLOW simulation.

Figure 4.11: Heads for non-porous region flow configuration, comparison of measured to modeled values along the AA and BB transects seen in Figure 4.10.
4.4 Tracer Plumes

Sodium bromide tracer plume transport through the synthetic aquifer was modeled using the numerical transport code MT3DMS. Only the one solute species was included in the analysis and it was treated as being fully conservative and non-reactive. In the physical synthetic aquifer, electrolyte tracer was introduced into the system by instantaneously adding a precisely measured mass of fine grained, solid sodium bromide to a supply reservoir. If tracer was being introduced to a single reservoir the solution in that reservoir would be kept continuously mixed by a paddle-type paint mixer attached to a stirring motor. Only one stirring motor was available so if tracer was to be introduced into multiple supply reservoirs a forced air bubbler system was placed at the bottom of the reservoir to maintain a constant mixing action.

Tracer would only be added to the synthetic aquifer after steady state flow operation had been verified. At steady state aquifer outflow, it can be assumed that a steady state
flow rate occurs into each supply reservoir and out into the aquifer inlet boundary screen. Each reservoir which has had the sodium bromide tracer added therefore can be modeled as a continuously stirred tank reactor. The tracer concentration will instantaneously spike at the moment of introduction and decay according to an exponential time function until no tracer is left. The tracer concentration decay function is:

\[
C(t) = C_0 \exp \left(-\frac{Q}{Vol} t \right)
\]

(4.4)

where:

- \(C(t)\) = tracer concentration as a function of time (ML\(^{-3}\))
- \(C_0\) = initial concentration added (ML\(^{-3}\))
- \(Vol\) = volume of reservoir (L\(^3\))
- \(Q\) = volumetric flow rate through reservoir (L\(^3\)T\(^{-1}\))

In MT3DMS the tracer decay was modeled in a stair-step fashion using 31 stress periods to exponentially decay the inlet concentration from the initial value down to zero concentration at the 31\textsuperscript{st} stress period.

All MT3DMS models used in this investigation employed the 3\textsuperscript{rd} order total variation diminishing (TVD) and implicit generalized conjugate gradient (GCG) solver options. The parameters of grid-scale dispersivities and aquifer porosity used in the forward models are listed in Table 4.4. The grid-scale longitudinal dispersivity value was estimated based on a factor of approximately 60% of the numerical grid size which was 1.27 cm in the longitudinal and transverse directions. The transverse and vertical dispersivity multipliers were initially set according to recommendations listed in the MT3DMS Users Guide (Zheng and Wang, 1999)

<table>
<thead>
<tr>
<th>Table 4.4: MT3DMS forward model parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>longitudinal dispersivity (cm)</td>
</tr>
<tr>
<td>transverse dispersivity (cm)</td>
</tr>
<tr>
<td>vertical dispersivity (cm)</td>
</tr>
<tr>
<td>aquifer porosity (-)</td>
</tr>
</tbody>
</table>
4.4.1 Centerline Plume

The first tracer flow modeled was a plume issuing from the center supply reservoir (S4). It was created to be a straight centerline plume with all supply and all drain reservoirs open, that is, the baseline subsurface flow configuration. Point in time color contour snapshots of the tracer numerical simulation and physical synthetic aquifer measurements are presented in this and subsequent sections. The color scales all refer to normalized concentration \( (C/C_0) \), where \( C_0 = 1000 \text{ mg/L} \) which was the initial tracer concentration used for all transport simulations and experiments. In the snapshots of the numerical simulation, wall sections between reservoirs and at the ends of the reservoir banks are shown as either white squares or white “X’s.” The longitudinal and transverse distance labels refer to the numerical grid number. Wells are depicted as white circles. The reservoirs are ordered sequentially and are labeled as follows, S1 – supply #1, S7-supply #7, D1 – drain #1, and D7 – drain #7.

A snapshot of the modeled tracer concentration taken at 12.5 hours after the instantaneous introduction of the sodium bromide is seen in Figure 4.13. The tracer plume is seen to have a long trailing section, or tail, due to the exponential decay of concentration at the reservoir inlet. The effect of the wells is clearly seen by a protrusion in the concentration contours resulting from the solute reaching the low flow resistance of the well interior.

In comparison, Figure 4.14 depicts a kriged contour plot of the normalized tracer concentration from the physical synthetic aquifer. This data was obtained from electrical conductivity sensors at a sample time 12.5 hours after sodium bromide was introduced to the S4 reservoir.

Similarly, Figure 4.15 is a snapshot of the MT3DMS simulation of the centerline plume 76.5 hours after tracer introduction. Figure 4.16 in comparison is a kriged contour plot of the tracer concentration measured by the in-well electrical conductivity sensors at 76.5 hours after tracer was introduced into the physical synthetic aquifer.
Figure 4.13: Animation of MT3DMS model of a centerline tracer plume. This snapshot is 12.5 hours after tracer introduction into reservoir S4. The white circles are well locations. The color scale is normalized concentration (C/C₀).

Figure 4.14: Contour plot of normalized NaBr tracer concentration (C/C₀) obtained by kriging measurements taken with EC sensors. Centerline plume, 12.5 hours after tracer introduction.
Figure 4.15: Animation of MT3DMS model of a centerline tracer plume. This snapshot is 76.5 hours after tracer introduction into reservoir S4. The white circles are well locations. The color scale is normalized concentration ($C/C_0$).

Figure 4.16: Contour plot of normalized NaBr tracer concentration ($C/C_0$) obtained by kriging measurements taken with EC sensors. Centerline plume, 76.5 hours after tracer introduction.
4.4.2 Diagonal Plume

Diagonal plume transport is important to this investigation because it is not dominated by a single advection and dispersion direction; instead it has significant longitudinal and transverse movement. From a modeling perspective, plume transport is often assumed to be axis-aligned; a diagonal plume will violate this assumption and provide a difficult test case for model calibration using WSN data. Diagonal plume movement will also prove to be a significant test case for the ultimate goal of an autonomous system which uses WSN data and real-time model calibration to predict plume transport behavior. Such a system which could accurately predict the transition from a predominately longitudinal transport to a predominately transverse one would be a dramatic advancement in technology.

The following 6 figures (Figure 4.17 – 4.22) compare MT3DMS simulation results of tracer flow to kriged contour plots derived from physical measurements taken with electrical conductivity sensors in the wells of the synthetic aquifer. The flow condition is the “diagonal” configuration as discussed previously. All 7 supply reservoirs are open to flow and only D7 drain reservoir is open to outflow. Sodium bromide tracer was added to supply reservoir S2. A preliminary numerical simulation released tracer in reservoir S1, however this simulation showed considerable wall effects as the plume migrated to the aquifer boundary and so this condition was not attempted experimentally in the synthetic aquifer.

Figures 4.17 and 4.18 represent the plume transport 25 hours after tracer introduction. Figures 4.19 and 4.20 depict the plume 116 hours after tracer introduction. The plume is seen to be curving towards the open D7 drain reservoir and the primary transport direction is transitioning from the longitudinal to transverse direction. Figures 4.21 and 4.22 show the plume 130 hours after tracer introduction, the plume is seen to be considerably stretched in the transverse direction. The plume seen in Figure 4.21 appears to be exiting the aquifer from drain reservoir D6; however this is not what is occurring. The plume becomes considerably diluted as it reaches reservoir D7 and so the exiting plume concentration does not appear in this color contour plot.
Figure 4.17: Animation of MT3DMS model of the “diagonal” tracer plume. This snapshot is 25 hours after tracer introduction into reservoir S2. The white circles are well locations. The color scale is normalized concentration ($C/C_0$).

Figure 4.18: Contour plot of normalized NaBr tracer concentration ($C/C_0$) obtained by kriging measurements taken with EC sensors. “Diagonal” plume, 25 hours after tracer introduction.
Figure 4.19: Animation of MT3DMS model of the “diagonal” tracer plume. This snapshot is 116 hours after tracer introduction into reservoir S2. The white circles are well locations. The color scale is normalized concentration (C/C₀).

Figure 4.20: Contour plot of normalized NaBr tracer concentration (C/C₀) obtained by kriging measurements taken with EC sensors. “Diagonal” plume, 116 hours after tracer introduction.
Figure 4.21: Animation of MT3DMS model of the “diagonal” tracer plume. This snapshot is 130 hours after tracer introduction into reservoir S2. The white circles are well locations. The color scale is normalized concentration ($C/C_0$).

Figure 4.22: Contour plot of normalized NaBr tracer concentration ($C/C_0$) obtained by kriging measurements taken with EC sensors. “Diagonal” plume, 130 hours after tracer introduction.
The next 6 figures (Figure 4.23 - Figure 4.28) depict the same diagonal subsurface flow configuration, however for this case the sodium bromide tracer solution was introduced at supply reservoirs S2 and S3. Numerical simulations of the previous scenario where tracer was released only from reservoir S2 indicated that the plume would intersect with relatively small number of the wells in the synthetic aquifer. Therefore a plume which was wider in the transverse direction was simulated. The same three snapshots as before are depicted, at times of 25, 116, and 130 hours after tracer introduction into the reservoirs, while MT3DMS simulations are compared to physical concentration measurements obtained in the synthetic aquifer.

Comparing the numerical simulation in Figure 4.23 to the experimental results from Figure 4.24, qualitatively it appears that the plume center of mass moves faster nearer to the centerline of the aquifer in the experimental result. This is seen in the contour plot of Figure 4.24, where the plume has just arrived at well W22 while the peak concentration measurement is obtained in well W32. The numerical simulation indicates that the opposite trend is occurring, showing the plume center of mass approaching well W22 before well W32.

At 116 hours after tracer introduction, as seen in Figures 4.25 and 4.26, the plume is more stretched in the longitudinal direction than in the previous case where tracer was introduced only in reservoir S2. Peak relative concentration as measured in the physical aquifer is seen to be nearly double of the peak value resulting from the numerical simulation.

From Figures 4.27 and 4.28, each at 130 hours after tracer introduction, it can be seen that numerical simulation indicates the leading edge of the plume is traveling faster that what experimental results indicate. The plume is seen exiting the D7 reservoir in the modeled snapshot, where as sensor measurements have just detected the arrival of the plume in well W58 and no sodium bromide was measured in the drain reservoirs. The experimental measurements also show that the tail of the plume remains resident in the aquifer longer than the numerical simulation indicates. No tracer is present in the wells of row 6 as predicted by the numerical simulation while significant tracer concentrations were physically measured in wells W26 and W36.
**Figure 4.23:** Animation of MT3DMS model of the “diagonal” tracer plume. This snapshot is 25 hours after tracer introduction into reservoirs S2 and S3. The white circles are well locations. The color scale is normalized concentration (C/C₀).

**Figure 4.24:** Contour plot of normalized NaBr tracer concentration (C/C₀) obtained by kriging measurements taken with EC sensors. “Diagonal” plume, tracer introduced in S2 and S3, 25 hours after tracer introduction.
Figure 4.25: Animation of MT3DMS model of the “diagonal” tracer plume. This snapshot is 116 hours after tracer introduction into reservoirs S2 and S3. The white circles are well locations. The color scale is normalized concentration (C/C₀).

Figure 4.26: Contour plot of normalized NaBr tracer concentration (C/C₀) obtained by kriging measurements taken with EC sensors. “Diagonal” plume, tracer introduced in S2 and S3, 116 hours after tracer introduction.
Figure 4.27: Animation of MT3DMS model of the “diagonal” tracer plume. This snapshot is 130 hours after tracer introduction into reservoirs S2 and S3. The white circles are well locations. The color scale is normalized concentration \((C/C_0)\).

Figure 4.28: Contour plot of normalized NaBr tracer concentration \((C/C_0)\) obtained by kriging measurements taken with EC sensors. “Diagonal” plume, tracer introduced in S2 and S3, 130 hours after tracer introduction.
4.4.3 Bi-Modal Plume

Numerical simulations and experimental measurements of the synthetic aquifer with the imbedded non-porous regions are depicted in the next 6 figures (Figures 4.29 – 4.34). This plume configuration was created by opening all supply and drain reservoirs to flow. The non-porous regions were created as described in section 4.3.3. This configuration was constructed with the intention of creating a single plume which would split into a bi-modal form as it transports through the synthetic aquifer and recombine to a single mode prior to exiting out of the drain reservoirs. Initial simulations showed that a wide plume would be easier to split into two lobes and would also intersect with more synthetic aquifer wells providing greater experimental data resolution. Ultimately the plume was created by releasing sodium bromide tracer into supply reservoirs S3, S4, and S5.

Figures 4.29 and 4.30 depict the plume 45 hours after tracer introduction. The numerical simulation in Figure 4.29 clearly shows how the plume is split by the first non-porous region and is further separated by the second region. The plume thins considerably as it is forced to go around the flow obstructions. The tracer also forms a boundary layer near the first obstruction where tracer slowly diffuses into the stagnant flow around the flat faces of the obstruction. This level of detail is missing from the well measured concentrations seen in Figure 4.30. Two plume lobes can be identified in Figure 4.30 however the kriging data analysis tends to connect well concentrations together. The size and exact location of the non-porous regions would not be readily identifiable from the kriged well data.

Figures 4.31 and 4.32 depict the plume 90 hours after tracer introduction. Both the numerical simulation and experimental data both show how the tracer tends to stay stagnant near the flat faces of the non-porous obstructions. Two distinct plumes are seen behind the large obstruction in the numerical simulation, whereas measured aquifer data indicates the plume has reformed into a single lobe by well row 5.

Figure 4.33 and 4.34 depict the plume 161 hours after tracer introduction. Maximum relative tracer concentrations are below 0.1 in both the numerical simulation and measured data, while at the same time discernable tracer concentrations can be detected throughout nearly the entire length of the aquifer.
Figure 4.29: Animation of MT3DMS model of the tracer plume with non-porous regions. This snapshot is 45 hours after tracer introduction into reservoirs S3, S4, and S5. The white circles are well locations. The color scale is normalized concentration (C/C₀).

Figure 4.30: Contour plot of normalized NaBr tracer concentration (C/C₀) obtained by kriging measurements taken with EC sensors. Non-porous regions plume, tracer introduced in S3, S4, and S5, 45 hours after tracer introduction.
Figure 4.31: Animation of MT3DMS model of the tracer plume with non-porous regions. This snapshot is 90 hours after tracer introduction into reservoirs S3, S4, and S5. The white circles are well locations. The color scale is normalized concentration \((C/C_0)\).

Figure 4.32: Contour plot of normalized NaBr tracer concentration \((C/C_0)\) obtained by kriging measurements taken with EC sensors. Non-porous regions plume, tracer introduced in S3, S4, and S5, 90 hours after tracer introduction.
Figure 4.33: Animation of MT3DMS model of the tracer plume with non-porous regions. This snapshot is 161 hours after tracer introduction into reservoirs S3, S4, and S5. The white circles are well locations. The color scale is normalized concentration (C/C₀).

Figure 4.34: Contour plot of normalized NaBr tracer concentration (C/C₀) obtained by kriging measurements taken with EC sensors. Non-porous regions plume, tracer introduced in S3, S4, and S5, 161 hours after tracer introduction.
4.5 Results and Discussion

The numerical simulation for the baseline flow as depicted in Figure 4.3 indicates a very uniform distribution of equipotential lines with only slight curving of the lines owing to corner boundary effects. The experimentally measured hydraulic head profile depicted in figure 4.35 for the baseline flow configuration shows some variability in the equipotential lines. This variability indicates that the synthetic aquifer sand field is less than perfectly homogeneous. Inconsistent sand packing and compression as well as air trapped in the sand pores are possible causes of some degree of heterogeneity within the aquifer.

Figure 4.35: Head pressure contour plot of baseline flow configuration. Contours were generated by applying a kriging technique to heads measured in the wells and reservoirs.

The application of the DuPuit equation to the baseline hydraulic heads measured in the synthetic aquifer as listed in Table 4.3 provides further indications of possible heterogeneity within the synthetic aquifer. Lower than average hydraulic conductivities were calculated from the inlet to well row 1 and from well row 8 to the outlet, this is
consistent with the UCODE inverse modeling results which predicted reduced hydraulic conductivity in a narrow band close to the reservoir screens. The DuPuit calculation also determined that the hydraulic conductivity in the band between well rows 6 and 7 is significantly greater than the hydraulic conductivity of the overall synthetic aquifer. This can be seen in Figure 4.35 as a wider section between equipotential lines in addition to wavier equipotential lines in the vicinity of well rows 6 and 7.

For the diagonal flow profile, numerical modeling as depicted in Figure 4.5 indicates very uniform equipotential lines which smoothly transition to an elliptical shape near the D7 drain reservoir. In contrast, the experimentally measured hydraulic heads as depicted in Figure 4.36 create equipotential lines which become more angled and do not fully curve until just before the D7 reservoir. This indicates that a tracer released from reservoir S2 would tend to stay on a longitudinal track and not begin to curve significantly before well row 7.

**Figure 4.36:** Head pressure contour plot of the diagonal flow configuration. Contours were generated by applying a kriging technique to heads measured in the wells and reservoirs.
In the case of the flow with the non-porous obstructions, the experimentally
determined equipotential lines are asymmetric near the large obstruction and appear to be
skewing the flow towards the higher numbered wells (towards the southern boundary as
seen in Figure 4.12).

In examining the tracer transport simulations and experimental results, several
observations can be made. First, from a purely qualitative observation of the
concentration plots, the center of mass of the plumes from measured experimental data
have progressed further into the aquifer than the numerically simulated plumes. This
would indicate that the simulation parameters which effect solute transport velocity,
particularly hydraulic conductivity and porosity, require a calibration effort to improve
their characterization. Hydraulic conductivity was determined through an inverse
modeling effort, employing hydraulic heads and volumetric outflow rates as measured
observations, therefore it is believed that hydraulic conductivity is adequately
characterized and so further inverse modeling efforts should focus on the porosity value.

The next observation from examining the tracer plume data is that the experimentally
measured relative concentrations are consistently greater than the values calculated by
numerical simulation. Two possible explanations for this effect are; excessive dispersive
forces in the simulated models or density sinking of the sodium bromide plume in the
wells of the physical synthetic aquifer. Comparing the plume spread and distribution
between numerically modeled results and experimentally measured results indicates that
excessive dispersion in the simulated models is not the cause of the discrepancy in plume
mass between modeled and measured data sets. The maximum sodium bromide tracer
concentration of 1000 mg/L was selected to ensure that density sinking did not occur in
the synthetic aquifer, however, this analysis was based on a purely homogeneous media
assumption and did not account for the free-flow of solution in the wells themselves.
Further examination of possible density sinking effects will be discussed in the next
chapter.

It can also be noticed that plume shape is not adequately depicted by kriging analysis
of the measured well concentrations. The synthetic aquifer has a fairly dense well
distribution but given the relatively narrow width of the plumes in the transverse
direction, a plume can easily pass between wells and not be detected by the emplaced sensors.

During the course of taking electrical conductivity sensor measurements in the synthetic aquifer, it was observed that data taken in the drain reservoirs was greatly affected by the placement of the sensor in the reservoir. An attempt was made to prevent the sensors from coming into contact with the reservoir screen to avoid any electrical interference between the sensor contacts and the stainless steel screen material. The drain reservoirs were not stirred and so solute density sinking in the reservoirs is a considerable risk. Also without reservoir stirring, preferential flow paths between the screen face and the reservoir exit port is likely. The drain reservoirs contain approximately 9 liters of water therefore dilution of the tracer as it exits the aquifer would have to be taken into account. For these reasons drain reservoir sensor readings should not be used for data analysis and should only be used to give an indication if tracer is still present in the aquifer.

4.6 Conclusions

The most significant conclusion to be drawn from the work presented in this chapter is that the synthetic aquifer is capable of performing the task for which it was designed; that is, as an experimental test bed for evaluation of WSN technologies. Complex, time and spatially variant subsurface plumes were created with single or bi-modal lobes as designed through numerical simulation.

Another significant conclusion is that the assumption that the synthetic aquifer is homogeneous and isotropic is not fully applicable. Variability in heads across well rows and asymmetric equipotential lines provide evidence that some degree of heterogeneity exists in the synthetic aquifer. Anisotropy between the longitudinal and transverse flow directions is also possibly occurring in the tank as evidenced by the diagonal plume. The experimental measurements from the diagonal plume show that the tracer remains close to the north wall longer than the isotropic numerical model predicts.
CHAPTER 5
SENSOR NETWORK DATA ACQUISITION IN THE SYNTHETIC AQUIFER

The following chapter discusses the use of a network of electrical conductivity sensors to track complex plume movement through the synthetic aquifer test facility. Data processing is discussed, followed by results from the experimental procedures which are compared to traditional well sampling methods. Various issues encountered during the experimentation and data processing will be addressed.

5.1 Introduction

The procedures and methods used when testing in the physical synthetic aquifer have been discussed in several sections of chapters 3 and 4. This chapter will discuss the physical tracer experimentation and the results in more detail.

Sodium bromide tracer plumes were created in the synthetic aquifer by instantaneously releasing NaBr into well mixed supply reservoirs. The movement of the NaBr plume through the synthetic aquifer can be tracked by the increase in electrical conductivity of the aquifer solution due to the ionized tracer. To measure this effect Decagon 5TE electrical conductivity (EC) sensors were placed in the synthetic aquifer wells and reservoirs. Sensor readings were taken once every half hour and recorded with Decagon EM50 dataloggers. The synthetic aquifer instrumented with EC sensors and dataloggers is seen in Figure 5.1.

Each sensor was individually calibrated to relate measured electrical conductivity to equivalent NaBr concentration in Millipore deionized water. The water supplied to the synthetic aquifer had its own background level of electrical conductivity which had to be subtracted from the EC sensor data to obtain the pure NaBr concentration levels.
Traditional field or laboratory testing methods would entail the collection of grab samples which are then analyzed in a laboratory. The use of sensor networks aim to provide data which has much greater temporal resolution compared to sampled data and can be analyzed and interpreted on a real-time basis.

5.2 Manual Aqueous Samples

Solution grab samples were taken from the synthetic aquifer wells and reservoirs by pipette extraction. A section of vinyl tubing was added between a manual pipette filler and a pipette so that it could reach the full length of the well. The extended pipette was marked so that extraction of grab samples would occur at the same depth as the location...
where the EC sensors take their measurement. Each sample was placed into a 2 ml sample vial and capped for analysis with a Dionex DX-600 Ion Chromatograph. The ion chromatograph (IC) results required calibration to relate the bromide ion conductivities determined by chromatography back to known sodium bromide dilution standards. The linear calibration factors determined for the EC sensor standards were used for all IC analyses. The IC analytical process separates out each ionic species present in a sample and concentration values can be determined for a specific chemical species, therefore sodium bromide concentration is determined uniquely and assuming there is no sodium bromide in the background water, no background concentration subtraction is required. Background aquifer samples were processed with each IC analysis and no bromide ions were ever detected in the aquifer supply water.

5.3 Tracer Plumes

Five tracer plume configurations were created in the synthetic aquifer. The following section examines the results obtained from the EC sensor network for the centerline plume configuration. A discussion of the results for the remaining 4 plume configurations is presented in Appendix A. The data is presented in graphical format as time series breakthrough curves. Breakthrough curves (BTC) labeled as “equivalent NaBr concentration” indicate that background electrical conductivity has not yet been subtracted from the measured data. BTC plots are separated according to well row within the synthetic aquifer.

5.3.0 Centerline Plume

The centerline plume configuration was run twice as a back to back repeat. No changes to the flow configuration were made in between the tracer runs. The following 9 figures (Figure 5.2 - 5.10) plot the equivalent NaBr concentration measured as a function of time for the first run. The data as presented in these 9 figures is unprocessed other.
than the conversion of the directly measured electrical conductivity to NaBr concentration. It was left unprocessed to demonstrate the issues of step-function spikes and data drift which are discussed in detail in section 5.4.

The exponential decay character of NaBr in the S4 supply reservoir is clearly evident in Figure 5.2. A mass of NaBr was added to produce a maximum aqueous concentration in the supply reservoir of 1000 mg/L; however the EC sensor sampling rate of once every half hour failed to measure this peak value. Temporal resolution of the measurements proved to be quite adequate for tracking plume movement and BTC characteristics.

![Centerline Plume Run 1: Tracer Decay in Supply Reservoir](image)

**Figure 5.2:** Equivalent NaBr concentration decay trend for the centerline plume configuration, run 1, decay in supply reservoir S4.

Figure 5.3 shows the tracer concentration as it moves through the centerline well in well row #1, which has well ID W31. The dramatic concentration reduction spike occurring at approximately 115 hours elapsed time is attributed to a datalogger read error. A key feature of the W31 BTC plot is the rapid increase in NaBr concentration at the leading edge of the plume. The concentration shows a moderate rate of increase for a few hours and then increases at a near vertical rate slope till achieving a peak level. This
dramatic increase in tracer concentration is seen in subsequent plots whenever the NaBr plume center of mass intersects a well. Following the BTC peak, the plot begins to exhibit a long-tailed reduction in concentration typical of a conservative, dispersive tracer media. But instead of following a power-law type decay down to background levels of equivalent NaBr concentration, the concentration begins to oscillate. The tracer concentration continues to have an overall decaying trend, but with short-term oscillations. Tracer density effects are theorized as being the cause of this oscillatory behavior. Wells W21 and W41 are outside of the path of the plume and so only show some drift in background concentration measurements.

![Figure 5.3](image.png)

**Figure 5.3:** Equivalent NaBr concentration BTC for the centerline plume configuration, run 1, well row 1.

Concentration measurements for well row #2 are seen in Figure 5.4. Wells W32 and W42 straddle the centerline of the synthetic aquifer. A distinct BTC for well W32 can be seen, but none is evident for well W42, indicating that the plume is not fully symmetric. The rise in W32 concentration is approximately 35 mg/L over background levels therefore it can be assumed that only the lateral end of the plume contacts well W32 and
the plume boundary just misses well W42. A considerable amount of background concentration drift is observed in this figure along with a dramatic step-like spike in concentration measured in well W32. These phenomena will be discussed in a later section.

**Figure 5.4:** Equivalent NaBr concentration BTC for the centerline plume configuration, run 1, well row 2.

The remaining figures for the centerline plume case show similar trends as just addressed. The odd numbered well rows, which have a well at the synthetic aquifer centerline, lie in the path of the tracer plume center of mass, and so show a dramatic, rapid increase in concentration at the leading edge of the BTC. This rapid increase in concentration is likely due to the free flow of solution within the well, with a possible additional effect due to density sinking of the NaBr electrolyte in the free flowing solution. The even numbered well row plots beginning with row #4 show BTC at the 3rd and 4th wells indicating that the plume has spread in the transverse direction and now comes into contact with the wells which straddle the synthetic aquifer centerline. Background EC drift and step-like spikes are frequently seen throughout this data set.
Figure 5.5: Equivalent NaBr concentration BTC for the centerline plume configuration, run 1, well row 3.

Figure 5.6: Equivalent NaBr concentration BTC for the centerline plume configuration, run 1, well row 4.
Figure 5.7: Equivalent NaBr concentration BTC for the centerline plume configuration, run 1, well row 5.

Figure 5.8: Equivalent NaBr concentration BTC for the centerline plume configuration, run 1, well row 6.
Figure 5.9: Equivalent NaBr concentration BTC for the centerline plume configuration, run 1, well row 7.

Figure 5.10: Equivalent NaBr concentration BTC for the centerline plume configuration, run 1, well row 8.
The next nine figures (Figure 5.11 – 5.19) display comparisons between run 1 and run 2 for the centerline plume configuration. The data sets from run 1 and run 2 are labeled as R1 and R2 respectively. The BTC plots have been adjusted to absolute NaBr concentrations with the time scales matched to the instant of tracer introduction to provide a one-to-one comparison of the data.

Figure 5.11 plots the decay of tracer in the S4 supply reservoir. Grab samples were taken from reservoir S4 during centerline plume run 2 and analyzed in the ion chromatograph (IC) discussed previously. The IC grab sample data is plotted along with the EC sensor derived concentration data from both runs. An exponential curve fit was applied to the decay data which resulted in the decay rate coefficients listed in Table 5.1.

<table>
<thead>
<tr>
<th>Data Set</th>
<th>Exponential Decay Rate (1/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Run 1 EC sensor data</td>
<td>0.13069</td>
</tr>
<tr>
<td>Run 2 EC sensor data</td>
<td>0.12877</td>
</tr>
<tr>
<td>IC grab sample data – run 1</td>
<td>0.14386</td>
</tr>
<tr>
<td>IC grab sample data – run 2</td>
<td>0.14683</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Difference Analysis</th>
<th>% Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>% Difference EC run 1 to run 2</td>
<td>1.48</td>
</tr>
<tr>
<td>% Difference IC run 1 to IC run 2</td>
<td>2.04</td>
</tr>
<tr>
<td>% Difference means of IC and EC data</td>
<td>11.35</td>
</tr>
</tbody>
</table>

The decay rate as measured by EC sensors is very repeatable between runs 1 and 2 with a percent difference between the two of 1.48%. The IC processed grab sample data results in a significantly larger decay rate which has an 11.35% difference between the means of the IC acquired data to the EC measured data. The grab sample data measures a higher peak NaBr concentration than the EC sensor data and grab sample collection terminated too early to achieve an adequate curve fit at low concentration levels. The higher peak concentration values measured by the IC samples would tend to skew the decay curve fit and this likely leads to the higher calculated decay rate.
Well row 1 BTC are compared between runs 1 and 2 in Figure 5.12. From a qualitative sense, repeatability appears to be excellent in centerline well W31 until the point when concentration oscillations begin. The fact that oscillatory behavior itself repeats is a significant finding and it is noted that oscillations begin at nearly the same elapsed time and concentration values. The oscillations also have a very similar frequency between runs 1 and 2; however run 2 concentrations decline at a steeper rate.

Well row 2 comparisons are seen in Figure 5.13. No tracer is detected in well W42 in either run, whereas a distinct BTC is seen in well W32 for both runs. The peak concentration in W32 from run 2 is approximately 60% greater than the run 1 peak value. The run 2 BTC is also much wider than run 1 indicating either greater transverse movement or transverse dispersivity for run 2. Transport time of the center of mass for the two BTC appears to repeat very well. Some concentration rebound is noted in the tail of each curve and is likely due to the oscillations seen in well W31.
**Figure 5.12**: NaBr concentration BTC for the centerline plume configuration, comparing the repeatability of runs 1 and 2, in well row 1.

**Figure 5.13**: NaBr concentration BTC for the centerline plume configuration, comparing the repeatability of runs 1 and 2, in well row 2.
Centerline well W33 comparisons are seen in Figure 5.14. BTC characteristics repeat quite well, except for the peak concentration value is lower for run 2 resulting in a smaller total mass of NaBr moving through well W33. The decrease in peak concentration and total mass in W33 run 2 could support the hypothesis that an increase in transverse dispersive movement led to the increased concentration in well W32 run 2. The step BTC leading edge is continuing to be seen in centerline wells, whereas no oscillatory trends are observed at the BTC tails.

Repeatability between the centerline plume runs 1 and 2 breaks down further at well row 4 as seen in Figure 5.15. Tracer transport times repeat fairly well however peak concentrations and BTC total mass is seen to be greater for run 2 in both wells W34 and W44. As these two wells straddle the synthetic aquifer centerline, transverse dispersion is more likely the driving force. Transverse advection would tend to move the plume towards one off-center well or the other. This data indicates plume spreading in both directions away from the centerline.

Figure 5.14: NaBr concentration BTC for the centerline plume configuration, comparing the repeatability of runs 1 and 2, in well row 3.
**Figure 5.15**: NaBr concentration BTC for the centerline plume configuration, comparing the repeatability of runs 1 and 2, in well row 4.

Figures 5.16 – 5.18 continue to exhibit these trends, with centerline wells seen in the odd numbered well rows repeating fairly well between runs 1 and 2 except for a reduction in peak concentration and overall mass for run 2. While peak concentrations and total mass are greater in the centerline straddling wells for run 2. BTC characteristics of transport time and general curve shape repeat well between the two runs.

Well row 8 as seen in Figure 5.19 indicates transverse advection is shifting the plume towards well W38. A significantly greater concentration of NaBr is measured in the off-center well W38 than would be expected from the data seen in the preceding well rows. Additionally significantly lower concentrations were measured in well row W48 indicating the plume has shifted from centerline towards well W38.

BTC results for the other plume configurations can be seen in Appendix A, which contains sections: A1-Diagonal Plume Introduced in Reservoir S2, A2-Diagonal Plume Introduced in Reservoirs S2 and S3, A3-Wide Centerline Plume, and A4-Bi-Modal Plume.
Figure 5.16: NaBr concentration BTC for the centerline plume configuration, comparing the repeatability of runs 1 and 2, in well row 5.

Figure 5.17: NaBr concentration BTC for the centerline plume configuration, comparing the repeatability of runs 1 and 2, in well row 6.
Figure 5.18: NaBr concentration BTC for the centerline plume configuration, comparing the repeatability of runs 1 and 2, in well row 7.

Figure 5.19: NaBr concentration BTC for the centerline plume configuration, comparing the repeatability of runs 1 and 2, in well row 8.
5.4 Electrical Conductivity Sensor Issues

Several issues were encountered while tracking the sodium bromide tracer plumes with a network of electrical conductivity sensors. A lack of available sensors was a manageable inconvenience; however it led to some inefficiency and prevented fully automatic data processing. The synthetic aquifer contains 44 wells and 14 reservoirs plus the two constant-head devices for a total of 60 possible measurement locations. This project had 38 sensors available for data acquisition, which generally provided adequate coverage of the wells and sensors. For some plume configurations the sensors were moved from one location to another during the course an experiment. If interpretation of the sensor data indicated that a specific well was outside of the plume boundary or that the plume had fully passed by a well or reservoir; then the sensor in that well or reservoir was moved to a new measurement location. This process was financially beneficial as it increased sensor utilization and reduced overall sensor costs for the project. It did require greater diligence with data processing and analysis to ensure measured data corresponded to the correct measurement location.

The calibration accuracy and the stability of the electrical conductivity measurements were also of concern and possible sources of error. Two main stability issues were encountered with the EC data, step-like measurement spikes and data drift. While the accuracy of the sensor calibrations was questioned because background measurements between sensors were not equivalent under equivalent conditions. Additionally IC grab samples taken from tracer supply reservoirs consistently measured peak concentrations that were significantly greater than the peak concentration values calculated from EC sensor data.

5.4.1 Electrical Conductivity Spikes

The first use of the EC sensors after calibration was the centerline plume experiment in the synthetic aquifer. The data frequently exhibited a sudden and dramatic shift in electrical conductivity which was not due to electrolyte tracer flow through the aquifer.
The W32 plot shown in Figure 5.20 provides an illustrative example of this phenomenon. In the time series plot for well W32 a distinct BTC is observed followed by two small scale downward shifts and then a dramatic step-function-like increase in the electrical conductivity. The background EC in well W32 is seen to be drifting downward at a rate comparable to the drift seen in well W42 until after the large step increase. After the step, EC in well W32 becomes fairly steady and after some time begins to drift upwards.

These spikes in measured EC values were problematic for data analysis. An automated procedure was desired to subtract out the background conductivity and bring different experimental data sets to a common base point for comparison, but the EC spikes made this nearly impossible. Manual manipulation of the data was required to isolate BTC trends and process the measured data into a usable format. The spikes in EC data also made it difficult to discern if a change in the measured value was a real effect or a sensor error.

**Figure 5.20:** Electrical conductivity measurements from the centerline plume experiment run #1. Example data set to demonstrate EC measurement issues.
5.4.2 Electrical Conductivity Drift

Figure 5.20 also demonstrates the issue of EC drift. The data sets from both W32 and W42 show significant downward drift in the background EC readings, which was thought to be a real effect caused by drift in the EC of the water supply. When the drift slope would change dramatically after an EC spike, as seen in W32, it was unknown which effects were real and which were due to sensor error. An accurate measurement of the background electrical conductivity was vital in order to subtract this value from tracer BTC and determine the NaBr concentration.

Fortunately the EC spikes became less severe and less frequent over time. The cause of the EC spikes and why they dissipated over time is not known. The downward drift in background EC measurements continued through late winter and spring. It is believed that snowpack runoff into the surface water sources which supply the local municipal water utility is the cause for the reduction in background water electrical conductivity. The background EC values remained relatively constant and low through the months of May and June and then began to increase in July.

A linear curve fitting method was developed to account for drift in the background EC measurements. Once a complete EC sensor data set had been collected for an experimental run, a linear least squares slope and intercept was calculated based on data measured at the beginning and end of the data set. This provided a linear equation which calculated background EC as a function of time. The background levels were subtracted off of the measured values at each measurement point leaving only the values due to the NaBr tracer plume. This method would have some degree of inaccuracy due to the linear curve fit and would produce some negative concentration values, so a cut-off value of 2 mg/L was established. Any concentration value calculated to be less than the cut-off value was set equal to zero. This method provides a procedure for automatic processing of the EC sensor data assuming spikes in the data are minimal. For the early experiments where step-function spikes were common, the same linear method was applied but it required manually isolating a BTC and using only the data adjacent to it.
5.4.3 Sensor Calibration

Figure 5.20 presented the raw EC sensor data which was processed with a sensor specific, linear calibration curve fit to calculate the equivalent NaBr concentration data seen in Figure 5.21. Note that Figure 5.21 is a repeat of Figure 5.4. The equivalent NaBr concentrations calculated for wells W32 and W42 in Figure 5.21 ideally should have the same background levels, but as the plot demonstrates well W42 has a background concentration level approximately 30 mg/L higher than well W32, at least until the sensor spike is encountered. This trend is observable in all of the well rows presented in Figures 5.2 – 5.10. The EC sensor calibration, if accurate to an absolute scale, should have resulted in equivalent NaBr plots for wells within the same row which lied on top of each other except for when tracer electrolyte was detected. In the unprocessed results shown in Figures 5.2 – 5.10, most wells have a unique background concentration level. The slopes of the background concentrations within well rows are fairly consistent, indicating that the sensor calibration slopes are accurate while the intercept value may not be.

Figure 5.21: Equivalent NaBr measurements from the centerline plume experiment run #1. Example data set to demonstrate EC sensor calibration issue (repeat of Figure 5.4).
Further evidence of EC sensor calibration inaccuracy can be seen by re-examining Figure 5.11 which shows EC sensor data compared to IC analyzed grab samples. Both plots on this figure show that EC derived concentrations for NaBr match IC grab sample values very well for concentrations below 500 mg/L, while EC measurements fall below IC values at concentrations above 500 mg/L. The level of under prediction from EC measurements increases as the concentration increases. This trend can also be seen in reservoir decay plots from other plumes shown in Appendix A.

5.5 Tracer Density Effects

Based on the analysis presented in section 3.2.4, density sinking of the tracer plume as it moves through the synthetic aquifer should not have occurred, however several BTC plots demonstrated recession rebounds in concentration which indicated that density sinking was occurring. The critical density ratio as calculated by Equation 3.2 assumed a continuous, homogeneous porous media and did not take into account the free flow of solute in the wells of the synthetic aquifer. It is believed that density sinking, if occurring, only takes place in wells; however this will impact solute concentrations down gradient from any affected well.

To investigate if density sinking of the tracer plume was occurring, several wells were instrumented with two or three EC sensors. The normal procedure for EC sensor placement was to locate the sensor at the bottom of the well. The offset of the sensor’s measurement terminals would put the point of actual EC reading at approximately 4.5 cm above the floor of the synthetic aquifer. Multiple sensors in wells are designated by the well ID followed with a “d”, “m”, or “s” for deep, mid, or shallow respectively. The deep mounted sensors are in the standard position at the bottom of the well. Mid designated sensors are located at a well depth which is equivalent to the aquifer mid-thickness point. Shallow sensors are located at a depth were the water in the well just covers the top of the sensor at the base of the cable.

The following figures present the results obtained from wells containing multiple EC sensors for several tracer plume configurations. Figure 5.22 displays the NaBr
concentration measured in wells W26 and W27 at the standard deep sensor location and at a shallow sensor mounting depth. The tracer plume configuration for this figure is the diagonal flow with tracer released in the S2 supply reservoir. For both wells, the shallow mounted EC sensor measurements produce a BTC that matches the fundamental character of the deep mounted sensor BTC; however the peak concentrations measured at a shallow well are considerably reduced. Comparing to the deep mounted sensor, the peak concentration is reduced by 70% for the shallow depth sensor in well W26 and by 65% for the shallow depth sensor in well W37. The BTC arrival time at the sensor is also delayed by approximately 26 hours for the shallow mounted sensor compared to the deep mounted sensor.

Figure 5.23 presents a sensor depth comparison for well W22. This data was taken during the diagonal-S2S3 tracer plume experiment. The mid and shallow depths BTC are seen to be scaled down versions of the deep sensor BTC. Comparing to the deep mounted sensor, the peak concentrations are reduced by 22% for the mid-depth sensor and 33% for the shallow mounted sensor.

Figure 5.22: NaBr concentration BTC for the diagonal-S2 plume configuration, comparison of deep and mid depth sensor locations in wells W26 and W27.
Figure 5.23: NaBr concentration BTC for the diagonal-S2S3 plume configuration, comparison of deep, mid, and shallow depth sensor locations in well W22.

Figure 5.24 displays sensor depth comparisons for well number W32 at the diagonal-S2S3 plume configuration. Similar to the previous example, the mid and shallow depth sensor results appear as if they are scaled down versions of the deep mounted EC sensor results. Comparing to the deep mounted sensor, the peak concentrations are reduced by 46% for the mid-depth sensor and 60% for the shallow mounted sensor. The arrival front of the shallow depth sensor is not as steep as that seen in the mid and deep mounted sensors.

Similar trends are seen in Figure 5.25 which compares sensor depth measurements in well W23 again for the diagonal-S2S3 plume configuration. Comparing to the deep mounted sensor, the peak concentrations are reduced by 44% for the mid-depth sensor and 57% for the shallow mounted sensor. Again, the shallow depth sensor data shows a breakthrough curve concentration arrival front that is less steep than the mid and deep sensor fronts.
Figure 5.24: NaBr concentration BTC for the diagonal-S2S3 plume configuration, comparison of deep, mid, and shallow depth sensor locations in well W32.

Figure 5.25: NaBr concentration BTC for the diagonal-S2S3 plume configuration, comparison of deep, mid, and shallow depth sensor locations in well W23.
Figure 5.26 compares sensor depth concentration results in well W36 for the diagonal-S2S3 plume configuration. It can be seen the BTC shape characteristics are not as similar from one depth to the other as they were in previous sensor depth comparisons. The mid-depth BTC does not have as steep of an arrival front and the BTC from the deep sensor, while the shallow sensor BTC has a fundamentally different shape than the other two BTC presented. The mid and shallow depth BTC do not appear to be scaled down versions of the deep mounted sensor BTC as seen previously. Comparing to the deep mounted sensor, the peak concentrations are reduced by 51% for the mid-depth sensor and 68% for the shallow mounted sensor.

![Graph of Sensor Depth Comparison](image)

**Figure 5.26:** NaBr concentration BTC for the diagonal-S2S3 plume configuration, comparison of deep, mid, and shallow depth sensor locations in well W36.

Grab sample were taken in several wells which contained EC sensors at multiple depths. The following plots compare the results obtained from NaBr concentration measurements taken from these wells. All of the plots comparing EC sensors at different depths with grab samples are from an additional run of the bi-modal plume configuration. Figure 5.27 plots concentration values from a deep and mid depth EC sensor against IC
analyzed grab samples. The grab sample data set has a low level of temporal resolution compared to the sensor data which leads to missing key features of the tracer BTC. The IC grab samples appear to match the BTC recession of the mid depth sensor concentrations. Some of the oscillatory rebound effects are seen in the IC data, but not in the mid depth EC sensor data.

Arrows point out two locations where the taking of grab samples caused a noticeable reduction in tracer concentration in the deep mounted sensor. A direct correlation between grab sample timing and reduction in EC measured concentration was noticed in other wells. It is believed that insertion of the grab sample pipette causes mixing within the well affecting any concentration density stratification that may exist.

![Measurement Method Comparison](image)

**Figure 5.27:** NaBr concentration BTC for a repeat run bi-modal plume configuration, comparison of deep and mid depth EC sensors with IC grab samples in well W31.

Figure 5.28 shows a similar plot comparing concentration measurements taken in wells W24 and W54. It can be seen that the IC grab sample data corresponds well with the mid depth EC sensor measured concentrations.
Figure 5.29 displays a comparison of EC sensor data taken at deep and mid depths to IC grab sample concentrations in well W37. No discernable correlation between these three data sets can be identified.

**Figure 5.28:** NaBr concentration BTC for a repeat run bi-modal plume configuration, comparison of deep and mid depth EC sensors with IC grab samples in wells W24 and W54.

**Figure 5.29:** NaBr concentration BTC for a repeat run bi-modal plume configuration, comparison of deep and mid depth EC sensors with IC grab samples in well W37.
5.6 Observations and Conclusions

The size and scope of developing the CESEP synthetic aquifer is fairly unprecedented in laboratory scale research and as such, the initial experimental procedures presented in this chapter represent a significant gain in experiential knowledge on how to conduct subsurface experiments at this scale. Observations made during the course of these investigations are noted along with any conclusions that may be drawn.

The synthetic aquifer was packed with homogeneous sand with the objective of creating a porous media field that was fully homogeneous and isentropic. One of the conclusions of Chapter 4 was that the synthetic aquifer is less than ideally homogeneous, the results of the present chapter provides further evidence of this. Experimental measurements of head and temporal changes in tracer concentration show a small degree of non-uniformity and asymmetry exists within the synthetic aquifer. It would be difficult to quantify the degree of heterogeneity within the synthetic aquifer, but it can be concluded that some level of non-uniform flow results from these heterogeneities.

Density sinking of the tracer plume is likely occurring within the wells. EC sensors placed at mid and shallow well depths consistently measured electrical conductivities which were dramatically lower than values measured from sensors placed at the well bottom. The arrival time and BTC duration within a well were also highly dependent upon the sensors depth. The general shape of BTC within a well were often similar as the depth varied indicating that a method of moments based scaling factor may be appropriate for relating concentration data sets acquired at different depths.

Grab samples from wells were taken at the same depth as the EC sensor measurement point for the standard deep sensor location. This depth was used for all grab samples taken. An extended pipette was inserted into the well to extract each grab sample and it is likely that some depth-wise mixing occurred which would obscure any density sinking observations made based on IC measurements. As was noted in Figure 5.27, sudden, step-like reductions in tracer concentration could be directly correlated to the taking of grab samples which gives further evidence to density stratification within
the wells. Once this effect had been noticed, extra care was taken to prevent excess
disturbance of the well water when procuring grab samples.

The comparison of EC sensor data taken at mid and deep well locations to IC grab
sample concentrations indicates that it would probably have been preferable to mount the
EC sensors at the mid aquifer depth.

The tracer concentration data seen in Figure 5.29 shows no discernible correlation
between the three measurement methods used. The well in this figure is W37 which is a
centerline well located behind and down gradient of the large PVC obstruction. The
concentration measurements taken by the deep mounted EC sensor, W37-d, shows that
the bi-modal plume is recombining much sooner and at a much higher concentration than
numerical modeling predicts. Therefore it is speculated that tracer flow may be occurring
beneath the large PVC obstruction.

5.7 Implications to WSN Applications

The development of robust, automatic data processing and error checking protocols
would be a necessary step in the development of a WSN linked to real-time automatic
calibration of transport models. In the work presented here, considerable manual data
manipulation was required to extract useful plume BTC data from the raw sensor data.
An automatic system would need to:

- recognize real changes in sensor data due to contaminant transport
- identify background drift and account for any shift in sensor data
- provide sensor error detection and account for missing or faulty data.

Density sinking of the experimental tracer plume was shown to be a significant issue
in this study. For field application of a WSN similar issues could also be of concern.
Typical field extraction sampling involves removing a purge volume prior to extraction
of the sample. Careful attention to purge volume, sampling time and pumping rates is
recommended by Puls and Paul (1997) in order to extract a representative sample. A
WSN application would use emplaced sensors taking continuous sample data. If the
sensors were located in wells, then density effects or cross-depth mixing is likely to occur and needs to be accounted for in the data analysis.

Calibration of the EC sensors determined that a unique calibration slope and zero offset existed for each sensor. As the number of sensors employed in a WSN increases, issues related to unique sensor calibrations becomes more cumbersome. Performing a multi-point calibration of each sensor is time consuming; therefore for field application it is recommended that a WSN contain protocols for fixing the calibration with a single point reference measurement prior to installation of the sensor.
CHAPTER 6
TRANSPORT MODEL CALIBRATION AND PREDICTION

In Chapter 4, comparison of plume transport model results to measured tracer data indicated the need to calibrate the transport model input parameters of grid-scale dispersivity and porosity. This chapter presents a transport model calibration method suitable for application to a WSN and automatic model calibration system. The calibration methodology developed uses temporal method of moments analysis to characterize experimentally measured BTC. Calibrations were performed on the centerline plume configuration and the resulting parameter estimates were used as inputs in predictive numerical models of the other plume configurations. The results of these predictive models are compared to experimental results.

6.1 Introduction

Solute concentration break through curves as discussed in the previous chapter are equivalent to a probability density function (PDF) where the random variable is the measured concentration which can be cast as a function of time or space. As a result of examining concentration data as a PDF, the statistical properties of the BTC can be used as characterizing parameters in solute transport equations.

The moments of a PDF are related to its measures of central tendencies such as mean and variance. Similarly the moments of a solute tracer BTC are related to total solute mass, the mean position of the solute, and the degree of dispersion within the porous media.

Spatial moments analysis is frequently used to characterize subsurface plumes at the field scale (Adams and Gelhar 1992). This investigation uses temporal based moments to provide a characterization of sensor measured BTC. This characterization is then used as observation data for calibration of numerical transport models. Data provided by sensor networks has a high degree of temporal resolution. Employing a temporal moments
based method then takes advantage of this high temporal resolution with the underlying assumption that greater data resolution should lead to improved accuracy.

6.2 Solute Transport Model Calibration

Calibration of flow models of the synthetic aquifer were discussed in Chapter 4. The calibrations employed the numerical tool UCODE linked to a forward model of the synthetic aquifer created in MODFLOW for the purpose of determining hydraulic conductivity. Hydraulic heads and volumetric outflow were used as measured observations for the flow model calibrations. It was assumed that the calibrated flow models were valid and appropriate to use as input to the MT3DMS solute transport models. The calibration of solute transport models therefore use MODFLOW results as an input to MT3DMS.

Three input parameters were involved in the solute transport model calibration: grid-scale longitudinal dispersivity ($\alpha_{L-grid}$), grid-scale transverse dispersivity ($\alpha_{T-grid}$), and porosity ($\phi$). Temporal method of moments analysis was applied to EC sensor data to calculate two observation values per each well, these observations were: center of mass transport time ($\mu'_t$) and breakthrough curve scale dispersivity ($\alpha_{BTC}$).

6.2.1 Temporal Method of Moments

From a probability theory perspective the expectation of a continuous random variable can be expressed as:

$$E[X] = \int xf(x)dx$$  \hspace{1cm} (6.1)

where $x$ is a random variable in the sample space $X$ and $f(x)$ is a probability density function (PDF). For the case of a time series in solute transport, the random variable
sample space \((X)\) is replaced by a time variable and the PDF is replaced by solute concentration. Absolute temporal moments are then defined as (Govindaraju and Das, 2007):

\[
\mu_n = \int_0^\infty t^n C(z, t) dt
\]  

(6.2)

where \(\mu_n\) is the absolute temporal moment of order \(n\), \(t\) is time, and \(C(z, t)\) is solute concentration as a function of a length variable \(z\) and time. Normalized moments are defined as:

\[
\mu'_n = \frac{\mu_n}{\mu_0}
\]

(6.3)

and central moments as:

\[
m_n = \frac{1}{\mu_0} \int_0^\infty (t - \mu'_1)^n C(z, t) dt
\]

(6.4)

The zero order moment (when the subscript \(n = 0\)) equates to the total mass, and for a conservative solute tracer the normalized zero\(^{th}\) moment \(\mu'_0 = 1\), that is mass is conserved. The first normalized moment is a measure of the center of mass. For temporal based moments applied to BTC, as discussed here, the first normalized moment is the travel time of the center of mass for that BTC. The second normalized moment can be expressed as:

\[
m_2 = \mu'_2 - (\mu'_1)^2
\]

(6.5)

which is equivalent to the definition of the variance for a random variable. Following the derivation of Butters and Jury (1989), the coefficient of variation (CV) is:
\[ CV = \left( \frac{\mu'_2 \mu'_0}{(\mu'_1)^2} - 1 \right)^{\frac{1}{2}} \]  \hspace{1cm} (6.6)

and the dispersivity localized to the BTC is:

\[ \alpha_{BTC} = \left( \frac{2}{z} \right) (CV)^2 \]  \hspace{1cm} (6.7)

In the synthetic aquifer the length scale term \((z)\) was set equal to the longitudinal distance from the inlet to the center of the well.

Two temporal moments terms were used to characterize BTC measured in the synthetic aquifer. The first normalized moment \((\mu'_1)\) is a time scale measure of how long it took for the BTC center of mass to travel from the inlet to the well where the concentrations were measured. The BTC dispersivity term \((\alpha_{BTC})\) is a measure of dispersivity scaled by longitudinal distance, localized to the specific well. Employing these two characteristics as observations in transport model calibration is convenient because they provide a measure of two distinct physical quantities related to both advection and dispersion.

To compute moments from experimentally measured solute concentration data Equation 6.2 is integrated numerically using the trapezoidal rule, so that:

\[ \mu_0 = \Delta t \left[ \left( \frac{C_1 + C_k}{2} \right) + \sum_{i=2}^{k-1} C_i \right] \]  \hspace{1cm} (6.8)

\[ \mu_1 = \Delta t \left[ \left( \frac{t_1 C_1 + t_k C_k}{2} \right) + \sum_{i=2}^{k-1} t_i C_i \right] \]  \hspace{1cm} (6.9)

\[ \mu_2 = \Delta t \left[ \left( \frac{(t_1)^2 C_1 + (t_k)^2 C_k}{2} \right) + \sum_{i=2}^{k-1} (t_i)^2 C_i \right] \]  \hspace{1cm} (6.10)
\[ \mu'_{0} = 1 \]  \hspace{1cm} (6.11)

where \( k \) is the total number of measurement points.

### 6.2.2 Calibration Procedure

To perform a solute transport model calibration based on the center of mass transport time and the BTC dispersivity required the creation of a computer script which generated BTC data sets from the numerical model output file. Time series concentrations were stripped from the MT3DMS output file at the numerical grid points corresponding to the well centers. Temporal moments were calculated based on numerical integration just as they were for experimentally measured data according to Equations 6.8 – 6.10. The model predicted \( \mu'_{1} \) and \( \alpha_{BTC} \) terms were then written to a text file as input to UCODE. The executable file called by UCODE was a batch file which executed MT3DMS and then the moment analysis script. The observed data consisted of the \( \mu'_{1} \) and \( \alpha_{BTC} \) terms calculated from EC sensor measurements taken in the synthetic aquifer. The observed BTC dispersivities were assigned a 10% coefficient of variation while the center of mass transport times were assigned a 5% coefficient of variation.

Transport model calibrations were conducted on the centerline plume model and the associated experimental observations taken from the second run of this configuration in the synthetic aquifer. Tracer BTC were measured in 10 wells in the centerline plume experiment, the 4 centerline wells; W31, W33, W35, W37 and 6 off-center wells; W32, W34, W44, W36, W46, and W38. Calibration of the centerline plume model was conducted with six levels of observation data. Two calibration runs were conducted using observation data from all 10 wells where tracer was detected. The first of these two runs was initialized using parameter values that were artificially low while the second run initialized parameter values that were artificially high to determine if a unique solution would be reached by each run. The next calibration run used observation data from the 4 centerline wells. The forth calibration employed observation data taken from the off-center wells in row 6 (W36, W46) and the centerline well in row 7 (W37). The fifth
calibration used observation data taken from well W37 only. Each well produced two observation values $\mu_i'$ and $\alpha_{BTC}$. A sixth calibration using 9 wells was added based on the findings of the first two 10 well calibrations.

Center of mass transport time ($\mu_i'$) values and BTC dispersivities ($\alpha_{BTC}$) are listed in the following tables, comparing experimentally measured data to the final values produced after calibration of the transport model. Table 6.1 lists the method of moments BTC characteristics calculated when all 10 observation wells were used in the calibration and low initialization values were used for the parameters $\alpha_{L-grid}$, $\alpha_{T-grid}$, and $\phi$. The percent difference between the experimental and modeled values is also listed. There is a 109.75% difference between the experimental and modeled center of mass transport time from the BTC in well W31. This large difference is due to the long tail and oscillations measured in well W31 which are likely due to a density sinking effect. Other than well W31, somewhat lower percent difference values are seen for the center of mass transport times at centerline wells, however no discernable trends can be derived from the difference data.

Table 6.2 lists the same data for a 10 observation well calibration where the $\alpha_{L-grid}$, $\alpha_{T-grid}$, and $\phi$ parameters were initialized with artificially high values. No discernable trends can be derived from the percent difference data from this calibration model either. The modeling result for the center of mass transport time for well W31 is again much lower than the experimental value, resulting in a 111.52% difference.

An additional calibration was conducted based on 9 observation wells. Data from well W31 was removed from the 10 observation well data set because of the excessive density sinking effects. Results from this calibration run are listed in Table 6.3. For this calibration, the percent difference between modeled and experimental center of mass transport times is less than 10% for 7 of the 9 wells. While percent differences in BTC dispersivities are generally quite large.
### Table 6.1: Centerline Plume Model Calibration, 10 Well Low Initialization

<table>
<thead>
<tr>
<th>Well ID</th>
<th>$\mu_1$ (hr)</th>
<th>$\alpha_{BTC}$ (cm)</th>
<th>$\mu_1$ (hr)</th>
<th>$\alpha_{BTC}$ (cm)</th>
<th>% Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>W31</td>
<td>45.85</td>
<td>12.00</td>
<td>13.36</td>
<td>10.66</td>
<td>109.8</td>
</tr>
<tr>
<td>W33</td>
<td>38.04</td>
<td>4.38</td>
<td>36.00</td>
<td>7.06</td>
<td>5.52</td>
</tr>
<tr>
<td>W35</td>
<td>59.45</td>
<td>2.53</td>
<td>59.79</td>
<td>5.91</td>
<td>0.57</td>
</tr>
<tr>
<td>W37</td>
<td>85.54</td>
<td>4.69</td>
<td>83.26</td>
<td>5.26</td>
<td>2.71</td>
</tr>
<tr>
<td>W32</td>
<td>34.76</td>
<td>2.47</td>
<td>25.99</td>
<td>7.87</td>
<td>28.87</td>
</tr>
<tr>
<td>W34</td>
<td>45.74</td>
<td>2.70</td>
<td>49.63</td>
<td>6.21</td>
<td>8.14</td>
</tr>
<tr>
<td>W44</td>
<td>57.16</td>
<td>6.26</td>
<td>51.07</td>
<td>6.17</td>
<td>11.26</td>
</tr>
<tr>
<td>W36</td>
<td>66.69</td>
<td>4.84</td>
<td>73.38</td>
<td>5.25</td>
<td>9.55</td>
</tr>
<tr>
<td>W46</td>
<td>69.02</td>
<td>0.74</td>
<td>73.03</td>
<td>5.28</td>
<td>5.64</td>
</tr>
<tr>
<td>W38</td>
<td>88.04</td>
<td>2.98</td>
<td>97.03</td>
<td>4.79</td>
<td>9.71</td>
</tr>
</tbody>
</table>

### Table 6.2: Centerline Plume Model Calibration, 10 Well High Initialization

<table>
<thead>
<tr>
<th>Well ID</th>
<th>$\mu_1$ (hr)</th>
<th>$\alpha_{BTC}$ (cm)</th>
<th>$\mu_1$ (hr)</th>
<th>$\alpha_{BTC}$ (cm)</th>
<th>% Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>W31</td>
<td>45.85</td>
<td>12.00</td>
<td>13.02</td>
<td>3.22</td>
<td>111.5</td>
</tr>
<tr>
<td>W33</td>
<td>38.04</td>
<td>4.38</td>
<td>36.7</td>
<td>2.25</td>
<td>3.54</td>
</tr>
<tr>
<td>W35</td>
<td>59.45</td>
<td>2.53</td>
<td>60.33</td>
<td>1.90</td>
<td>1.46</td>
</tr>
<tr>
<td>W37</td>
<td>85.54</td>
<td>4.69</td>
<td>83.74</td>
<td>1.69</td>
<td>2.13</td>
</tr>
<tr>
<td>W32</td>
<td>34.76</td>
<td>2.47</td>
<td>26.23</td>
<td>2.58</td>
<td>27.99</td>
</tr>
<tr>
<td>W34</td>
<td>45.74</td>
<td>2.70</td>
<td>49.48</td>
<td>2.08</td>
<td>7.85</td>
</tr>
<tr>
<td>W44</td>
<td>57.16</td>
<td>6.26</td>
<td>44.12</td>
<td>0.90</td>
<td>25.75</td>
</tr>
<tr>
<td>W36</td>
<td>66.68</td>
<td>4.84</td>
<td>73.10</td>
<td>1.75</td>
<td>9.17</td>
</tr>
<tr>
<td>W46</td>
<td>69.02</td>
<td>0.74</td>
<td>68.16</td>
<td>1.18</td>
<td>1.26</td>
</tr>
<tr>
<td>W38</td>
<td>88.04</td>
<td>2.98</td>
<td>97.12</td>
<td>1.59</td>
<td>9.81</td>
</tr>
</tbody>
</table>
Table 6.3: Centerline Plume Model Calibration, 9 Well

<table>
<thead>
<tr>
<th>Well ID</th>
<th>Experimental Data</th>
<th>MT3D Modeled Data</th>
<th>% Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\mu_1'$ (hr)</td>
<td>$\alpha_{BTC}$ (cm)</td>
<td>$\mu_1'$ (hr)</td>
</tr>
<tr>
<td>W33</td>
<td>38.04</td>
<td>4.38</td>
<td>36.78</td>
</tr>
<tr>
<td>W35</td>
<td>59.45</td>
<td>2.53</td>
<td>60.43</td>
</tr>
<tr>
<td>W37</td>
<td>85.54</td>
<td>4.69</td>
<td>83.89</td>
</tr>
<tr>
<td>W32</td>
<td>34.76</td>
<td>2.47</td>
<td>26.26</td>
</tr>
<tr>
<td>W34</td>
<td>45.75</td>
<td>2.70</td>
<td>49.57</td>
</tr>
<tr>
<td>W44</td>
<td>57.16</td>
<td>6.26</td>
<td>44.24</td>
</tr>
<tr>
<td>W36</td>
<td>66.69</td>
<td>4.84</td>
<td>73.23</td>
</tr>
<tr>
<td>W46</td>
<td>69.02</td>
<td>0.74</td>
<td>68.30</td>
</tr>
<tr>
<td>W38</td>
<td>88.04</td>
<td>2.98</td>
<td>97.30</td>
</tr>
</tbody>
</table>

Examining the percent differences between the experimental and modeled $\mu_1'$ and $\alpha_{BTC}$ characteristics for the 4, 3, and 1 well calibrations revealed no discernable trends in the data. The parameter terms calculated by the 6 calibrations are listed in Table 6.4. The 4 and 1 well calibrations used only centerline wells and the calibrations proved to be unstable until the transverse grid-scale dispersivity was set to a fixed value. It should be noted that the value of $\alpha_{T-grid}$ as used here is a multiple of $\alpha_{T-grid}$. For the case of the single well calibration only two observations were available and so only one parameter could be estimated by UCODE. The transverse dispersivity parameter was fixed at 0.01 and the porosity was fixed to the original estimated value of 0.4446 listed in Table 4.2.

Table 6.4: Transport Model Parameters For Each Calibration

<table>
<thead>
<tr>
<th>Number of wells used in calibration</th>
<th>$\alpha_{L-grid}$ (cm)</th>
<th>$\alpha_{T-grid}$ (multiple of $\alpha_{L-grid}$)</th>
<th>$\phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 (low initial values)</td>
<td>1.024</td>
<td>0.0097</td>
<td>0.4442</td>
</tr>
<tr>
<td>10 (high initial values)</td>
<td>1.024</td>
<td>0.0096</td>
<td>0.4439</td>
</tr>
<tr>
<td>9</td>
<td>1.017</td>
<td>0.0098</td>
<td>0.4448</td>
</tr>
<tr>
<td>4</td>
<td>2.792</td>
<td>0.01 fixed</td>
<td>0.4568</td>
</tr>
<tr>
<td>3</td>
<td>3.312</td>
<td>0.0009</td>
<td>0.4357</td>
</tr>
<tr>
<td>1</td>
<td>4.550</td>
<td>0.01 fixed</td>
<td>0.4446 fixed</td>
</tr>
</tbody>
</table>
Comparisons of experimentally measured to numerically modeled BTC are seen in Figures 6.1 – 6.3. The numerical model results are from the 10 well, low initial value calibration of the centerline plume configuration. Figure 6.1 presents BTC measured in centerline wells.

**Figure 6.1:** Comparison of experimental to model data BTC, centerline wells, 10 well low initial value calibration of centerline plume configuration.
Figure 6.2: Comparison of experimental to model data BTC, off-center wells in rows 2 and 4, 10 well low initial value calibration of centerline plume configuration.
6.3 Solute Transport Model Predictions

The parameters determined from the 6 calibrations of the centerline plume were inputted into the forward models of the diagonal-S2, diagonal-S2S3, bi-modal, and wide centerline plumes. Calibrated parameters of hydraulic conductivity, grid scale dispersivities, and porosity were now available to these models and so they could be considered predictive in nature. To quantify the accuracy of their predictions, sum of squared weighted residuals (SSWR) were calculated at for each prediction. Residuals
were calculated at each well location based on the sensor data already collected. Table 6.5 lists the SSWR values for each plume configuration based on the calibration used.

<table>
<thead>
<tr>
<th>Number of wells used in calibration</th>
<th>Diagonal Plume-S2</th>
<th>Diagonal Plume-S2S3</th>
<th>Bi-Modal Plume</th>
<th>Wide Centerline Plume</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 (low initial values)</td>
<td>2,891.4</td>
<td>5,179.8</td>
<td>3,939.2</td>
<td>7,408.2</td>
</tr>
<tr>
<td>10 (high initial values)</td>
<td>2,888.6</td>
<td>5,180.5</td>
<td>3,937.4</td>
<td>7,420.1</td>
</tr>
<tr>
<td>9</td>
<td>2,863.2</td>
<td>5,173.2</td>
<td>3,938.4</td>
<td>7,340.0</td>
</tr>
<tr>
<td>4</td>
<td>34,970.9</td>
<td>6,403.9</td>
<td>4,562.4</td>
<td>58,796.6</td>
</tr>
<tr>
<td>3</td>
<td>19,205.9</td>
<td>8,744.6</td>
<td>7,328.4</td>
<td>34,402.7</td>
</tr>
<tr>
<td>1</td>
<td>62,257.6</td>
<td>14,791.9</td>
<td>9,270.2</td>
<td>107,779.0</td>
</tr>
</tbody>
</table>

Figure 6.4 demonstrates the SSWR data from Table 6.5 for the predictive plume models. The first observation from this plot is the expected result that fewer observation data points results in a larger SSWR and a less accurate predictive model. Of note is the influence of off-centerline wells to the predictive capability of the models. The calibrations involving centerline wells only show dramatic increases in SSWR for the diagonal-S2 and wide centerline plume configurations. These large SSWR values are primarily due to well measurements at the transverse edges of the plumes. Experimental measurements detect tracer in these wells where as the predictive models indicated no tracer concentration. Particularly large residual values resulted when tracer BTC were seen by either modeling or experiment and not seen by the other.
6.4 Conclusions

Using temporal method of moments to characterize plume BTC transport times and dispersivity was shown to be a useful technique for integrating high temporal resolution WSN data into model calibrations. Spatial resolution and sensor distribution also needs to be taken into account to ensure a contaminant plume is adequately captured and that the WSN is providing enough data to ensure a meaningful model calibration. Time series BTC are taken at a point in space and have no particular spatial scaling, therefore dispersivity information derived from them will tend to be heavily weighted by the dominant direction of plume transport and transverse dispersivity values may be underestimated.

Figure 6.4: Bar chart of SSWR from plume predictive models.
CHAPTER 7
LESSONS LEARNED AND RECOMMENDATIONS

This chapter summarizes and concludes this study. Significant results and lessons learned along with their implications to WSN implementation are addressed. Finally, recommendations for future work are discussed.

7.1 Summary

The goals of this work were to (1) design and construct a large lab-scale synthetic aquifer capable of acting as a WSN research and development test bed. The synthetic aquifer should have control mechanisms enabling the creation of complex plume geometries; and (2) develop a methodology for transport model calibration employing macro-scale dispersivity and plume transport time as the objective function observation metrics.

Chapter 3 described the construction of the CESEP large-scale synthetic aquifer. The design and function of individual parts and sub-systems were discussed along with how they all work together to form the overall synthetic aquifer system. The sensors and data acquisition methods were also presented.

Chapter 4 addressed the use of numerical modeling in both the design of the synthetic aquifer and as a tool for designing experiments prior to running them in the physical test bed. Head and outflow measurements were used as observation data to calibrate MODFLOW subsurface flow models. A series of 5 plume configurations were developed both through numerical simulation and later physically in the synthetic aquifer. Discrepancies between the modeled results and experimental measurements were discussed.

Chapter 5 discusses the physical tracer plume experiments in more detail. Issues relating to WSN data acquisition and processing were highlighted. Evidence of heterogeneity in the synthetic aquifer and density sinking of the plume were uncovered.
Chapter 6 concerns the use of WSN data to calibrate transport models. A method is presented which uses temporal method of moments to characterize the transport time and global dispersivity of breakthrough curves. These two characteristics are then employed as observation data for the parameter estimation of porosity, longitudinal grid-scale dispersivity, and transverse grid-scale dispersivity.

7.2 Lessons Learned and Recommendations

The key lessons learned during the course of this investigation and corresponding recommendations are:

- The operation of a synthetic aquifer requires continual maintenance and care. Daily degassing of the supply lines was required along with filtering and filling of the supply tank. Prevention of bio-film and algae growth required frequent attention. If tap water is used as the supply source, it is recommended that it is monitored closely for seasonal changes in composition.

- Small changes in synthetic aquifer outflow rates were noticed, these were most likely due to changes in ambient laboratory temperatures. The synthetic aquifer has a sand and water weight of over 8 tons, which is a considerable thermal mass. Changes in ambient temperatures would cause a slowly changing temperature distribution within the aquifer, which intern could be cause of some of the heterogeneous effects observed. Maintaining a constant ambient temperature of the synthetic aquifer and the supply water is recommended to reduce variability.

- Sensor calibrations are critical to obtaining accurate data; however it is often difficult to obtain absolute value precision from sensors. Often they perform better at measuring changes and change rates, therefore applying relative measurement scales is frequently more advantageous than using absolute scales. For WSN applications an absolute sensor measurement scale is preferred because it provides a baseline for comparison. It is recommended
that WSN employ an absolute value reference adjustment to all sensors. This could be accomplished electronically if the sensors prove to be sufficiently robust or it could be accomplished by placing each sensor in a control solution for a reference reading prior to site installation.

- The EC sensors used in this study required some break-in time. Whenever a sensor was moved from one well location to another, the first 2 or 3 readings were typically low and these data points were ignored. Also, spikes in the sensor data occurred frequently when the sensors were new but then diminished over time. Allowing sensors to acclimatize to a steady state condition prior to beginning an experiment is recommended.

- Homogeneity is a useful concept but it rarely occurs, even in tightly controlled environments. Account for variability in any system.

- WSN data analysis procedures must account for drifting and faulty data. A WSN must make use of protocols which can identify background or sensor drift and account for the time rate of drift. Faulty sensor data is going to occur at some point in any WSN application, therefore protocols should be prepared for when they occur and ensure they do not skew the data set.

- Plume shape and transport behavior can be effectively manipulated by fluidic control in a homogeneous media. The 7 supply and 7 drain reservoirs in the synthetic aquifer enabled the creation of several complex plume configurations. The creation of a single mode plume which split and later recombined did however require the addition of non-porous inclusions into the aquifer field.

- Fluid density differences in open hole wells have a considerable influence on the depth-wise aqueous concentration distribution within the well. Long term emplacement of sensors will have to account for possible density driven distributions. Sensors located at multiple depths within a single well may be required to accurately assess the mass of a contaminant.

- Temporal method of moments analysis shows promise as a method to characterize BTC in a global sense for use in automated calibrations. It is
recommended to add the zero\textsuperscript{th} moment to calculate mass and higher order moments to provide more information on BTC characteristics.

- Temporal method of moments looks to be particularly useful in laboratory scale experiments when time scales are on the order of days or weeks, and data analysis can be conducted after the BTC has passed through a well. Field applications may not have the luxury of complete BTC. This method also is ill suited to real-time calibrations because it requires a complete BTC for global characterization. Point source concentrations in combination with spatial moments characterization may prove more applicable to WSN deployment at the field scale.

7.3 Recommendations for Future Studies

The study presented here was a continuing step towards the goal of building autonomous plume monitoring networks of sensors which communicate wirelessly and have the ability to make predictive evaluations of plume transport. Before such a system will be ready for field deployment, many cross-discipline advances need to be made. Data quality protocols need to be investigated which can distinguish desirable “real” data from drifts, faults, or sensor errors.

This investigation performed flow model and transport model calibrations completely separate from each other. A next step in WSN technology development would be to conduct physical experiments and concurrent modeling studies which perform coupled calibrations of flow and transport; with a further goal of conducting real-time calibrations based on multiple types of observation data, (i.e. heads, flows, concentrations, etc.).

The experiments conducted in this study were essentially static in nature. Adding a dynamic component would provide a formidable test of WSN capabilities. The addition of transient well pumping or injection or transient changes to the flow boundaries could be used to add this dynamic aspect to the problem.
WSN promise near immediate access to field data at high levels of temporal and possibly spatial resolution; however the data provided by sensors may not be as accurate as data obtained by traditional sampling means. It is therefore proposed that a cost-benefit analysis be conducted to ascertain the financial and technical implications of employing a WSN which provides less accurate but high resolution data compared to using traditional sampling methods. For critical situations where contaminants risk human health and safety, accuracy will be of primary importance; but for site assessments and monitoring situations, WSN data and predictions have the potential to provide more information at a lower cost.
REFERENCES


APPENDIX A
SUPPLIMENT TO CHAPTER 5

The following material is supplemental to Chapter 5; it includes breakthrough curves and analysis of the tracer plume experiments. Refer back to the end of Chapter 5 for observations and conclusions.

A1 Diagonal Plume Introduced in Reservoir S2

The plume configuration presented in this section is the “diagonal” plume created by releasing the sodium bromide tracer from the S2 supply reservoir. The subsurface flow is controlled with all 7 supply reservoirs open to inflow while only the D7 drain reservoir is open to outflow. The vent valves on the supply lines to drain reservoirs D1 - D6 were opened to prevent outflow and the reservoir gates were not used.

The following 9 figures (Figure A1 – A9) present the equivalent NaBr concentrations measured by the EC sensor network. These concentration data are referred to as equivalent NaBr because the background water conductivity was not subtracted from the data before it was converted from bulk electrical conductivity to calibrated NaBr aqueous concentration.

Figure A1 demonstrates the tracer concentration decay measured in supply reservoir S2, also plotted is the background measurements from reservoir S3. An exponential decay rate of 0.115 hr⁻¹ was calculated by curve fitting the S2 data. This decay rate is 88.7% of the mean decay rate from the centerline plume configuration as measured by EC sensors. This reduction in decay rate is as expected because the total flow rate for the synthetic aquifer is reduced for the diagonal flow configuration compared to the centerline plume which had all reservoirs open to flow.

Figure A2 shows the measured concentration values for the first row of wells. Distinct BTC are seen in wells W11 and W21. A larger amount of NaBr mass travels through well W11 than W21. The steep increase in concentration along the BTC leading
edge as seen in the previous centerline plume cases is again seen in wells W11 and W21. The oscillatory behavior seen in the first well row of the centerline plume configuration is not seen here; however, wells W11 and W21 straddle the transverse edges of the plume.

**Figure A1:** NaBr concentration decay trend for the diagonal-S2 plume configuration, decay in the supply reservoir S2.

**Figure A2:** NaBr concentration BTC for the diagonal-S2 plume configuration, data from well row 1.
Figure A3 displays the NaBr concentration BTC measured from well row number 2. The tracer is only detected in well W22, which exhibits breakthrough behavior as seen previously. Beginning at approximately 75 hours elapsed time an increase in concentration can be seen. This could be another example of oscillatory behavior; however it is not as dramatic as the examples seen in the centerline plume cases.

**Figure A3:** NaBr concentration BTC for the diagonal-S2 plume configuration, data from well row 2.

**Figure A4:** NaBr concentration BTC for the diagonal-S2 plume configuration, data from well row 3.
Examination of Figures A2 – A6 which correspond to well rows 1 – 5 indicates the tracer plume travels in a relatively straight path in a longitudinal direction from the S2 reservoir. NaBr is detected in the first two wells of the odd numbered rows and only the second well in even numbered well rows. At the 6th well row as seen in Figure A7, the plume begins to move in a transverse direction towards the higher numbered wells. This
is demonstrated by the existence of a BTC for well W36. Transverse movement towards the D7 drain reservoir is further demonstrated in the 7th well row depicted in Figure A8, where tracer concentrations are detected in wells W17, W27, and W37.

**Figure A7:** NaBr concentration BTC for the diagonal-S2 plume configuration, data from well row 6.

**Figure A8:** NaBr concentration BTC for the diagonal-S2 plume configuration, data from well row 7.
Figure A9 shows that NaBr tracer is detected in wells W38 and W48 and just slightly in well W28. Qualitatively the measured data corresponds well with the numerical modeling results as seen in Figure A10. The tracer detected in well W28 and W17 indicates that the plume remains closer to the north boundary wall of the synthetic aquifer than what the numerical model would indicate. Qualitatively the measured experimental data detects NaBr at concentrations than are close to double the peak concentrations produced by the numerical model. It should be kept in mind that the numerical simulations presented so far were calibrated to subsurface flow and head measurements and were not yet calibrated to any solute transport parameters.

![Figure A9: NaBr concentration BTC for the diagonal-S2 plume configuration, data from well row 8.](image-url)
Figure A10: Animation of MT3DMS model of the “diagonal” tracer plume. This snapshot is 142 hours after tracer introduction into reservoir S2. The color scale is normalized concentration (C/C₀).

A2 Diagonal Plume Introduced in Reservoirs S2 and S3

A repeat of the diagonal plume configuration was run, however in this experiment 1000 mg/L of tracer was introduced in both supply reservoirs S2 and S3. This was done to create a wider plume which would come into contact with a larger number of wells and provide greater data resolution.

Figure A11 is a plot of the NaBr tracer as it decays in the supply reservoirs. Tracer concentrations were measured by two methods, EC sensors and grab samples processed in an IC. As can be seen there was considerable difference between the decay rates in reservoirs S2 and S3 due to differences in reservoir flow rates. The exponential decay rates determined from curve fitting along with the percent difference values between EC and IC data sources is listed in Table A1. The EC sensor and IC data sets correspond
well at lower concentrations but deviate from each other as the concentration increases to values greater than 500 mg/L.

**Figure A11**: NaBr concentration decay trend for the diagonal-S2S3 plume configuration, decay in the supply reservoirs S2 and S3.

**Table A1: Tracer Supply Exponential Decay Rates – Diagonal S2S3 Plume**

<table>
<thead>
<tr>
<th>Data Set</th>
<th>Exponential Decay Rate (1/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S2 – EC sensor</td>
<td>0.118</td>
</tr>
<tr>
<td>S3 – EC sensor</td>
<td>0.134</td>
</tr>
<tr>
<td>S2 – IC samples</td>
<td>0.118</td>
</tr>
<tr>
<td>S3 – IC samples</td>
<td>0.155</td>
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</table>

<table>
<thead>
<tr>
<th>Difference Analysis</th>
<th>% Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>S2 EC to IC data</td>
<td>0.10</td>
</tr>
<tr>
<td>S3 EC to IC data</td>
<td>15.0</td>
</tr>
</tbody>
</table>
Figure A12 displays concentration BTC for the first row of wells in the synthetic aquifer. Trends similar to the diagonal-S2 case are seen with the plume being wider and extending transversely to the W31 well.

The BTC seen in Figure A13 for well row 2 shows a steeper recession in well W22 compared to well W32, indicating a greater level of dispersion in W32. This is likely due to the flow velocity being greater in W32 compared to W22.

Concentration BTC trends continue as before in well rows 2, 3, and 4 except for the plume being wider in the transverse direction and indications that plume dispersion becomes greater as you move towards the higher well numbers within a row.

**Figure A12:** NaBr concentration BTC for the diagonal-S2S3 plume configuration, data from well row 1.
Figure A13: NaBr concentration BTC for the diagonal-S2S3 plume configuration, data from well row 2.

Figure A14: NaBr concentration BTC for the diagonal-S2S3 plume configuration, data from well row 3.
Figure A15: NaBr concentration BTC for the diagonal-S2S3 plume configuration, data from well row 4.

Figure A16: NaBr concentration BTC for the diagonal-S2S3 plume configuration, data from well row 5.
In Figure A16 above, the NaBr concentration in well W35 is significantly greater than the concentration measured in well W33 seen in Figure A14, indicating the plume begins to move in the transverse direction before well row 5. The detection of NaBr tracer in well W46 seen in Figure A17 below gives further evidence that transverse plume movement is occurring. By well row 7, seen in Figure A18, significant transverse stretching of the plume has occurred. The bulk of the plume’s mass is located at wells W27 and W37, while traces of NaBr have been measured in W17, W47, and W57.

Further transverse movement of the tracer plume’s center of mass is seen in Figure A19 for the 8th well row. The bulk of the plume’s mass is measured in wells W38 and W48, with a distinct BTC at well W58.

Figure A17: NaBr concentration BTC for the diagonal-S2S3 plume configuration, data from well row 6.
Figure A18: NaBr concentration BTC for the diagonal-S2S3 plume configuration, data from well row 7.

Figure A19: NaBr concentration BTC for the diagonal-S2S3 plume configuration, data from well row 8.
A3 Wide Centerline Plume

In an effort to determine if preferential flow paths existed in the synthetic aquifer, a tracer configuration was created which would ideally move as a transverse wave across the field. The subsurface flow was set to the steady-state baseline condition with all 14 reservoirs open to flow. Tracer was introduced simultaneously to supply reservoirs S2 through S6. No tracer was introduced in reservoirs S1 and S7 to avoid wall effects at the transverse boundaries. This configuration was referred to as either “the wave profile” or more correctly a wide centerline plume. The tracer exponential decay rate in each supply reservoir is listed in Table A2. The increase in decay rates seen in this configuration compared to the original centerline plume configuration is attributable to higher ambient temperatures in the laboratory leading to lower fluid viscosities and slightly increased flow rates, and minor adjustments made to the elevations of the constant head devices.

<table>
<thead>
<tr>
<th>Data Set</th>
<th>Exponential Decay Rate (1/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S2 – EC sensor</td>
<td>0.193</td>
</tr>
<tr>
<td>S3 – EC sensor</td>
<td>0.231</td>
</tr>
<tr>
<td>S4 – EC sensor</td>
<td>0.190</td>
</tr>
<tr>
<td>S5 – EC sensor</td>
<td>0.202</td>
</tr>
<tr>
<td>S6 – EC sensor</td>
<td>0.200</td>
</tr>
</tbody>
</table>

Figure A20 displays the NaBr concentration values in the supply reservoirs as measured by EC sensors. Considerable variability exists between the decay rates of the reservoirs, with S2 having the slowest decay rate and the adjacent S3 reservoir having the highest rate.

Tracer is measured in all 5 wells of well row 1 as seen in Figure A21. All 5 BTC are aligned on the time axis indicating no preferential flow at this point in the synthetic aquifer. No oscillatory behavior is exhibited in the BTC tails, however wells W31 and W51 both show a convex kink in the BTC occurring at approximately 30 hours duration.
**Figure A20:** NaBr concentration decay trend for the wide centerline plume configuration, decay in the supply reservoirs S2 through S6.

**Figure A21:** NaBr concentration BTC for the wide centerline plume configuration, data from well row 1.
In Figure A22 it can be seen that the plume arrival and peak concentrations times are closely aligned between wells W22 – W52 and no tracer is detected in the end wells W12 and W62. Differences in dispersive character of the BTC are becoming pronounced. The wells at the center of the plume, W32 and W42, are showing a much longer recession compared to the wells on the edge of the plume, W22 and W52.

Differences in plume transport time are beginning to be seen at well row 3 as shown in Figure A23. Plume arrival and peak times for wells W23 and W33 are closely matched while the arrival time to well W13 lags by approximately 2 hours.

Figure A22: NaBr concentration BTC for the wide centerline plume configuration, data from well row 2.
As the plume continues to progresses through the synthetic aquifer as seen in Figures A24 – A28, the plume arrival times become more distributed with a maximum span of 5.5 hours difference between wells W38 and W58 in well row 8. The second and third wells in each row are reached by the plume first with the 4th and 5th wells tending to have later arrival times. Times to peak concentration follow somewhat similar trends but are more influenced by changes in the magnitude of the peak concentration. The center of the plume maintains a high NaBr concentration while the edges are more influenced by dispersive forces and so the peak concentration values decrease more rapidly at the edges.

A concentration rebound “hook” develops in the BTC of well W45 as seen in Figure A25. This rebound and continued recession is seen to carry through wells W56, W47 and then on to W48 and W58 in row 8. Well W38 from Figure A28 shows a shift in the BTC recession possibly due to this same rebound effect. It is hypothesized that density sinking and rebound into the transporting plume is a possible cause for this behavior.
Figure A24: NaBr concentration BTC for the wide centerline plume configuration, data from well row 4.

Figure A25: NaBr concentration BTC for the wide centerline plume configuration, data from well row 5.
Figure A26: NaBr concentration BTC for the wide centerline plume configuration, data from well row 6.

Figure A27: NaBr concentration BTC for the wide centerline plume configuration, data from well row 7.
A4 Bi-Modal Plume

A bi-modal plume was created by splitting a single, wide plume into two lobes. The tracer was introduced in supply reservoirs S3, S4, and S5. The 7 supply and 7 drain reservoirs were all open to flow. Four non-porous PVC boxes were placed in the synthetic aquifer to split and divert the plume into a complex bi-modal pattern. See Figure 4.7 for a planview image of the placement of the non-porous boxes within the synthetic aquifer.

The exponential decay of the tracer in the supply reservoirs is seen in Figure A29. The decay rate coefficients for each reservoir are listed in Table A3. As expected the lowest decay rate occurs in S4, the center reservoir which would be most affected by the placement of the 1st non-porous region. A larger decay coefficient was measured in reservoir S5 compared to reservoir S3, which indicates a more preferential flow towards the southern end of the synthetic aquifer.
Figure A29: NaBr concentration decay trend for the bi-modal plume configuration, decay in the supply reservoirs S3, S4, and S5.

Table A3: Tracer Supply Exponential Decay Rates – Bi-Modal Plume

<table>
<thead>
<tr>
<th>Data Set</th>
<th>Exponential Decay Rate (1/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S3 – EC sensor</td>
<td>0.159</td>
</tr>
<tr>
<td>S4 – EC sensor</td>
<td>0.139</td>
</tr>
<tr>
<td>S5 – EC sensor</td>
<td>0.176</td>
</tr>
</tbody>
</table>

Oscillatory behavior in the BTC recession of well W31 is again observed in Figure A30. Density effects and the influence of the broad face of the PVC box immediately down gradient of well W31 are likely causes of this behavior. A flow stagnation point is caused by the PVC obstruction keeping tracer concentrations elevated in this region, resulting in a longer BTC recession for well W31. The BTC of wells W21 and W41 indicate nearly ideal symmetric splitting of the plume.
Asymmetric plume transport is observed at well row 2 as seen in Figure A31. Wells W22 and W52 are symmetric pairs in the synthetic aquifer. A distinct tracer BTC was measured in well W52 while no tracer was detected in well W22. Wells W32 and W42 are also symmetric pairs. Plume arrival time is slightly sooner in W32 and its BTC recession is considerably longer than W42. Both wells W32 and W42 show a concentration rebound which is most likely due to the slow migration of tracer out of the stagnation zone around the 1st PVC obstruction.

The 3rd well row as seen in Figure A32 again shows an asymmetric plume split with tracer measured in well W53 but none in its symmetry pair well W13. The centerline well W33 shows a significantly delayed BTC with a rebounding recession due to the stagnation near the 2nd non-porous obstruction. The screen around well W23 broke filling the well with aquifer sand while an EC sensor was in place. The function and accuracy of this sensor cannot be confirmed and so data from well W23 will be ignored. The aquifer sand lost due to the well screen break was replaced.
Figure A31: NaBr concentration BTC for the bi-modal plume configuration, data from well row 2.

Figure A32: NaBr concentration BTC for the bi-modal plume configuration, data from well row 3.
The BTC from wells W24 and W54 as seen in Figure A33 indicate the two lobes of the bi-modal plume are close to symmetric as they move past the rear corners of the 2nd obstruction. There is a half hour difference in peak arrival time between these two wells and only a 10 mg/L difference in peak concentration values. The BTC timing of wells W34 and W44 however indicate significant asymmetry in the plume as it wraps around the back side of the long PVC obstruction.

In Figure A34, the southern lobe of the bi-modal plume is seen to have a greater concentration peak in well W45 compared to the northern lobe measured in well W25. The northern lobe is advancing more quickly, seen here reaching the 5th row of wells 3 hours before the southern lobe. The BTC for well W35 indicates that the plume has recombined at the synthetic aquifer centerline with a peak concentration greater than 300 mg/L, which is contrary to the numerical modeling results which predicted the plume would not reach well W35 until 116.5 hours with a peak concentration of 120 mg/L.

**Figure A33:** NaBr concentration BTC for the bi-modal plume configuration, data from well row 4.
The 6th well row as seen in Figure A35 continues trends seen in previous wells. The northern lobe of the plume has a quicker arrival time compared to the southern lobe. The BTC measured from well W56 indicates that the southern lobe is wider in the transverse direction.

The concentration measurements displayed in Figure A36 for well row 7 indicate the plume has recombined, but still retains a bi-modal character with lobes on either side of the centerline. These lobes precede the bulk of the plume which travels along the synthetic aquifer centerline. This behavior is seen by the early BTC peaks in wells W27 and W47 followed by a greater peak in well W37. The dual peaks of the W37 BTC can be accounted for by the faster traveling northern lobe reaching the centerline followed by the southern lobe. The last row of non-porous obstructions contains two PVC boxes. The wells in the vicinity of the northern obstruction indicate the northern lobe of the plume contacts only the edge of this obstruction. Tracer BTC seen in wells W56 and W57 indicate the wider southern lobe has more contact with the southern obstruction. The concentration rebounds seen in W27 and W47 is likely due to plume contact with the obstructions.
Figure A35: NaBr concentration BTC for the bi-modal plume configuration, data from well row 6.

Figure A36: NaBr concentration BTC for the bi-modal plume configuration, data from well row 7.
Figure A37: NaBr concentration BTC for the bi-modal plume configuration, data from well row 8.

Observations and conclusions based on the preceding BTC are found in Section 5.6, with implications as they relate to WSN applications are found in Section 5.7.