AN INVESTIGATION OF OIL-FIELD PRODUCED WATER MIGRATION IN GROUND WATER USING NUMERICAL MODELING AND PARAMETER ESTIMATION AT WELD COUNTY WASTE DISPOSAL, FORT LUPTON, COLORADO

by

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ABSTRACT

Oil-field produced water disposed in evaporation ponds near Fort Lupton, Colorado has seeped into an under-lying shallow aquifer, impacting ground-water resources. The objectives of this study are to: identify a non-reactive indicator of produced water, describe the migration of produced water, and provide recommendations to future investigations of similar contamination sites.

Chloride is used as a tracer to identify oil-field produced water within ground waters. Geophysical electromagnetics are also proven effective in identifying produced water in the subsurface. Twelve possible single-layer conceptual models are developed from analysis of data describing site conditions. The graphical user interface, Groundwater Modeling System, is used to convert conceptual models to numerical models. Ground-water flow and solute transport are simulated using the computer programs MODFLOW and $MT3D^{PD}$ respectively. Alternative models are calibrated to 650 field measurements of hydraulic head and chloride concentration measured in monitoring wells during the period from April 1978 to December 1998. Calibration is facilitated using UCODE, a parameter estimation code. Calibration statistics provided by UCODE show that single layer models are not capable of representing observed field conditions with acceptable accuracy and a twelve-layer model is more representative of

site conditions because it accounts for vertical components of flow and transport. When calibrated, the twelve-layer model simulates a plume that replicates the general characteristics of chloride distribution in space and time inferred from field measurements, but matches individual field measurements poorly.

Simulations of future plume migration indicate that the plume remains narrow as it migrates down-gradient at an average rate of 0.4 ft/day. No existing water supply wells are in the direct path of the plume and chloride concentrations exiting the study area are at low levels suggesting that the chloride plume is not a significant threat to ground-water users. Organic contaminants have been identified in ground water at the site and are not studied in this project. Confidence intervals determined by UCODE indicate that predicted chloride concentrations are highly uncertain due a lack of vertically distributed data and data describing seepage from a nearby canal.

While there exists a large amount of data describing conditions at WCWD, the use of numerical modeling and parameter estimation identified that the data does not describe certain aspects of the system that are needed for the development of representative models that can accurately simulate the migration of produced water. Investigations of similar produced water contamination sites should use these tools to guide data collection. As conceptual models are derived and revised according to data collected, additional data that are needed to improve parameter sensitivity and break correlation will be identified. This process will limit expenditures, maximize the understanding of the system, and lead to accurate numerical model predictions.

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I would like to thank four individuals who contributed to this study at a level beyond what may be reasonably expected: Dr. George Breit of the U.S. Geological Survey for his keen insight; Steve Laudeman of the Colorado Department of Health and Environment for providing up-to-date information on site activity; Jeff at BYU for supplying many customized versions of MODFLOW and MT3D on rush order; and my advisor, Dr. Eileen Poeter for guidance.

CHAPTER 1.0 INTRODUCTION

Water co-produced with oil and gas, or produced water, is being generated in increasing quantities from hydrocarbon reservoirs. Total U.S. production of produced water in 1993 was over 25 billion barrels. Presently, every barrel of oil produced yields approximately 10 additional barrels of produced water (Wanty and Kharaka, 1997), generating an annual volume roughly equivalent to nine days of flow over Horseshoe Falls at Niagra. This water is generally very saline, having total dissolved solids (TDS) concentrations from less than 1,000 ppm to over 400,000 ppm. If improperly managed, small quantities of produced water are capable of impacting large ground-water reservoirs. Produced water disposal is therefore an issue of increasing concern to energy resource developers and to regulators.

In the Denver Basin more than 125 million barrels of produced water have been generated from the early 1950's to 1995 (Colorado Oil and Gas Conservation Commission, 1996; Higley, et al., 1995; Gas Research Institute, 1995). While produced water disposal today is primarily through deep well injection, the majority of produced water in the Denver Basin has been disposed via surface impoundment in evaporation ponds, many of which are still in use (Gas Research Institute, 1990). The goal of such disposal is to evaporate pure water from the produced water and recover the residual salt precipitate for proper disposal or sale.

1.1 Statement of the Problem

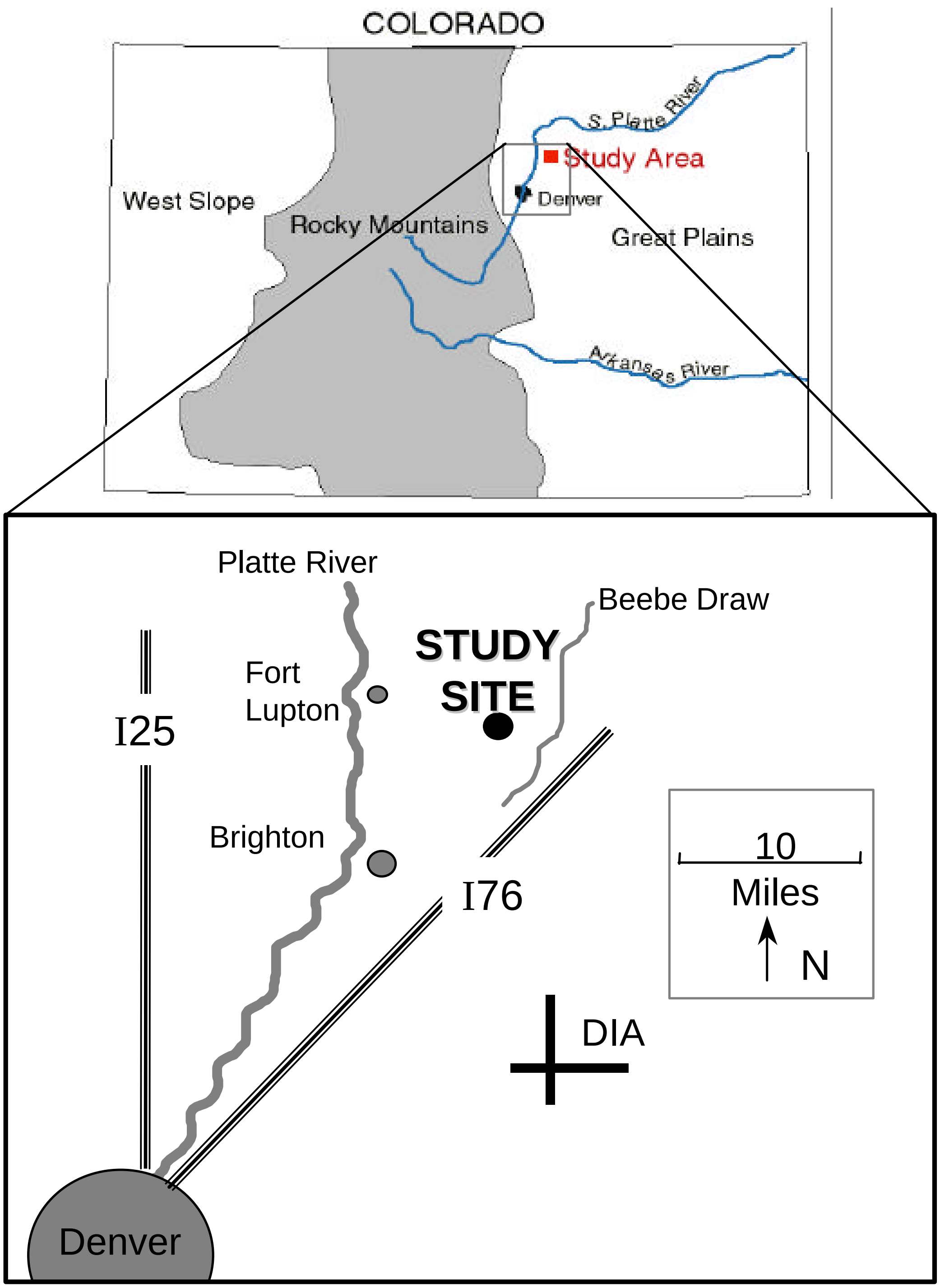
Many of the disposal ponds in the Denver Basin were constructed without low permeability liners and directly overlie permeable unconsolidated sediments. In 1963, unlined ponds received 32% of the 202,194 barrels of produced water generated in the Denver Basin (EPA, 1991). Former Director and State Geologist of Colorado, John W. Rold (1970), reported that 27 million barrels of produced water were disposed in unlined ponds in Colorado in 1969.

It is likely that a significant portion of all evaporation ponds leak to some degree, allowing produced water to mix with shallow ground water at various locations throughout the Denver Basin. Denver Basin communities rely heavily on ground water for agriculture, industry, and domestic use; and unconsolidated, surficial aquifers supplied approximately 91 percent of all fresh water pumped from wells in 1989 (Robson, 1989). Considering the high pace of residential development in the Denver area, the demand for shallow sources of potable water may increase dramatically. Therefore, responsible land and resource planning in the Denver Basin requires better understanding of produced water migration in ground water.

1.2 Study Objectives

Weld County Waste Disposal (WCWD), is a commercially owned produced water disposal facility 35 miles northeast of Denver (Figure 1) which is being investigated by the EPA, for violations of RCRA (Title 7003). Third party site characterization work has revealed anomalous ground-water chemistry at some locations which resembles produced water chemistry. This project is an investigation of the dispersion of the suspected produced water within the aquifer at WCWD.

Figure 1. Location of Weld County Waste Disposal.



The purpose of this study is to:

1) identify an indicator of produced water contamination;
2) assess the fate of the contamination plume within the aquifer and as it enters the larger Beebe Draw alluvial aquifer three miles down-gradient from WCWD;
3) and extend the findings of this study to other produced water disposal facilities in similar geologic and climatic settings.

This is accomplished through the development and evaluation of conceptual models describing the geohydrologic system, and subsequently through the calibration and simulation of numerical ground-water flow models (using the computer code, MODFLOW [McDonald and Harbaugh, 1983]) and numerical solute transport models (using the computer code MT3D [Zeng, 1990]). Calibration of the models is facilitated by use of UCODE parameter estimation code, which provides statistical measures of the accuracy of both the estimated parameter values and predictions made using those parameter values (Poeter and Hill, 1997).

The procedure is to 1) develop alternative viable conceptual models describing the geohydrology of WCWD; 2) develop MODFLOW and MT3D numerical models simulating ground-water flow and solute transport; 3) calibrate and discriminate between the models using the available data and UCODE; and 4) predict future contaminant concentrations using the calibrated numerical models.

1.3 Organization of Report

This report is divided into 10 chapters including this introduction. Chapter 2 provides a review of relevant studies and introduces the geohydrology of Weld Country Waste Disposal. Chapter 3 outlines the methodology used to achieve the study objectives. Chapter 4 discusses the collection and analysis of field data used to develop alternative conceptual models of the ground-water system. Chapter 5 presents alternative conceptual models. Chapter 6 discusses numerical model setup, simulation, and calibration. Chapter 7 presents results of numerical model simulations. Chapter 8 presents a multi-layer model derived from the results of previous modeling and discusses simulation and prediction results. Chapter 9 summarizes the conclusions of the study and how the objectives of the study are achieved. Chapter 10 provides recommendations for future work.

A compact disk is provided in the back cover of this report which includes geochemical data, geophysical data, monitoring well completion data that is not presented in this report, and MODFLOW, MT3D, and UCODE input files for selected models and all applications needed to run simulations and regressions for these models.

CHAPTER 2.0 SITE GEOHYDROLOGY

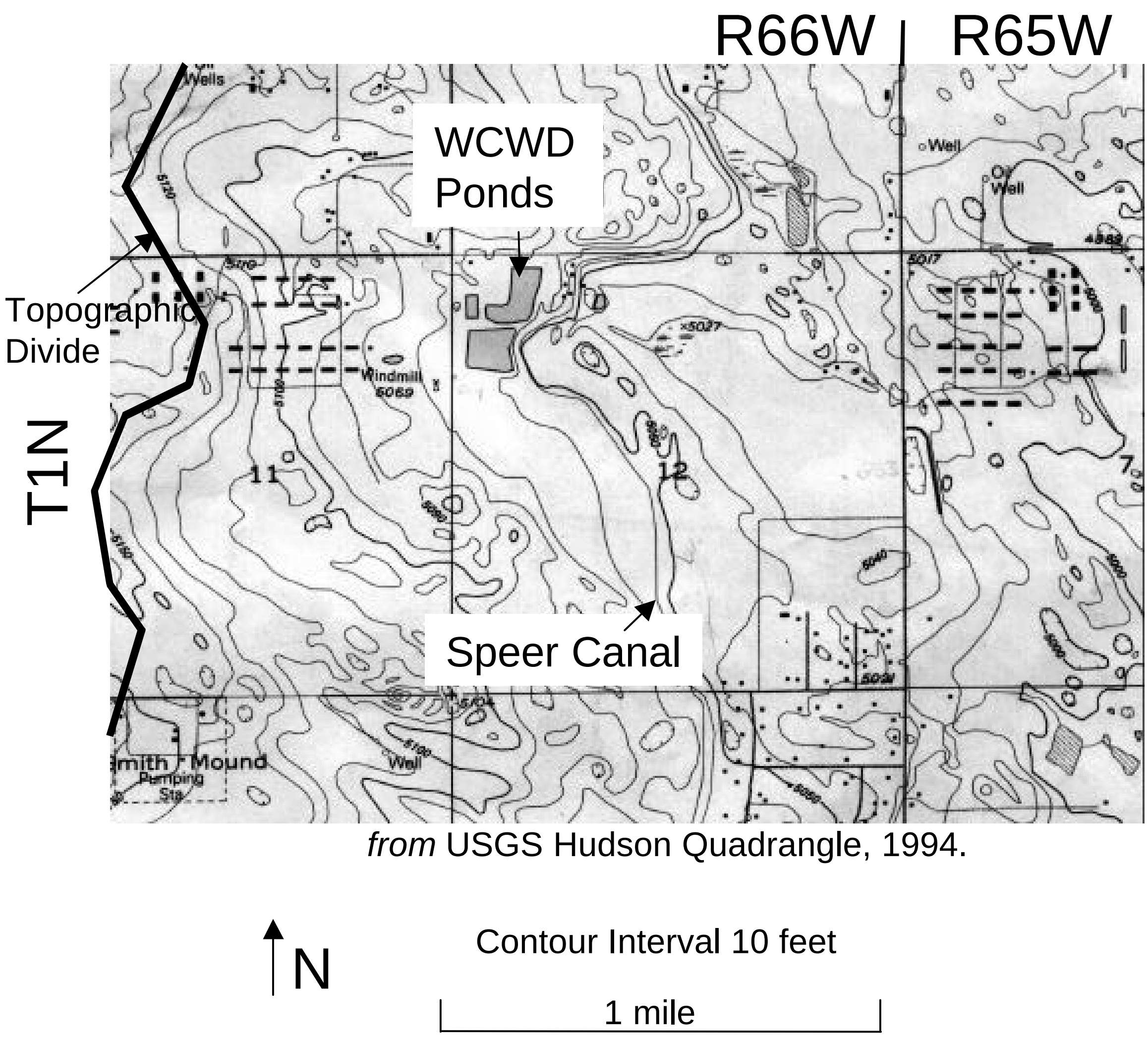
Weld County Waste Disposal (WCWD) is located five miles east of Fort Lupton, Colorado, in the high plains of the northern Denver Basin and occupies approximately 33 acres in the northwest corner of Section 12, Township 1 North, Range 66 West (Figures 1, 2, and 3). This chapter reviews relevant studies consulted in this project, discusses the setting and history of WCWD, describes the regional geology and ground-water conditions, and defines the study area boundaries.

2.1 Literature Review

While there has been substantial investigation of salt scarred soils resulting from produced water contamination, studies of produced water dispersion in a shallow unconfined aquifer are not common. Pertinent studies consist of geologic and hydrologic investigations of the area, geochemical and geophysical studies addressing the detection of produced water, and regional studies of the quantity and quality of produced water being generated and its means of disposal.

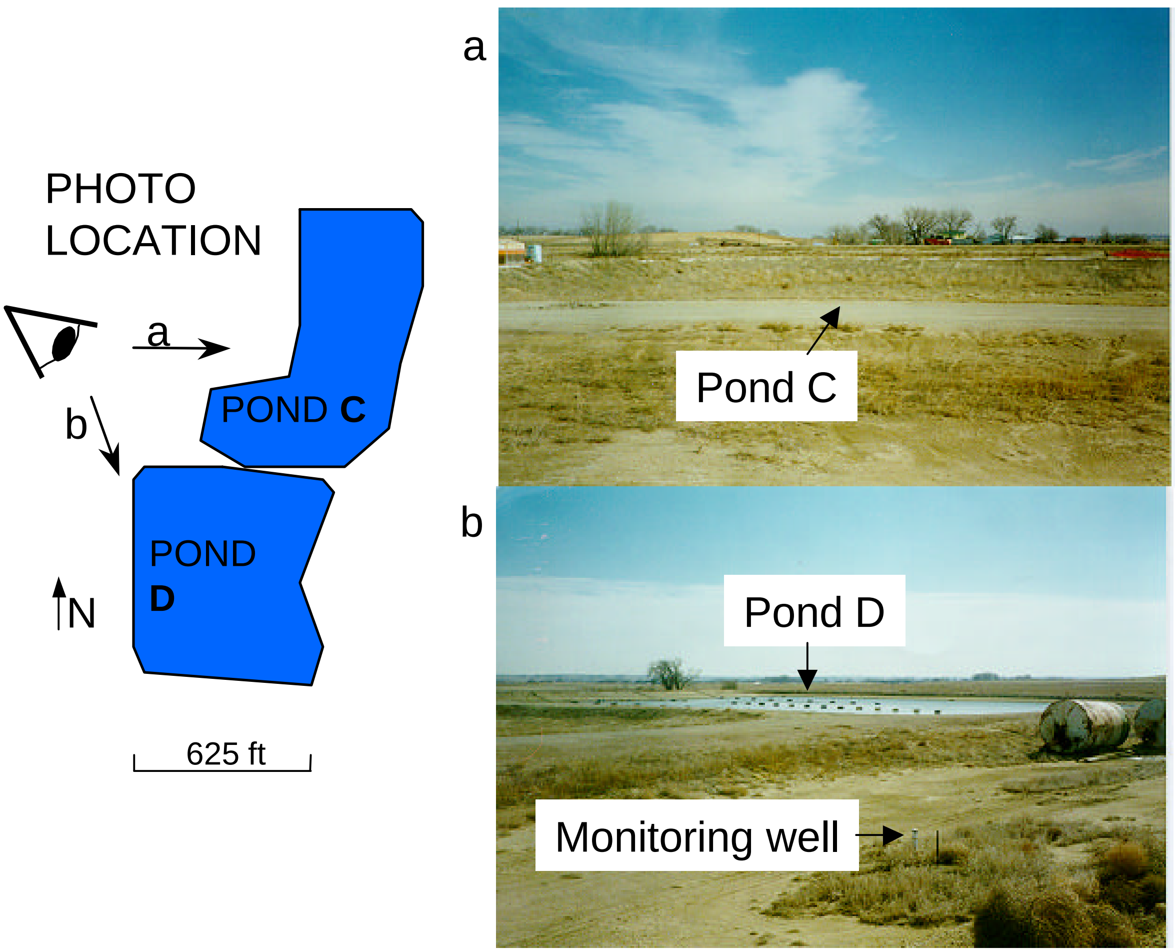
Because WCWD is a RCRA site, a major data source for this study is the publicly available information generated by LT Environmental Inc. (LTE), the environmental engineering company performing the characterization work on site as directed by the EPA. LTE began work at WCWD in 1995 and has installed shallow (less than 50 feet deep) monitoring wells, described the lithology in those wells, conducted aquifer (slug) tests, recorded water levels monthly, analyzed water chemistry quarterly, and produced a report (Draft On Site Characterization Report, 1997) which analyzes the geohydrology of WCWD. Earlier site investigations include water quality studies conducted by Chen and

Figure 2. Portion of the USGS Topographic Map of Hudson Quadrangle showing the Weld County Waste Disposal site and surface drainage divide.



from USGS Hudson Quadrangle, 1994.

Figure 3. Photographs of study area in February, 1997. a) viewing east toward Pond C (dry) and b) viewing southeast toward Pond D.



Associates in 1984 and by Parsons Engineering Science, Inc. in 1995 and aquifer (slug) tests conducted by Ground Water Technology Inc. in 1993 (Shosky, 1993).

The surficial geology of the study area is reported by Soister (1965) as consisting primarily of Holocene and Pleistocene eolian deposits less than 35 feet thick overlying indurated Cretaceous siltstones. Maps by Colton (1978) expand the coverage of eolian sheet sands and included parabolic and longitudinal dune traces. Additional geologic analysis of the quaternary deposits is provided by Madole (1994, 1995). Crabb (1980) maped and described the properties of the soil in the area to a depth of five feet as permeable, silty loams.

Regional ground-water studies of surficial and bedrock aquifers in the Denver Basin have been conducted by Smith, et al. (1964); Hurr, et al. (1975); Hillier and Schneider (1980); and Robson (1989). These reports outline the general boundaries of aquifers present in the study area, describe recharge and discharge areas, list average values of transmissivities, and provide some geochemical analyses of the ground water. A study at a site ten miles to the north of WCWD by Gaggiani (1995) described the hydraulic properties and water chemistry of a highland aquifer and precipitation rates.

Produced water has been identified in aquifers using conservative (non-reactive) constituents, such as chloride and bromide, as geochemical tracers (Whittemore, 1988; Novak, 1988; and Stossell, 1997). Geophysical surface electrical resistivity surveys (Zhody, et al., 1974; Urish, 1983) and surface electromagnetic surveys (Thamke, et al., 1998) have proven valuable at identifying continuous areas of low resistivity associated with high TDS produced water plumes. Both surface and airborne electromagnetic surveys have been successful in detecting produced water contamination at the Brookhaven Oilfield in Mississippi (Smith, et al., 1997) and in west Texas (Paine, et al., 1997).

2.2 Physiography

The site is slightly more than 5,000 feet above mean sea level (amsl), on the east flank of a north-south trending ridge separating the Platte River to the west, from Beebe Draw, a remnant stream of an ancestral channel of the Platte River, to the east. The topography at WCWD is gently rolling, dipping a maximum of 5 degrees to the southeast, with a maximum relief of 160 feet (Figure 2). The physiography of the region may be divided into rolling highlands and planar lowland valleys. The site is situated in a small drainage basin of approximately 1.4 square miles. Speer Canal, an irrigation supply canal, flows north along the eastern border of the ponds, at rates ranging from 30-87 cubic feet per second (cfs) from late April to late October (M. Montoya, Farmers Irrigation Corp., verbal communication 9/15/98).

Average annual precipitation is 12.6 inches per year, and over 70% of the precipitation falls from April to September (Gaggiani, 1995). Mean daily temperatures range from lows of 27 ^{o}F to highs of 73 ^{o}F (National Oceanic and Atmospheric Administration, 1995). The prevailing winds are from the northwest and occasionally reach speeds over 50 miles per hour (Robson, 1989). Parabolic sand dunes, trending southeast and rising up to heights of 15 feet are common in the area (Colton, 1978). Dominant native vegetation is sand bluestem, sand reedgrass, and blue grama (Crabb, 1975). The few trees present are cottonwoods and occur along canals or where the water table is near the land surface. The surrounding land is used for dry-land agriculture, with the exception of a compost facility to the immediate west of WCWD which has also been used as a turkey farm (Figure 2) (Driscoll, Linda, 1974). Irrigation farming in the lowland valleys produces sugar beets, corn, beans, alfalfa and other grains.

2.3 Site History

From the late 1970's, until it was closed by the EPA in May of 1995, WCWD operated as a commercial waste water disposal facility permitted to receive saline waters co-produced with oil and gas extraction. During this time, WCWD received, stored, and evaporated produced water, and to a much lesser degree, other associated oil-field waste fluids (drilling mud, 'frac' water, etc.). Receipts indicate that for a 6 year period from October, 1988 to September, 1994, over 162 million gallons of produced water were received (LT Environmental, Public Involvement Plan, 1996). There is no record of salt residue removal from the ponds.

WCWD began receiving produced water in late 1978 (LTE, Draft Characterization Work Plan, 1997). For the first four years of operation produced waters were disposed in a variety of small ponds. In 1982 two large ponds, referred to Ponds C and D (Figures 2 and 3), replaced earlier ponds and increased the storage capacity of WCWD by an order of magnitude, from 110,000 ft^3 to approximately 1,840,000 ft^3 (assuming an average pond depth of 3 ft). Because of this dramatic change in capacity, and because disposal activity prior to 1982 is poorly documented, this study considers Ponds C and D as the sole sources of infiltration to the aquifer. The remaining produced water in Pond C was pumped into Pond D in December of 1995, and Pond D was empty (due to evaporation and/or percolation) by April, 1997 (LTE, 1997).

In 1984 a water quality study by Chen and Associates indicated that the water chemistry of the underlying aquifer was impacted by produced water, but no mitigative action was taken. New requirements for pond lining in 1989 brought WCWD under the scrutiny of the Colorado Department of Public Health and Environment, but no significant action resulted. However, in early 1995, the EPA was notified by a field investigator of the Fish and Wildlife Service that the facility was in violation of several titles under RCRA 7003, 40 CFR, and the EPA issued Administrative Orders to WCWD on May 11, 1995, closing the facility (EPA, 1995). The Administrative Orders specified that produced water contamination in the area must be characterized and, if necessary, remedied.

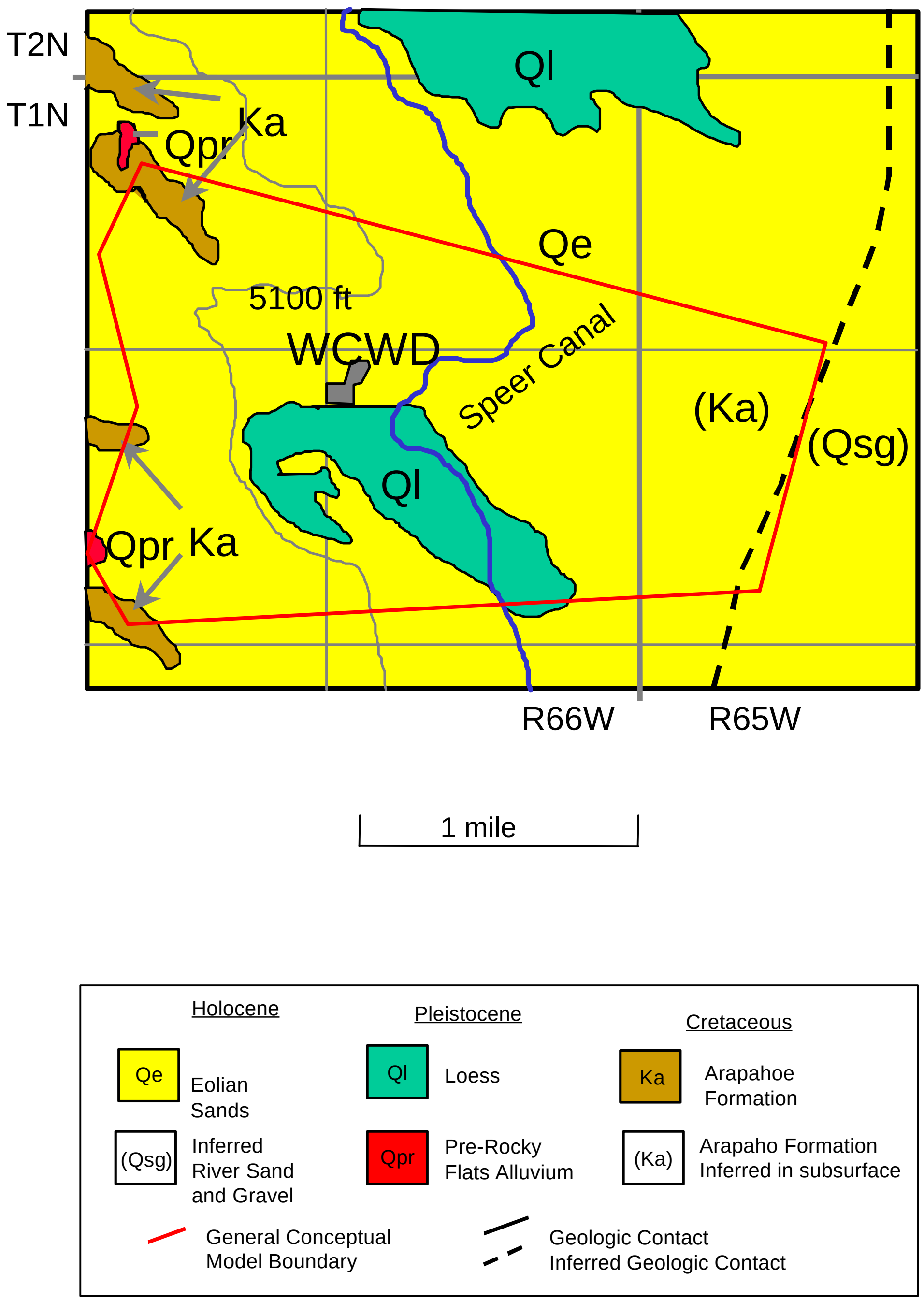
Work by LTE identified halogenated compounds in the ground water that are not normally present in produced waters, suggesting that these solvents were illegally disposed in the ponds. These compounds, as well as all organic compounds associated with produced water, are not considered in this study. This study focuses on the inorganic constituents of produced water.

To date, LTE has evaporated all the remaining water from the ponds, contained all sources of hydrocarbon contamination, and monitored ground-water levels (monthly) and water quality (quarterly) in the existing network of 20 monitoring wells. Due to ongoing litigation between LTE and the EPA regarding the scope of characterization and remediation work WCWD requires, third party access to the site is currently denied. This study therefore is restricted to publicly available data.

2.4 Stratigraphy and Soils

The surficial geology of the area is shown in Figure 4 (*after* Soister, 1965). The study area is outlined in red and will be discussed at the end of this section. The area includes widespread unconsolidated deposits of Pleistocene loess and Holocene eolian sands overlying the indurated Upper Cretaceous Arapahoe Formation. The Arapahoe Formation consists of over 1,000 feet of olive-gray claystones and siltstones, inter-bedded with tuffaceous sandstones and conglomerate (Colton, 1978). Early Pleistocene Rocky Flats Alluvium overlays the Arapahoe Formation, tracing a narrow stream deposit which trends north-south along the topographic divide between the Platte River and Beebe Draw (Colton and Fitch, 1974). The localized, large cobbles of the Rocky Flats Alluvium proved more resistant to erosional scouring of the Platte River than the adjacent Arapahoe Formation during Pliocene uplift, resulting in an inverted stratigraphy where the topographic highs reflect outcrops of Arapahoe and Rocky Flats Alluvium.

Figure 4 . Surficial geology of the study area *(after* Soister, 1964).



Generally, depositional processes are eolian in the highlands, such as WCWD, and alluvial in the valleys, such as Beebe Draw (Smith et.al. 1964). The eolian deposits are generally less than 35 feet thick and consist of Pleistocene loess sheet deposits, which underlie southeast trending parabolic dunes composed of fine to coarse silty sand (Soister, 1965; Colton, 1978; Madole, 1995). Soil studies by the Soil Conservation Service (Crabb, 1980), identify the surficial deposits as permeable, eolian, sandy loam, derived from local alluvial fill. Synchronous with the eolian deposition, the ancestral Platte River was filling Beebe Draw to the east with alluvium up to 80 feet in thickness. The inferred contact between Beebe draw valley fill and highland eolian deposits is shown in the eastern portion of Figure 4.

2.5 Ground Water

There are generally two types of unconfined aquifers in the Denver Basin, highland aquifers and valley aquifers. In highland aquifers, as occur in the study area, well yields are generally less than 50 gallons per minute: sufficient only for domestic and livestock use (Hilliel, 1980). In contrast, valley aquifers, such as Beebe Draw, have transmissivities as large as 20,000 ft^2/day and well yields greater than 1,000 gallons per minute (Robson, 1989; Hillier, 1980).

Some intervals of the underlying Arapahoe Formation serve as aquifers, with hydraulic conductivities typically 200 to 300 times lower than those in the highland deposits. These aquifers are generally grouped together as the Arapahoe Aquifer and are confined throughout most of the basin except in areas where the Arapahoe Aquifer outcrops or subcrops (Robson, et al., 1981 and Robson, 1989). In the study area the Arapahoe Formation outcrops at the western boundary along a regional erosional remnant at elevations above 5,100 feet, and underlies Beebe Draw at the eastern boundary at approximately 4,100 feet (Soister, 1964). Beebe Draw is a regional discharge zone for aquifers in the Arapahoe Formation (Robson, et al., 1981).

Recharge to the study area occurs via: infiltration from precipitation; seepage from Speer Canal; seepage from the ponds; and possible ground-water inflow from aquifers within the Arapahoe Formation. Irrigation is a significant source of recharge in some areas, but in the highlands, up-gradient from WCWD, there is no irrigated farming (based on areal photography and field reconnaissance). The only discharges for ground water are evapo-transpiration and ground-water outflow to Beebe Draw. If aquifers in the Arapahoe Formation are in communication with the unconfined aquifer in the study area it may act as either a ground-water source or sink.

Ground-water quality in the highland areas is generally poor, with TDS levels generally between 1,000 and 2,000 mg/L (Robson, 1989). Dissolved solids commonly present in significant quantities are calcium, sodium, iron, magnesium, bicarbonate, sulfate, and nitrate (Robson, 1989).

2.6 Conceptual Model Boundaries

The conceptual models encompass the ground-water system, defined approximately as the saturated materials within the surface-water divide surrounding the site, referred to as the WCWD aquifer or the system. The general area of interest is defined by the 3.2 mi^2 drainage basin which surrounds WCWD as shown outlined in red in Figure 4. Vertically the study area is bounded by a low permeability base, either the surface of the Arapahoe Formation or some deeper low permeability interval. Lateral boundaries are the highland drainage basin and the facies change to valley alluvial deposits to the east. Approximately 1.4 miles of Speer Canal flows across the study area. Boundaries are defined more precisely through data analysis and model testing, and vary among the different conceptual models.

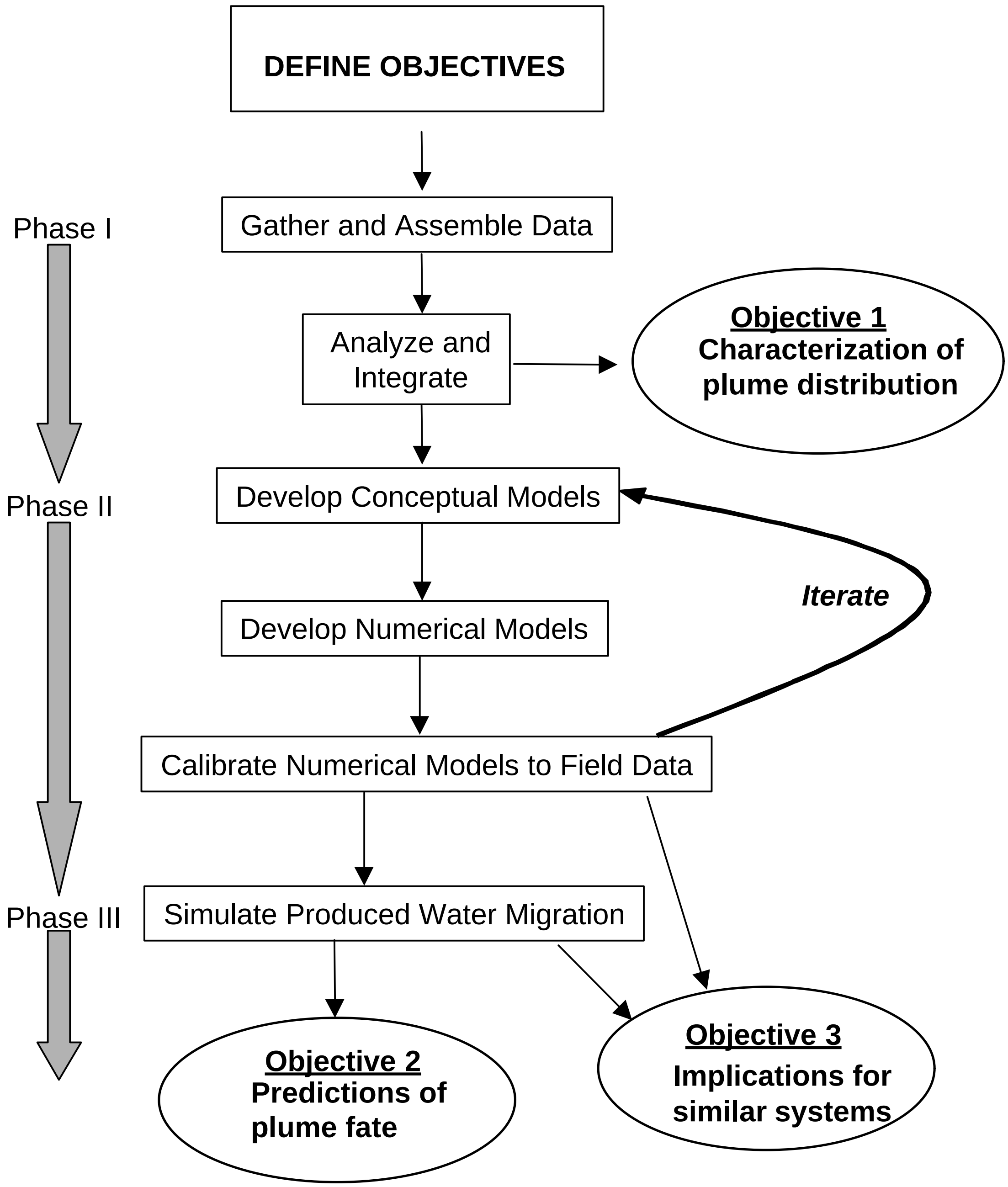
CHAPTER 3.0 STUDY METHODS

Study objectives are accomplished in three phases as described in the flow chart in Figure 5. Phase I consists of data collection and analysis, and accomplishes the first objective on the study: the characterization of the produced water contamination through identification of a tracer. In Phase II, using plume characterization data and other derived information describing the geohydrology of the system, conceptual models are developed that are viable representations of site conditions. These conceptual models are alternative representations of aquifer properties, such as hydraulic conductivity and recharge, in a manner which facilitates interpretation and manipulation by mathematical modeling. For each conceptual model, a numerical model is constructed and then refined using numerical inversion methods to ensure optimum model calibration, evaluate the confidence associated with the estimated parameter values, and identify those models which best represent the system. In Phase III viable conceptual models are used to predict the fate of the produced water plume, satisfying the second objective of the study. The final objective, to identify the implications of this project for other similar produced water contamination sites, is addressed through the analysis of the sensitivity of model predictions to input parameters, as well as the likely fate of the plume.

3.1 Data Analysis

Due to ongoing litigation between the EPA and LTE, access to the WCWD site has been denied, but sufficient data for this study is provided from the following three sources:

Figure 5. Flowchart of study methods.



1) Review of existing regional data sources including hydrologic, geologic, climatic, geochemical, and soils studies.
2) Existing site-specific public access data generated from studies conducted at WCWD by LTE and others, the most significant of which is the hydraulic head and geochemical measurements made in monitoring wells.
3) Independent data collection conducted on public and private lands with landowner permission, including:
   - "Grab" sediment samples collected and analyzed for grain size distribution and mineralogy;
   - Flow rates measured in Speer Canal;
   - Hydraulic heads measured in private wells;
   - Water samples collected and analyzed for major and trace chemical constituents from private wells and from Speer Canal; and
   - Electromagnetic induction (EM-34) surveys conducted in an effort to detect the relatively high conductance of the suspected produced water.

Analysis of these data provide the basis for development of alternative conceptual models. Analysis techniques include:

- Evaluation of the spatial distribution of hydrostratigraphic units and unit thickness, average potentiometric surface and gradients within the study area, chemical concentrations of tracers of produced water at selected times, and electrical conductivity distribution.
- Evaluation of the temporal variation of hydraulic head in monitoring wells and the variation of chemical concentration of a tracer of produced water in monitoring wells.
- Calculation of average and a likely range of aquifer parameter values within hydrostratigraphic units including: hydraulic conductivity, specific yield, and

dispersivity.

- Calculation of recharge rates of aquifer sources.

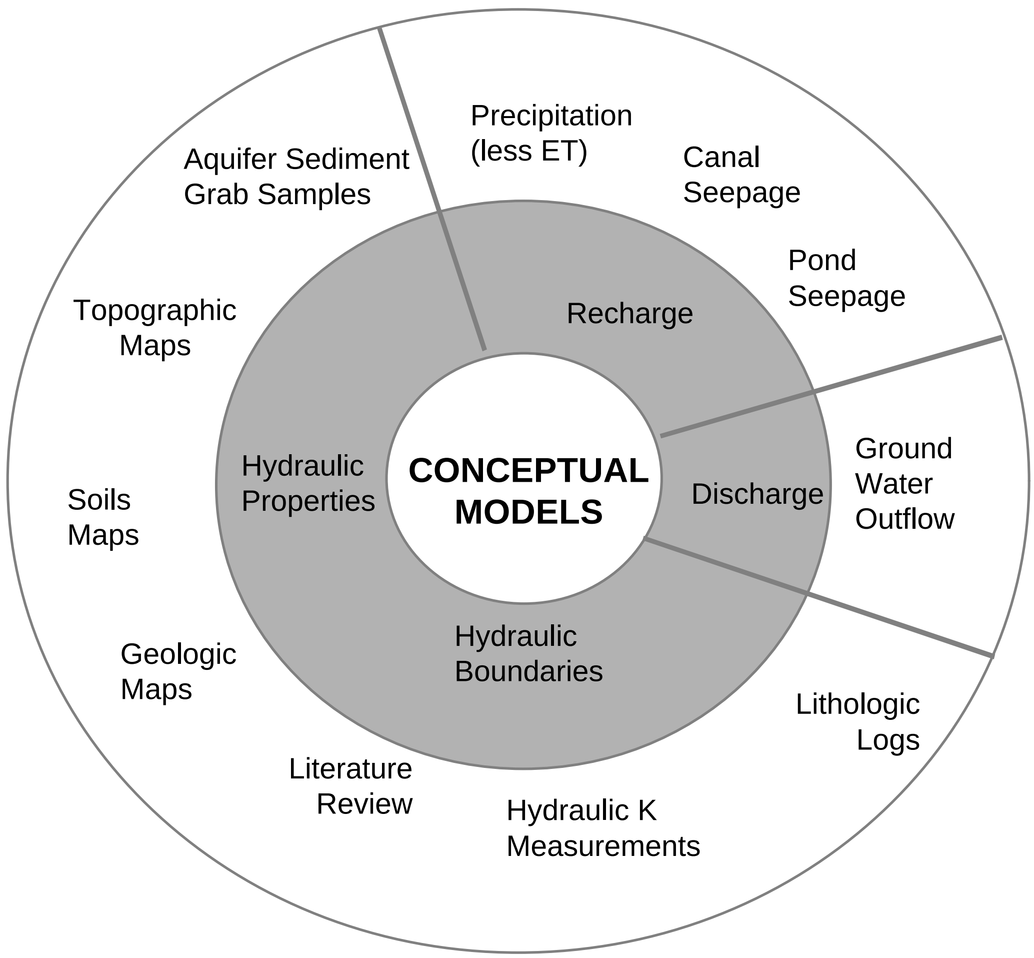
3.2 Conceptual Model Development

The results of the data analysis described in the above section do not define a unique system, rather they identify a range of aquifer geometries and distribution of aquifer properties. Consequently, several viable conceptual models are developed that describe likely geohydrologic systems. Figure 6 displays the construction of a conceptual model as a central hub of a wheel. Converging into the model are four input items which are required by the conceptual model. These are built from analysis and synthesis of the surrounding data defined on the outer ring of the diagram. Chapter 4 discusses the collection and analysis of the data and the generation of the four required modeling input items for the conceptual model. The conceptual models are developed using the Department of Defense's *Ground water Modeling System* (GMS). GMS is a computer program which is a spatially registered geographic information system (GIS) and a graphical user interface for the numerical models, MODFLOW and MT3D^{PD}, that facilitates the development of input files for the numerical models and allows for simulation results to be displayed graphically.

3.3 Numerical Modeling

Numerical models are used to integrate the data into a simulation of flow and solute transport. The requirements of the numerical model are that it be able to represent the geohydrologic system and predict migration of a conservative solute. The codes used in the study are:

Figure 6. Web diagram of conceptual model development. Conceptual model development begins with the collection of data identified in the outer circle, analyzing and synthesizing the data into the groupings in the next circle, and resulting in viable conceptual models.



1) MODFLOW (McDonald and Harbaugh, 1988, 1996)- a modular three dimensional finite difference ground-water flow model. This model calculates hydraulic heads and sub-surface flow rates for a given conceptual model.
2) $MT3D^{PD}$ (Zheng, 1996)- a modular three dimensional solute transport model which incorporates the MODFLOW output and aquifer dispersion characteristics. $MT3D^{PD}$ calculates the distributions of concentration at specified time intervals.

A third code used is UCODE, developed by Poeter and Hill (1998). UCODE is a parameter estimation code that is used to calibrate both MODFLOW and $MT3D^{PD}$ and to evaluate the confidence associated with estimated parameter values and predictions made using those values. The process of using MODFLOW and MT3D to calculate hydraulic heads or solute concentrations is referred to as simulation. The process of estimating optimum parameter values using UCODE is referred to as regression.

3.3.1 Governing Equations

MODFLOW calculates the flow of water of constant density through a porous medium in three-dimensions according the equation (McDonald and Harbaugh, 1988):

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

where:

K_{xx}, K_{yy}, and K_{zz} are the values of hydraulic conductivity along the x, y, and z coordinate axis, which are assumed to be parallel to the major axes of hydraulic conductivity [LT^{-1}];

h — hydraulic head, [L];

W — is a volumetric flux per unit volume and represents sources and/or sinks of water [T^{-1}];

S_s	is the specific storage of the porous material [L^{-1}]; and
t	time, [T];

The dissolved solute used to track produced water contamination is chloride. Justification for this is provided later in Chapter 4. Chloride is essentially non-reactive in ground water (Whittemore, 1988). Density differences between pond water and ambient ground water are related to chloride content. The average chloride concentration differences measured in WCWD disposal ponds and ambient ground waters in the study area (shown in Chapter 4 to be 13,000 mg/L and 85 mg/L respectively) are a magnitude of 1.0%, therefore density induced flow is not considered to be a significant process in the study area. The processes controlling solute transport at WCWD are therefore, advective transport and hydrodynamic dispersion. The equation used in MT3D^{PD} governing the three-dimensional transport of chloride is therefore reduced to (Freeze and Cherry, 1979):

$$\left[\frac{\partial}{\partial x}\left(D_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(D_z\frac{\partial C}{\partial z}\right)\right]-\left[\frac{\partial}{\partial x}\left(\bar{v}_x C\right)+\frac{\partial}{yx}\left(\bar{v}_y C\right)+\frac{\partial}{\partial z}\left(\bar{v}_z C\right)\right]+\frac{q_s}{\theta}C_s=\frac{\partial C}{\partial t}$$

where:

C	concentration of contaminants dissolved in ground water [ML^{-3}];
D_x, D_y, and D_z	hydrodynamic dispersion coefficient along the x, y, and z coordinate axis, which are assumed to be parallel to the major axes of hydrodynamic dispersion [$L^2\ T^{-1}$];
v_x, v_x, and v_z	seepage velocity along the x, y, and z coordinate axis, which are assumed to be parallel to the major axes of seepage velocity [LT^{-1}];
q_s	is the volumetric flux of water per unit volume of aquifer representing sources (positive) and sinks (negative) [T^{-1}] ;
C_s	concentration of the sources or sinks [ML^{-3}]; and
θ	porosity of the porous medium, dimensionless.

The estimation of optimal parameter values in UCODE is governed by minimizing the weighted least-squares objective function, S(b), defined by Hill (1998) as:

$$S(b) = \sum_{i=1}^{ND} \omega_i \left[y_i - y'_i(\underline{b}) \right]^2 + \sum_{p=1}^{NPR} \omega_P \left[P_p - P'_p(\underline{b}) \right]^2$$

where,

$\underline{b}$	vector containing values of each of the NP parameters being estimated;
ND	number of observations;
NPR	number of prior information values;
NP	number of estimated parameters;
y_i	ith observation being matched by the regression;
$y'_i(\underline{b})$	ith simulated value (a function of $\underline{b}$);
P_p	pth prior estimate included in the regression;
$P'_p(\underline{b})$	pth calculated value (a linear function of $\underline{b}$);
ω_i	weight of the ith observation; and
ω_p	weight of the pth prior estimate.

The differences $[y_i - y'_i(\underline{b})]$ and $[P_p - P'_p(\underline{b})]$ are residuals and represent the difference between simulated and observed values. The residuals are weighted to represent the relative importance of different observations in the regression. Weights are calculated as the square root of the inverse of the variance associated with the measured observation. Hill (1998) provides a complete discussion of the governing equations associated with UCODE.

In the process of minimizing the weighted least-squares objective function, UCODE calculates sensitivities of the estimated parameter values to simulated values such as hydraulic head. These sensitivities can also be used to derive valuable information about the model. UCODE utilizes both forward-difference and the more accurate central-difference sensitivities, respectively (Poeter and Hill, 1998):

$$\frac{\Delta y'}{\Delta b} = \frac{y'\left(\underline{b} + \Delta \underline{b}\right) - y(\underline{b})}{\Delta b}$$

and

$$\frac{\Delta_2 y'}{\Delta_2 b} = \frac{y'\left(\underline{b} + \Delta \underline{b}\right) - y(\underline{b} - \Delta \underline{b})}{2\Delta b}$$

where,

$\Delta y'$ change in the dependent variable value caused by the parameter value change, $\Delta \underline{b}$**;**

$\underline{b}$ vector, of the values of the estimated parameters;

$\Delta \underline{b}$ vector in which all values are zero except for one which corresponds to the parameter for which sensitivities are being calculated;

Δb nonzero value in $\Delta \underline{b}$, which is called the perturbation for this parameter; and

y'($\underline{b}$) and y'($\underline{b}$+$\Delta \underline{b}$) indicate that the value of y' is calculated using the parameter values represented by $\underline{b}$ or ($\underline{b}$+$\Delta \underline{b}$).

3.3.2 Model Calibration

Parameter values can differ significantly from measured values due to measurement error and aquifer heterogeneity. Calibration is the process of adjusting the model parameters, using measured and published parameter value ranges as guidelines, so that the difference between measured field conditions such as hydraulic head and contaminant concentrations and those simulated by a model are minimized. The data to which the models are calibrated include:

1) Water levels measured in wells. These consist of monitoring wells installed and monitored by LTE and independently sampled water levels in private wells.
2) Dissolved chloride levels from ground-water samples of LTE monitoring wells and independently collected water samples. The use of chloride as a tracer for produced water contamination is justified in Chapter 4.
3) Geophysical electromagnetic surveys performed in the study area. Measurements of soil conductivity identify concentration gradients and boundaries of produced water distribution within the study area.

The MODFLOW and MT3D^{PD} models are calibrated using UCODE. The basic purpose of UCODE is to statistically derive values for the input parameters of the models that minimize the objective function: the sum of squared weighted residuals of the difference between simulated hydraulic head and chloride concentrations and those observed in the field. The parameters to be estimated may include virtually any parameter assigned to a cell within the conceptual model (e.g. recharge and hydraulic conductivity). The code 1) substitutes specified starting values for the parameters to be estimated; 2) runs the application codes (MODFLOW and MT3D^{PD}); 3) calculates weighted residuals as the simulated minus measured value for each observation, multiplied by a user specified weighting factor; 4) sums the squared, weighted residuals to calculate the objective function; 5) perturbs each parameter value to calculate sensitivities; and 6) uses the weighted residuals and parameter sensitivities to estimate new parameter values that will decrease the objective function. This process is repeated until the estimated parameter values change less than a user specified tolerance, thus arriving at the optimal parameter values for the model. Additionally, UCODE reports statistical measures which can be used to evaluate the confidence associated with both the optimized parameter values and the predictions that are made using the optimized model.

For more information on parameter estimation and UCODE operation, consult Cooley and Naff (1990), Hill (1998), and Poeter and Hill (1998).

Besides greatly reducing the calibration effort, this tool facilitates evaluation and differentiation of conceptual models. Three general criteria are used to eliminate conceptual models that are not valid representations of the aquifer system: 1) estimated parameter values are not realistic, 2) poor fit of simulated values to measured values, and 3) biased residuals. These criteria are explained fully as they are used to accept/reject and rank results of conceptual model calibration in Chapter 6.

CHAPTER 4.0 SITE CHARACTERIZATION

The data analyses presented in this chapter are used to design conceptual models and calibrate numerical models. First, the data sources are presented, then each type of data is evaluated. A summary is provided in the final section.

4.1 Data Sources

The data include lithologic observations, hydraulic conductivity tests, hydraulic head measurements, water chemistry analyses, and electromagnetic measurements of material conductivity. The three main sources of data are: 1) existing regional studies, 2) work performed by LT Environmental and Parsons Engineering, described in Table 1 and located in Figure 7, and 3) data collected specifically for this study, described in Table 2 and Figure 8. Generally, the spatial distribution of data collected by LTE and Parsons Engineering is focused in the immediate vicinity of the disposal ponds and additional data collected for this study extends the data coverage throughout the study area. The majority of the data used in this study are measurements of hydraulic head and chloride concentration in LTE monitoring wells and in two monitoring piezometers. The locations of these data are shown in Figure 9.

4.2 Hydrostratigraphy

Analysis of the well log data and review of regional studies identifies three distinct lithologies that are likely to behave as individual hydrostratigraphic units. From oldest to youngest these are: the Arapahoe Formation, the Arapahoe gravel, and a loess.

Table 1. Data type and number of data points used in this study collected by LT Environmental and Parsons Engineering (see Figure 8 for locations).

Data (Source)	*Date(s)*	*Lithology*	*Hydraulic Conductivity*	*Hydraulic Head*	*Chemical Analyses*
Monitoring Well (LTE)	MW#1-13, 1984 MW#14-18, 1986 MW#19-23, 1997	12	4	22 (monthly pre-1997, quarterly post-1996)	22 (quarterly)
Monitoring Piezometer (Parsons Engineering)	1995	nm	nm	2	2
Borehole (LTE)	1997	12	nm	nm	nm
Shallow Corehole (LTE)	1997	13	nm	nm	nm
Geoprobe© Sampling Point (Parsons Engineering)	1995	292[1]	nm	29	29

nm = not measured
MW = monitoring well
[1] Based upon penetration resistance.

Table 2. Data type and number of data points collected for this study (see Figure 8 for locations).

Data Source	*Date(s)*	*Lithology*	*Hydraulic Head*	*Chemical Analyses*	*Electrical Conductivity*
Speer Canal Water	1996, 1998	nm	2[1]	2	nm
Private water wells	1998	nm	3	4	nm
Electromagnetic Geophysical Surveys using Geonics EM-34[2]	1998	nm	nm	nm	HML[3] and VML[4] at 20m spacing.

nm = not measured
[1] Flow velocity and cross-sectional area were also measured at these 2 locations.
[2] The EM-34 measures the conductivity of the earth material which is a function of lithology, hydaulic head, and water chemistry.
[3] Horizontal Magnetic Loop or Vertical Magnetic Dipole.
[4] Vertical Magnetic Loop or Vertical Magnetic Dipole.

Figure 7. Location of LT Environmental and Parsons Engineering Sample Points.

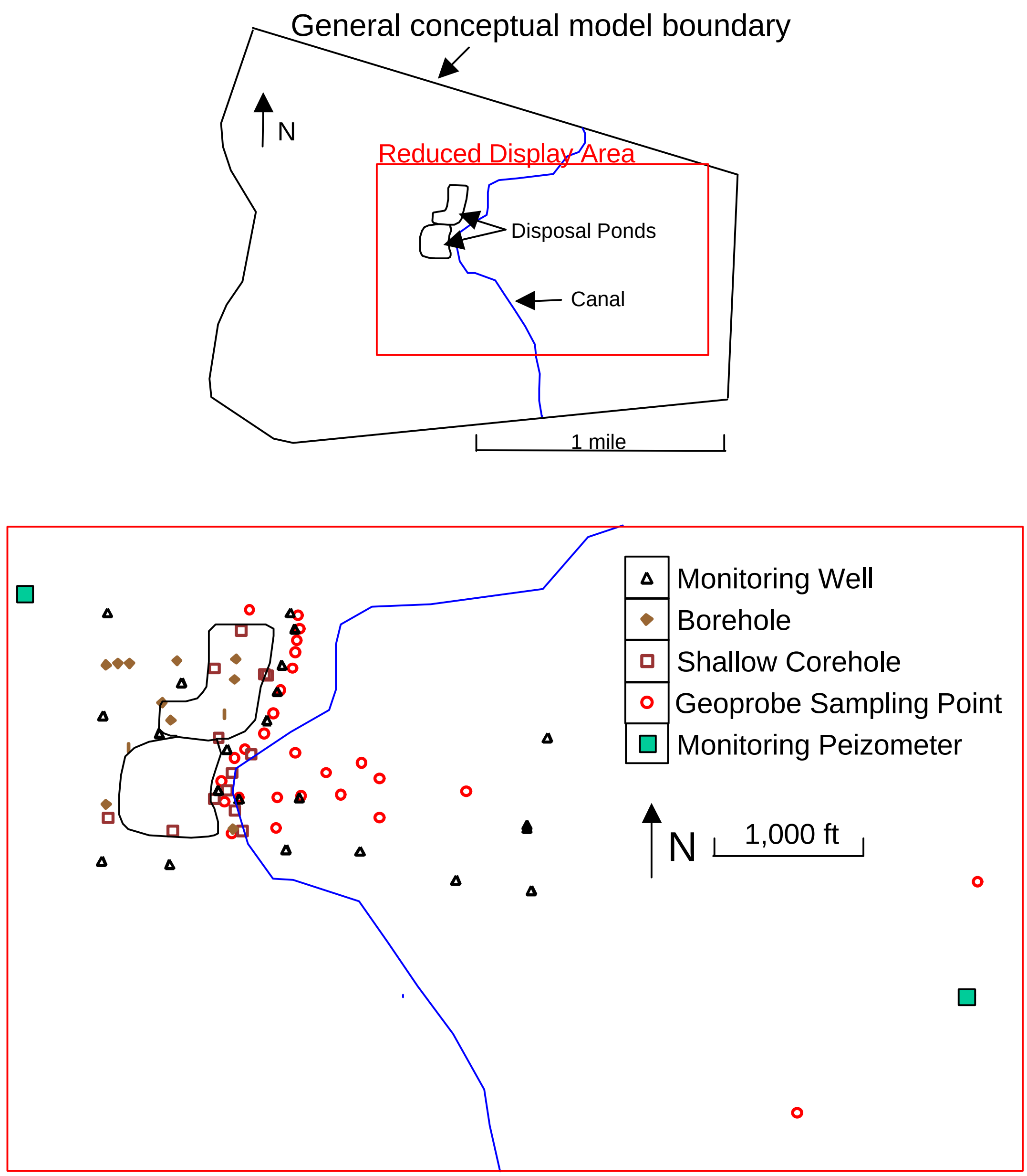


Figure 8. Location of study specific data sampling points. One canal chemistry sample location is located north outside the featured area as indicated by the arrow.

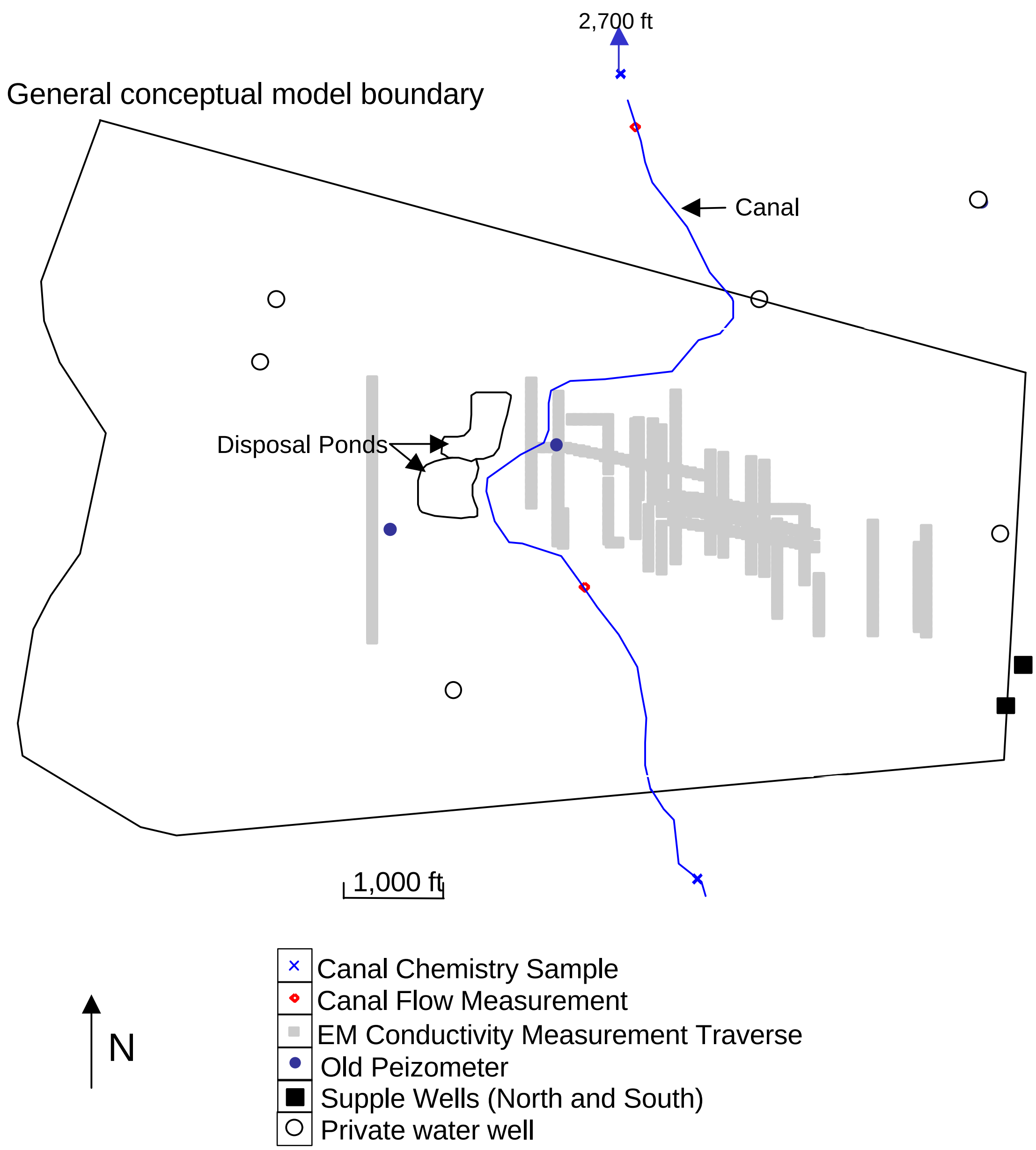
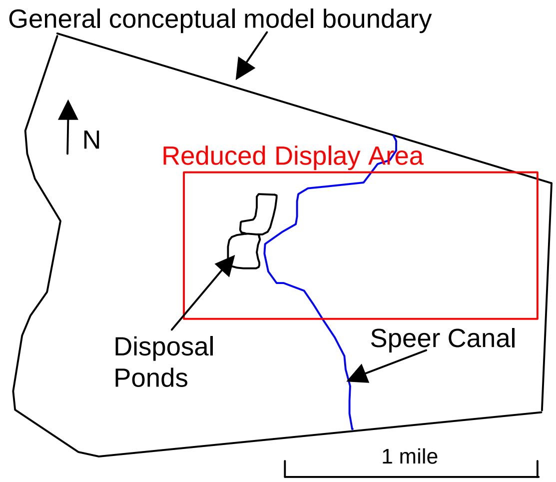
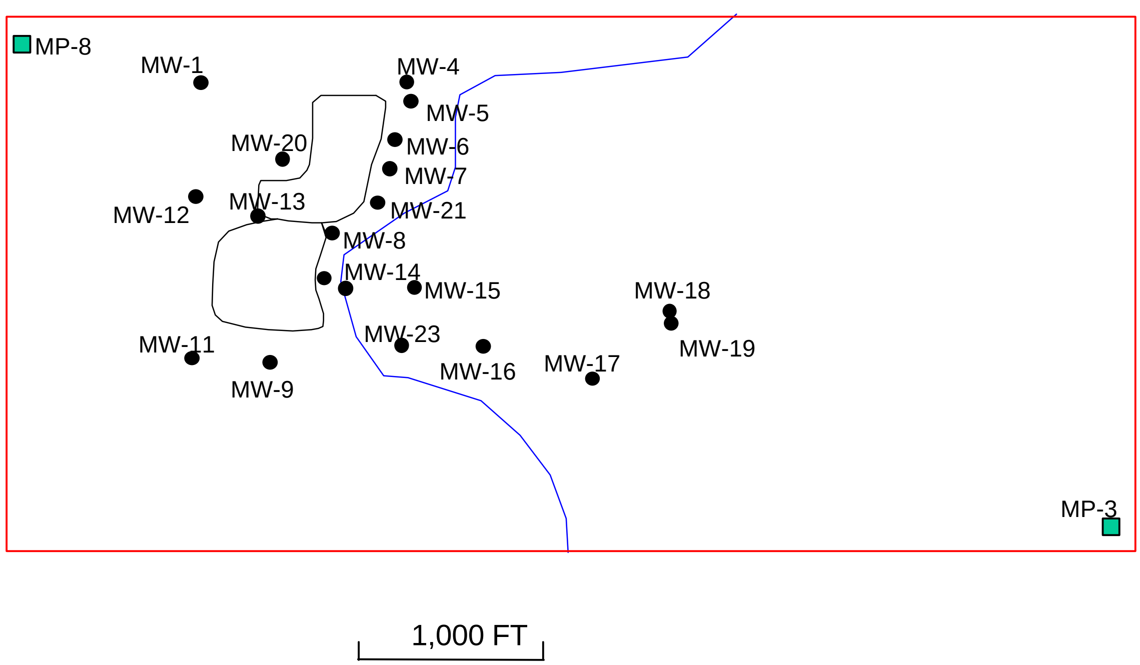


Figure 9. Location of LTE monitoring wells (shown as black circles) and Parsons Engineering monitoring piezometers (shown as green squares).



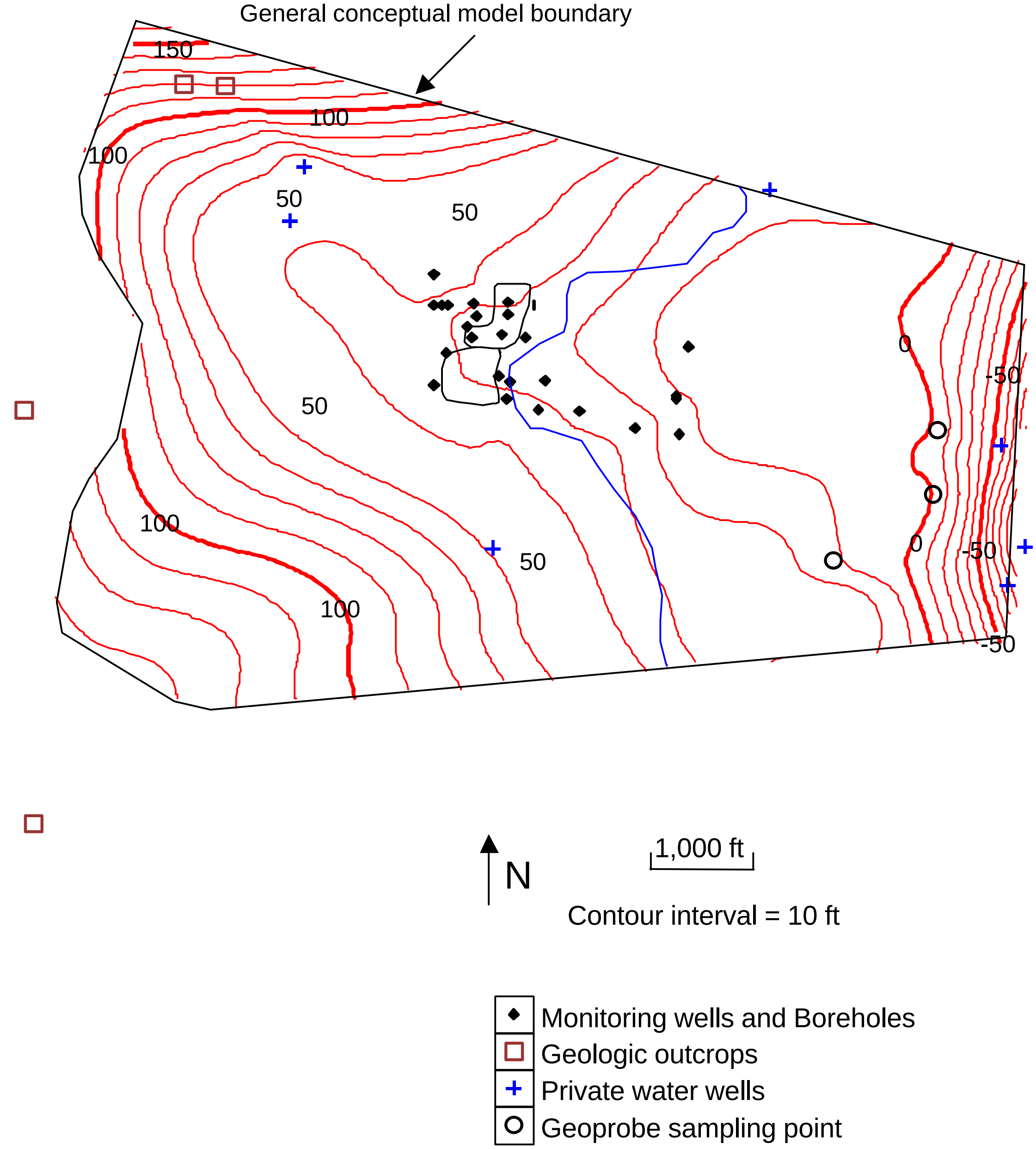


4.2.1 Arapahoe Hydrostratigraphy

The Upper Cretaceous Arapahoe Formation is approximately 250 feet thick in the study area, with approximately 50 feet of this interval comprised of permeable conglomerate, sandstone, and siltstone (Robson, 1981). Transmissivities range from 192,500 ft^2/day to 3,850,000 ft^2/day (Robson, 1981). The base of the formation dips at 0.003 ft/ft to the south, which is essentially horizontal at the scale of this study. The upper surface of the Arapahoe Formation is a Pleistocene fluvial erosional unconformity. Fourteen monitoring wells intersect the top of the Arapahoe Formation, completing at this surface within a hard, occasionally weathered claystone. Weathering during exposure of this surface may have enhanced permeability. Monitoring well 19 is the only well that penetrates the Arapahoe Formation, being completed 30 feet below the top of the formation (location shown in Figure 9). The well log for MW-19 indicates interbedded layers, one to ten feet thick, of sandstone, shale and claystone, with varying degrees of water saturation. Total depth of MW-19 is 54 feet below ground surface, terminating in a 5 ft interval of hard, dry, black shale. The well is screened in a 5 feet interval of sandstone immediately above the black shale. The surface of the Arapahoe Formation may act as an aquitard or aquiclude to ground-water flow in the overlying unconsolidated deposits, or it may be hydraulically connected with the WCWD aquifer.

In the immediate vicinity of the ponds the top of the Arapahoe Formation is identified by five data sources: 26 monitoring wells and boreholes, 7 private water well logs, surface outcrops in four locations, and three Parsons Geoprobe© sampling points (the remainder of the 29 data points are redundant). Contours of the data (Figure 10) delineate a basin similar to the surface drainage basin, with a south-east trending erosional channel that may control ground-water flow. The eastern portion of the Arapahoe Formation surface drops suddenly at 0.1 ft/ft into the valley fill channel of Beebe Draw at 4110 feet above mean sea level (Figure 10). The Parsons Geoprobe© data use penetration resistance to identify the Arapahoe contact which is prone to

Figure 10. Top of the Arapahoe Formation. Contours were generated by interpolating the data points shown using the natural neighbor quadratic routine in *GMS*. Elevations are referenced to 5,000 ft above mean sea level.



error, and when this data is not considered the slope of the Arapahoe Formation into Beebe Draw is much more gradual, sloping at approximately .04 ft/ft into Beebe Draw at 4110 feet above mean sea level.

4.2.2 Unconsolidated Hydrostratigraphy

The unconsolidated deposits in the study area contain two hydrostratigraphic units: Arapahoe gravel and loess. They are defined by integrating 22 well logs from LTE with geologic reports (Soister, 1965; Colton, 1974; 1978), Quaternary geologic studies (Madole, 1994 and 1995) and soils reports (Crabb, 1980). Eolian sand overlies these two hydrostratigraphic units, but is generally not saturated and therefore not considered in this study. The two hydrostratigraphic units are:

- Arapahoe Gravel- Well logs recorded by LTE identify a light brown, very fine-grained to coarse-grained sand and gravel unit with interbedded with silts and clays. LTE classifies the unit as a silty gravel (GM) based on the United Soil Classification System (USCS). Thickness of the Arapahoe gravel ranges from 0 to 12 feet. The unit does not outcrop in the study area. The unit is likely derived from fluvial scouring of the ancestral Platte River through the Rocky Flats Alluvium and the Arapahoe Formation. The thickness of this unit likely increases towards Beebe Draw to the east. While it is also reasonable to anticipate the thickness of this unit to increase in the location of the erosional channel in the surface of the Arapahoe Formation as a result of fluvial processes, this correlation is not evident from lithologic data.
- Loess- Pleistocene loess deposits described as, tan to dark brown, clayey and sandy silt, and silty and sandy clay, are continuous in the study area (Madole, 1995) and overly the Arapahoe Formation and Arapahoe gravel. This unit is likely derived from glacial processes along the front range (Madole, 1995). LTE classifies the units as a

silty clay of low plasticity (ML) based on the USCS. Thickness of the loess ranges from 5.0 feet to 18.8 feet and the unit is likely continuous in the study area.

Both units exhibit substantial variation in thickness over short distances (0 feet to 15 feet in less than 200 feet). Because of heterogeneities, and because no sources of hydrostratigraphic architecture exist other than monitoring well data in the immediate vicinity of the ponds, the units cannot be mapped accurately in the subsurface. Therefore, the Arapahoe gravel and loess are considered to compose a single hydrostratigraphic unit.

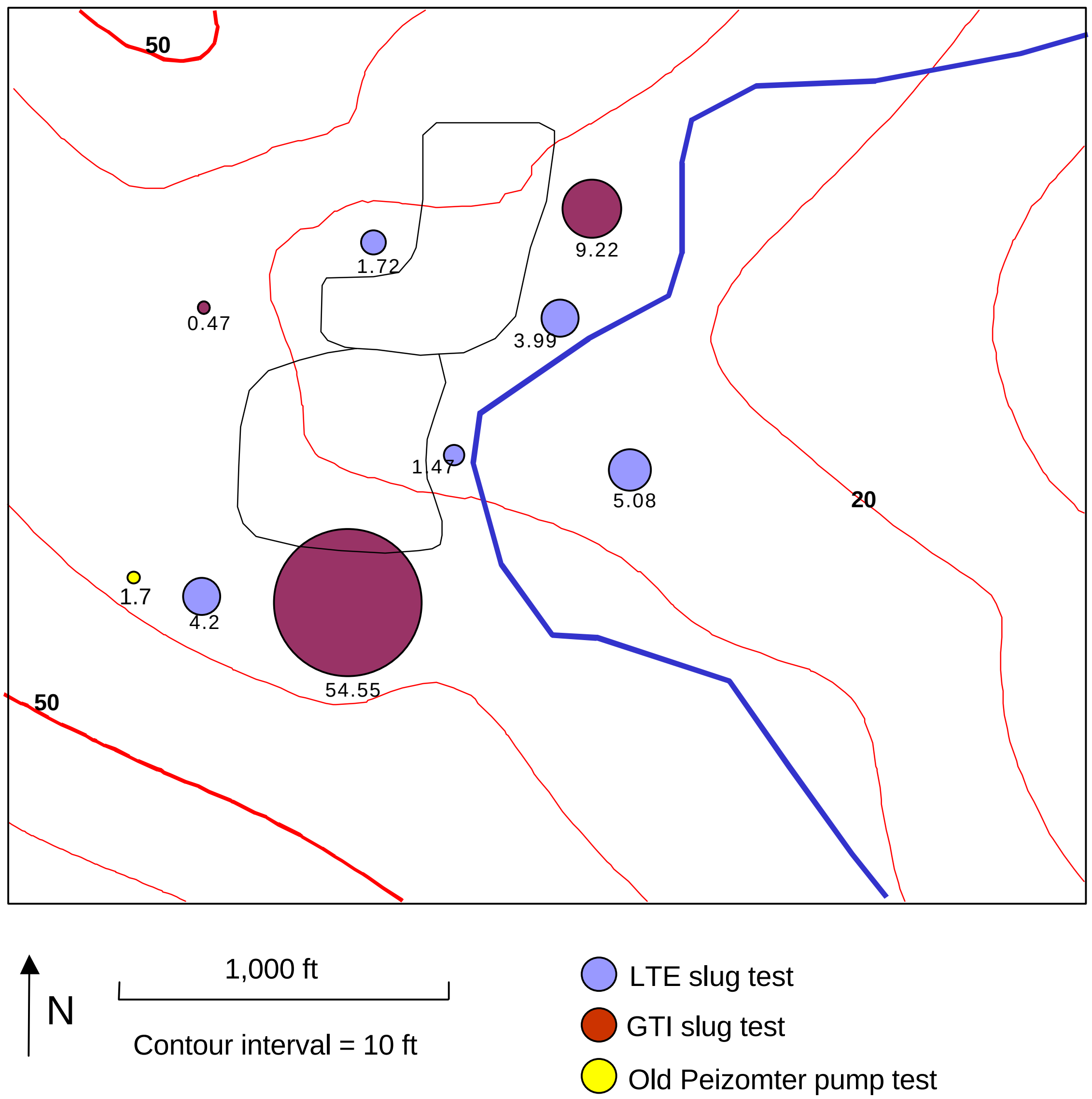
Effective porosity, or specific yield, is the amount of water that will drain from a unit volume of material by gravity. Specific yield values typically range from 0.01 to 0.10 for clays and from 0.10 to 0.30 for sands (Driscoll, 1986). To account for the significant amount of clay present in the unconsolidated hydrostratigraphic unit, an average value of 0.10 is assumed.

4.3 Hydraulic Conductivity

Hydraulic conductivity has been measured by Ground Water Technology Inc. (GTI) in three monitoring wells (1985), and by LTE in (1997) in 7 wells, using rising head slug tests. Additionally, a single well pump test was performed on an old piezometer, named Old Piezometer, just west of MW-11 by the investigator and interpreted using the Jacob straight line method. Completion schedules are not available for wells in which the GTI tests were performed or for the piezometer test. Therefore, these data are considered less reliable than the LTE data. The hydraulic conductivities calculated for tested wells are posted in Figure 11 with contours of the surface of the Arapahoe Formation.

Almost all of the wells are screened from above the water table to the surface of the Arapahoe Formation and therefore the tests do not reflect the hydraulic conductivity

Figure 11. Measured hydraulic conductivity in monitoring wells. All values are in ft/day. The size of the data point is proportional to the magnitude of the value. Contours describe the surface of the Arapahoe Formation referenced to 5,000 ft above mean sea level. The outline of the ponds is shown in black, and the canal location is shown as a blue line.



of individual units. The well tests provide only average hydraulic conductivities for the entire screened interval. Values range from 0.47 ft/day to 54.55 ft/day, with a geometric mean of 7.58 ft/day. The high value of 54.55 ft/day (GTI, 1985) is an outlier. Using only the LTE data, the geometric mean of the hydraulic conductivity measurements is 2.3 ft/day with a standard deviation of 1.8 ft/day. Although the values do not correlate with the erosional channel present in the surface of the Arapahoe Formation, the channel may significantly influence ground-water flow because of the increased thickness of the unconsolidated deposits in the channel area.

An aquifer test was performed in MW-19, which is screened in a five foot thick sandstone unit 30 feet below the top of the Arapahoe Formation. The geometric mean of four rising head tests gives a hydraulic conductivity value of 1.38 ft/day.

Because both unconsolidated deposits and the Arapahoe Formation contain fine-grained sands and coarse gravels, hydraulic conductivity values have a large range of reasonable values. Freeze and Cherry (1979) list typical values ranging as high as 3.0×10^{5} ft/day for gravels, and as low as 3.0×10^{-4} ft/day for loess. The slug tests in the study area indicate that this range may be reduced by two orders of magnitude to a maximum of 3.0×10^{3} ft/day and a minimum of 3.0×10^{-2} ft/day.

4.4 Hydraulic Head

The aquifer underlying WCWD may be comprised of both unconsolidated deposits and portions of the Arapahoe Formation. This sections analyzes hydraulic head in both units.

4.4.1 Arapahoe Aquifer

Approximately 60% of the total thickness of the Arapahoe Formation in the study area is considered a prolific aquifer (Robson, et al., 1981). In the region of the study area, the average hydraulic head in aquifers within the Arapahoe Formation is near the land surface, with a potentiometric gradient to the east/southeast ranging from 0.12 to 0.02 (Robson, et al., 1981). Based upon regional potentiometric contours, some of the lowest heads observed in the basin are in Beebe Draw, which acts as a regional discharge zone for the Arapahoe aquifers. Monitoring well MW-19 is the only monitoring well completed in the Arapahoe Formation. Hydraulic head levels in this well are on average 0.5 feet greater than that measured in the adjacent MW-18 which is completed in the unconsolidated deposits, 35 feet above the completed interval in MW-19. The gradient between these two completed intervals is 0.014 upward. This indicates that the study area is in a regional discharge zone.

4.4.2 Unconsolidated Aquifer

The average hydraulic head measured in monitoring wells and private water wells is shown in Figure 12. The potentiometric surface is hand-contoured as a solid line in the area of data coverage and dashed in other areas. Ground-water flow is to the east-southeast with an inflection point in the potentiometric surface in the vicinity of MW-18. Hydraulic gradients range from 0.016 in up-gradient areas, to 0.002 in down-gradient areas. The decreasing gradient may be due to an increase in aquifer thickness, an increase in hydraulic conductivity associated with thicker gravel deposits, or a decrease in discharge. Hydrographs for all monitoring wells are posted in Figure 13.

Hydrographs for all monitoring wells (Figure 13a) exhibit regularly oscillating water levels, with rising levels in the summer and decreasing levels in the winter. Oscillations are as large as 6 feet. This pattern correlates with the operation of Speer Canal and the amplitude of the oscillation within a well is directly related to the proximity of each well to the canal, both up and down-gradient. In the down gradient direction the amplitude of oscillation decreases from 5.6 feet in MW-14, located 20 feet down-gradient, to less than 2 feet in MW-18, located 1,750 feet down-gradient. In the up-gradient direction canal effects are apparent as far as 500 feet west in MW-13.

Figure 12. Average hydraulic head in monitoring wells and private wells manually-contoured to a datum of 5,000 feet above mean sea level. Dashed lines indicate areas of poor data coverage. The arrows depict the direction of the hydraulic gradient, with corresponding magnitudes posted.

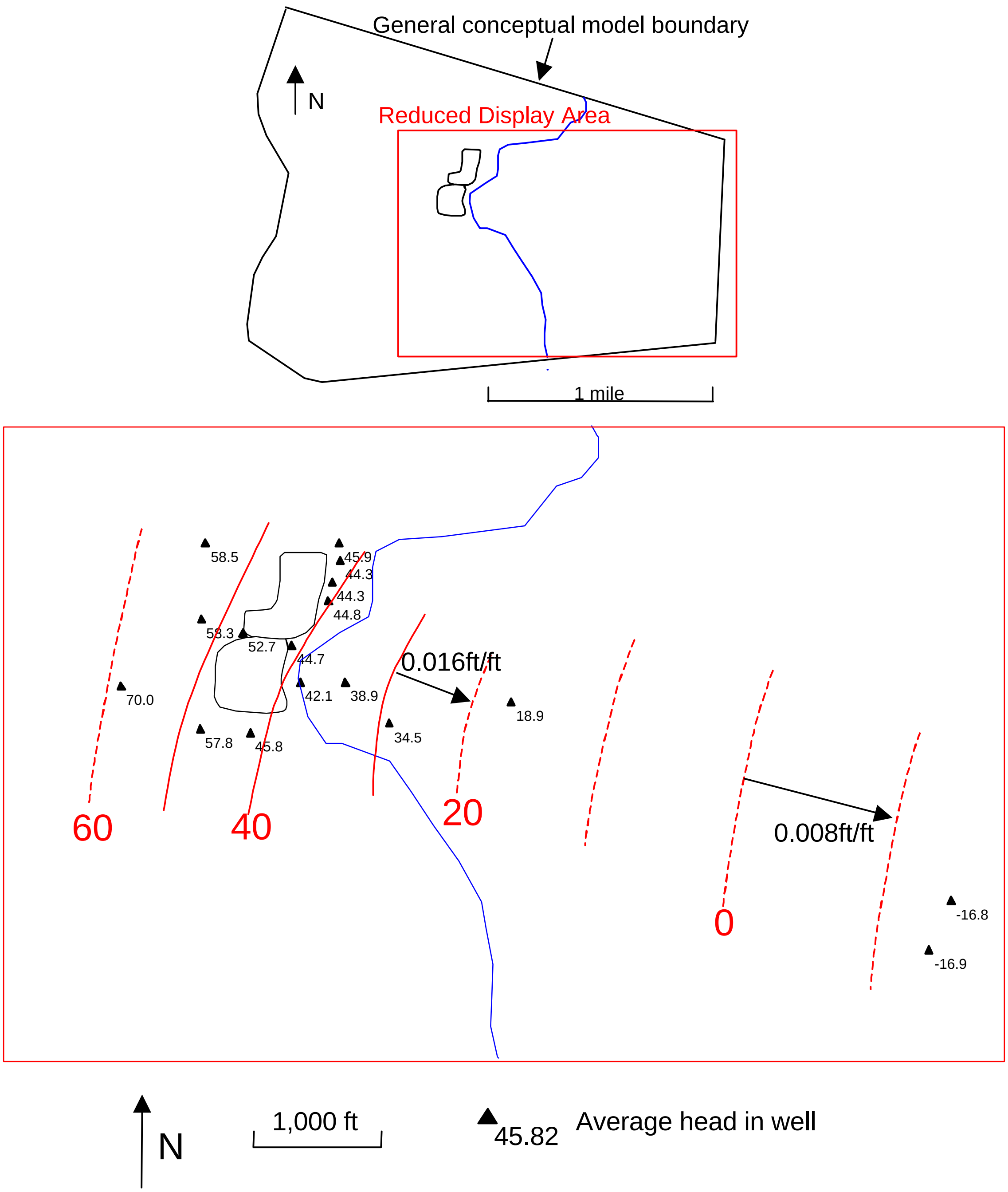
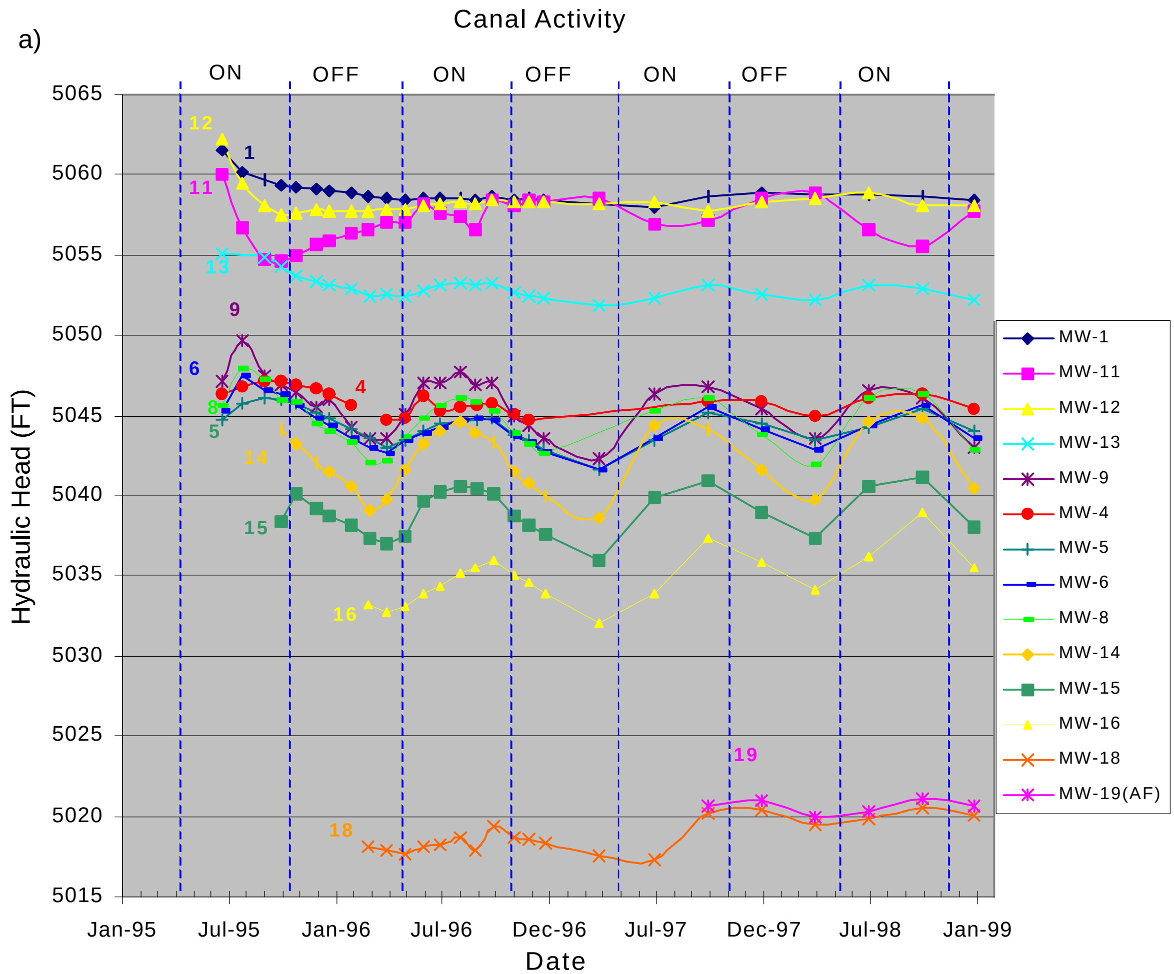
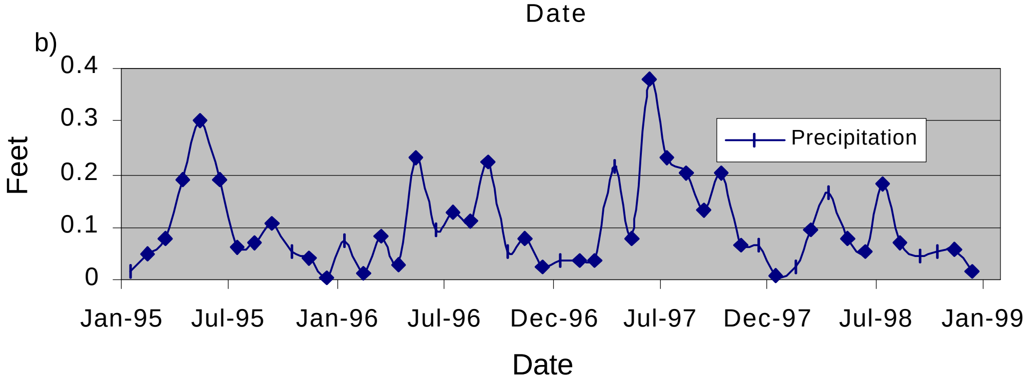


Figure 13. (a) Hydrographs for all monitoring wells and (b) precipitation from June of 1995 to December 1998 recorded 10 miles to the southwest at Brighton, CO (NOAA, 1998). The activity of Speer Canal, from late April to late October, is annotated with vertical divisions, indicating if the canal is "on" or "off". The location of the monitoring wells is shown in Figure 9.





Precipitation (Figure 13b) correlates with the hydrograph oscillations and may be contributing to the oscillation. The largest precipitation event was 4.56 inches in June of 1997. A maximum of 10% of this amount infiltrates to the water table (Hurr, et al., 1975). The porosity of the soil has been established to be 0.10. The maximum rise in ground-water levels attributable to precipitation is calculated to be only 4.56 inches, far less than the observed oscillation amount. Therefore, the canal is the principal source of recharge to the system and precipitation is a minor contributor.

Another water source to the aquifer are the evaporation ponds. The three most up-gradient wells, MW-1, MW-11, and MW-12, exhibit a steep decline by as much as 5 feet from maximum hydraulic heads in June of 1995, one month after the facility stopped receiving additional waste.

Additional head measurements were made at two domestic water supply wells, Supple North and Supple South, along the eastern border of the study area and at the Old Piezometer located in Figure 8. Water levels in these wells were recorded on four occasions during 1998 using a depth sounder. The elevations of the wells were estimated from topographic maps. The water levels in the Supple wells fluctuate very little over time and may be affected by both WCWD ground-water flow and flow in the Beebe Draw aquifer, which is interpreted by Soister (1954) to lie immediately to the east of the Supple wells. Measurements taken in the Old Piezometer fluctuate less than one foot over a six month period and the fluctuations correspond to seasonal canal activity.

4.5 Ground-water Sources and Sinks

Recharge comes from ground-water inflow, precipitation, canal seepage, and pond seepage. The possible sinks for ground water are evapotranspiration and ground-water outflow to Beebe Draw, which cannot be measured directly. Average values for these fluxes, and reasonable ranges of values, are estimated and later used as initial values for numerical modeling.

An initial average value of recharge may be estimated as a percentage of precipitation. Total annual precipitation is 12.6 inches a year. The percentage of precipitation which recharges the aquifer is likely less than 10% (Hurr, et al., 1975), or less than 3.45×10^{-3} ft/day. Because of the large uncertainty of this value, it is assumed that this value may vary +/- 50%, from 1.73×10^{-3} ft/day to 5.18×10^{-3} ft/day. Some of the models presented in this study do not directly simulate discharge from aquifers within the Arapahoe Formation or the process of evapotranspiration, but rather incorporate these processes into a single recharge value. Therefore, for these models it is possible that the value of recharge may be near zero or negative and a minimum reasonable value of recharge for these models is not presented.

Speer Canal operates from late April to late October, at rates of 30-85 cfs (Manuel Montoya, oral communication, FRI Corp., 9/15/98). The flow rate and cross-sectional flow area of Speer Canal was measured twice during the summer of 1998. The average width of the canal is 24 feet and the average depth is 2 feet. The average velocity is 156,000 ft/day through a measured cross-sectional area of 48 ft^2, giving an average flow rate of 7.5×10^{6} ft^3/day (87 cubic feet per second). The calculated average volumetric rate of seepage based upon up-gradient and down-gradient flow rate measurements made 7,500 ft apart is 193,000 ft^3/day, giving a seepage rate of 1.1 ft/day during the six months of canal operation over the length of the canal across the study area. This is 145% higher than the average rate loss quoted by the canal operators of 0.75 ft/day (Montoya, verbal communication 9/15/98), however, this value is not specific to the study area and the measured value is considered more accurate. Considering the error of the measured value, a reasonable range of 50% is assigned to this value, and canal seepage rates may vary from 0.55 ft/day to 1.7 ft/day.

Sampling of the pond bottoms by LTE failed to identify a continuous low permeability liner that was reported to have been installed. Vertical permeabilities measured in 5 samples from the pond bottoms ranged from 2.7×10^{-4} ft/day to 3.5 ft/day, with a geometric mean permeability of 8.3×10^{-4} ft/day. Assuming that: 1) the average depth of the ponds was 3 feet, an elevation of 5056 ft; and 2) the average elevation of the bottom of the pond liner is coincident with the average water table elevation below the ponds at 5049 feet (from Figure 12), the gradient is 1.75. The average rate of recharge from the ponds is calculated to be 1.5×10^{-3} ft/day, but could vary by as much as four orders of magnitude depending on the true hydraulic conductivity of the liner material, ranging from 1.5×10^{-5} ft/day to 0.15 ft/day.

4.6 Ground-water Chemistry

This study addresses only inorganic contaminants associated with produced water. This section discusses background-water quality, identifies chloride as an effective indicator of produced water contamination, and evaluates the distribution and fluctuation of chloride in monitoring wells.

4.6.1 Ground-water Quality

The majority of the geochemical data for the study area is from water samples from monitoring wells sampled by LTE. These wells are located in the immediate vicinity of the ponds. The first sampling of water for chemical analysis began in August of 1990. Monitoring wells were sampled quarterly by LTE beginning in August of 1990 for the following major inorganic constituents: chloride, iron, sodium, and total dissolved solids (TDS). Sources of background ground-water and surface-water quality in the study area come from published studies (Joncox and Gaggiani, 1992; Schneider, 1931; Gas Research Institute, 1990; Parsons Engineering, 1995; and LT Environmental, Monthly Progress Report, December, 1996) and water sampling performed for this study from locations shown in Figure 9. Major constituents are listed in Table 3.

Table 3. Water quality of eolian and alluvial aquifers and selected produced water sources. All measurements are in mg/L.

Sample Location	Source[1]	Date	Interval[2]	TDS	Ca	Mg	Na	K	Cl	HCO3	SO4	N (NO3 + NO2)
Platteville	JG	7/85	E/VF	4,270	380	330	360	30	90	2,800	2,400	330
Beebe Draw	Sch	9/31	VF	790	100	38	120	4.4	90	330	220	7.9
Martin	McC	3/98	E/VF	960	110	27	130	1.5	75	435	175	1.0
Supple South	McC	3/98	E/VF	2,080	210	77	270	6.8	150	220	1100	10
Supple North	McC	3/98	E/VF	1,940	220	83	220	5.8	162	225	980	10
Old Piezometer	McC	3/98	E	8,400	494	206	1,590	34	500	754	3,100	388
Trostel	McC	3/98	L/FH	900	1.6	0.6	220	1.5	93	585	nd	nd
Speer Canal South	McC	5/97	SC	580	75	17	91	8.6	31.3	180	57	1.6
Speer Canal North	McC	5/97	SC	580	71	15	84	7.9	44.5	183	92	1.8
Produced Water[3]	GRI	1990	K	7,790	72	34	2,940	nm	3,840	1,240	100	nm
Pond C	Par	9/95	PC	16,800	nm	nm	nm	nm	7,640	nm	nm	nm
Pond D	Par	9/95	PD	20,100	nm	nm	nm	nm	9,840	nm	nm	nm
Pond D	LTE	6/96	PD	43,000	nm	nm	6,420	nm	22,000	nm	nm	nm

nm – not measured; nd = not detected

[1] Source key: JG-Joncox and Gaggiani, 1992; Sch- Schneider, 1931; McC- author, 1998; GRI- Gas Research Institute, 1990; Par- Parsons Engineering, 1995; LTE, LT Environmental, December, 1996.

[2] Interval key: E- eolian; VF- valley fill; L/FH- Laramie/Fox Hills Formation; K- Cretaceous; PC- Pond C; PD- Pond D.

[3] Average produced water from the Denver Basin.

Methods of analysis are documented only for LTE water samples. Ground-water samples acquired by the author were collected and analyzed for the constituents listed in Table 3 according to the methods outlined in Table 4. Samples were collected using a peristaltic pump after approximately three well volumes were removed. Ground water samples collected by LT Environmental used the same analysis methods listed in Table 4, although documentation of collection protocols are not available.

Table 4. Geochemical sampling methods and analysis techniques for LTE samples and samples collected for this study.

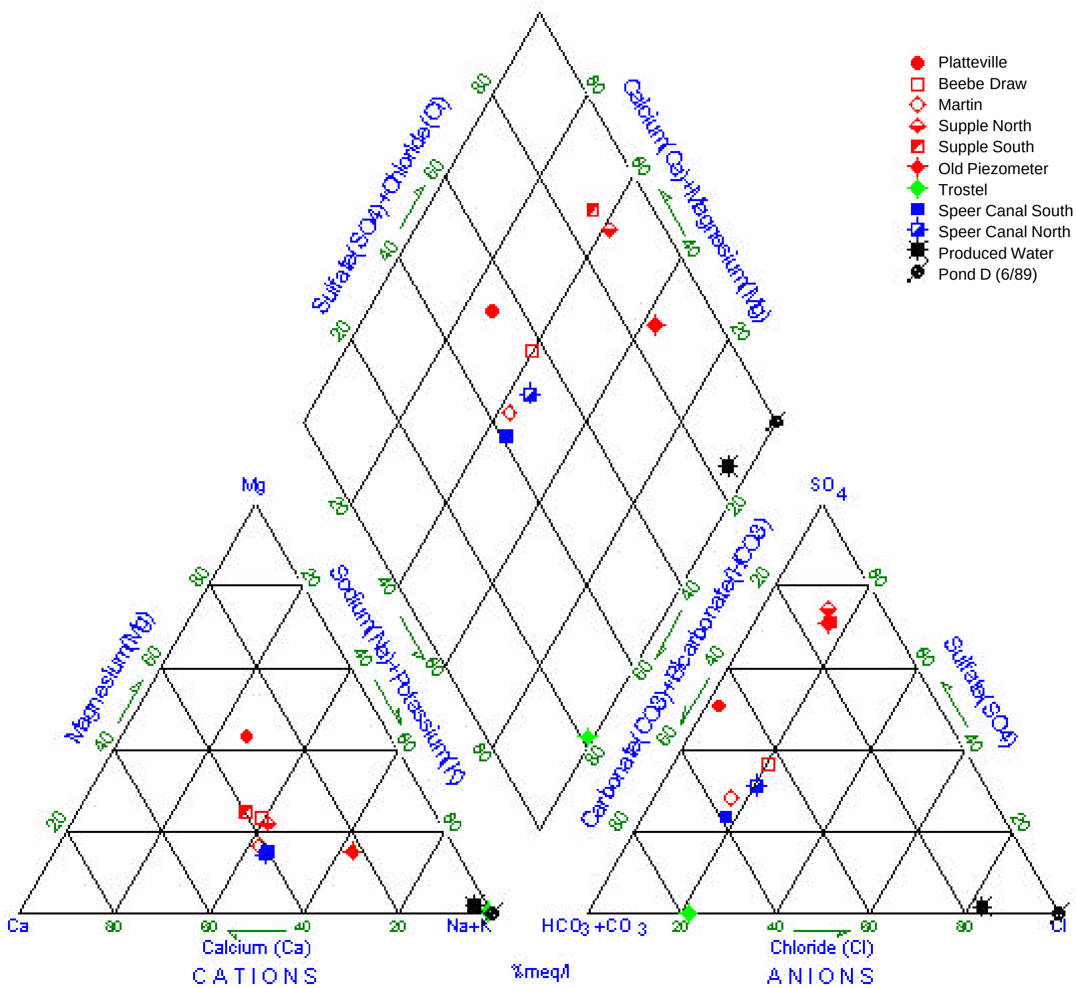
Constituent	*Volume*	*Filtered*	*Acidified*	*Analysis Method*
HCO_3	125 mL	not filtered	not acidified	Titration
Ca, Mg, Na, K[1]	125 mL	not filtered	acidified	Inductively Coupled Plasma
Ca, Mg, Na, K[1]	125 mL	0.2 ìm	acidified	Inductively Coupled Plasma
Cl, SO_4, NO_3	125 mL	0.2 ìm	not acidified	Ion Chromatograph

[1] Measured values for filtered and un-filtered samples do not differ significantly and values reported in Table 3 are those measured in filtered samples.

A Piper diagram in Figure 14 displays relative water composition for samples listed in Table 4 (except for samples from ponds C and D taken in 1995 due to limited constituent analysis). Ground-water samples from the eolian/valley fill aquifers (with the exception of the Old Piezometer sample), Arapahoe Formation, and Beebe Draw are sodium bicarbonate waters of similar composition, although different TDS. Speer canal water is also of this type and of low TDS. The produced water samples, in contrast, are sodium chloride waters of high TDS.

The average of three measurements of chloride concentration of produced water in ponds, or source strength, is 13,000 mg/L. The actual chloride concentration of produced water in ponds likely varies significantly over time due to evapotranspiration, dilution from precipitation, and the variable disposal rate and chloride content of waters disposed in the ponds. A reasonable maximum and minimum source strength is determined as 25% greater than the maximum measured chloride concentration in

Figure 14. Piper diagram comparing sources of background water quality with samples of produced water. Aquifer key: red = eolian and valley fill; green = Arapahoe Formation; blue = Speer Canal; black = produced water. Samples from ponds C and D taken in 1995 are not shown due to lack of data. Generally, all waters are sodium bicarbonate waters and produced waters are sodium chloride waters.



produced waters in Table 3 (Pond D, 1996 = 22,000 mg/L), and 25% less than the lowest chloride concentration of produced waters in Table 3 (Average produced water concentration in Denver Basin, = 3,840 mg/L); or a maximum of 27,500 mg/L and a minimum of 2,880 mg/L. These values are significantly greater than chloride contents of water from the canal and monitoring wells and ambient ground water.

4.6.2 Identification of Chloride as a Tracer of Produced-Water Migration

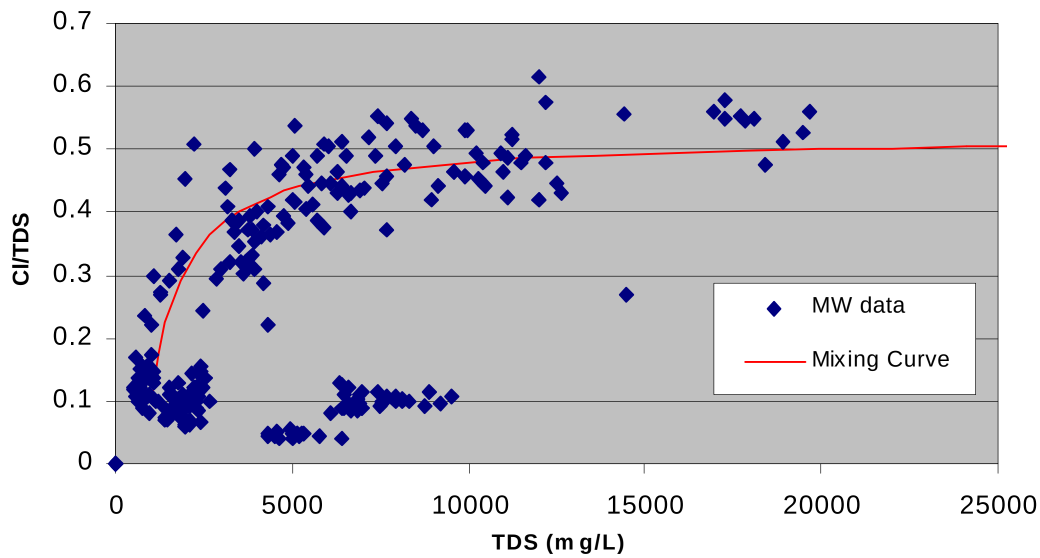
Chloride (Cl) is not a major constituent of highland ground waters near WCWD and is generally chemically non-reactive, therefore it may be an effective tracer of produced water migration (Stossell, 1997). TDS versus the ratio of Cl to TDS is presented in Figure 15 along with a curve calculated for mixtures of water from Pond D (1996) with a theoretical background water, consisting of 100 mg/L CL and 1,000 mg/L TDS. The trend of the mixing curve approximately matches the monitoring well data and suggests the presence of three distinct water compositions in the WCWD aquifer:

- a high TDS, high chloride water (produced water),
- a low TDS, low chloride water (ambient ground water),
- and a moderate TDS, low chloride water (a third water type not anticipated).

The third water type is present only in monitoring wells 9 and 11, located directly south of the ponds. Water samples taken from the Old Piezometer, located 50 feet west of MW-11, and a one-time sampling event in MW-9 and MW-11 (the only LTE sampling in monitoring wells that tested for nitrate) showed high nitrate levels in these wells. The past use of the property directly west of these well included turkey farming. Wastes from the farm may account for the high nitrate in ground waters.

At least two sources may account for increased TDS levels in ground water, however, high chloride does appear to be unique to monitoring wells near the WCWD site. A background chloride concentration of 85 mg/L is established from the average

Figure 15. TDS versus CL/TDS for all monitoring well data and mixing curve for theoretical ground water and Pond D water. The data closely follow a theoretical curve, derived from mixing increasing amounts of water from Pond D measured in 1996, with a hypothetical background water.



<u>Hypothetical Background Water</u>
Cl=100 mg/L
TDS=1,000 mg/L

<u>Pond D Water</u>
Cl=22,000 mg/L
TDS=43,000 mg/L

chloride content of samples taken from private wells within the eolian/valley fill aquifer listed in Table 4 (the Supple wells and Old Piezometer are excluded due to suspected influence from the WCWD).

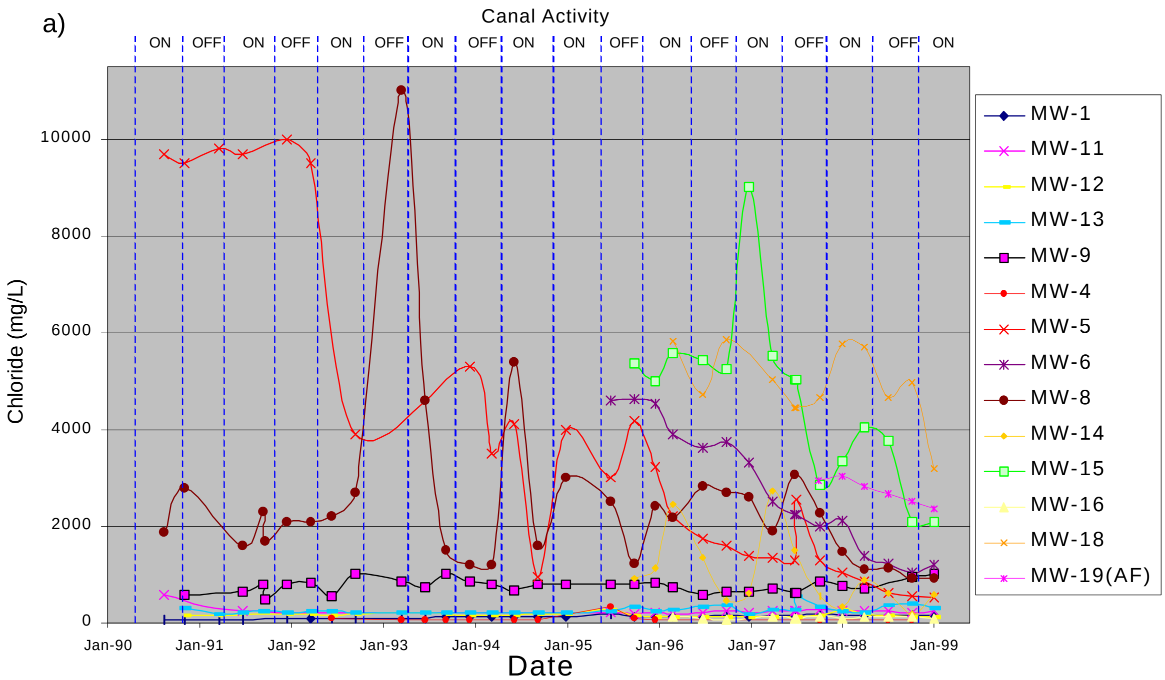
4.6.3 Chloride Distribution

Variations in chloride levels in monitoring wells over time are presented in Figure 16. A large scale is used in Figure 16a to show the entire data set, while the reduced scale of Figure 16b better displays low chloride concentration values. Generally, chloride levels decrease with time after the closure of WCWD in May of 1995. Canal activity is posted on the graph. There is a slight correlation between chloride levels and canal operation due to dilution of the ground water by the canal water during the summer months. The temporal variation of chloride concentrations is also affected by the source strength and depth of produced water in the ponds which may act to obscure this inverse correlation at times. Up-gradient monitoring wells MW-1, MW-11 and MW-12 are impacted by produced water, showing chloride concentrations as high as 190 mg/L, 575 mg/L, and 300 mg/L respectively. This may be due to contaminant transport when the hydraulic gradient is reversed by large canal or pond recharge rates or due to surface spills in the up-gradient area. The data set shown in Figure 16 is used subsequently to provide observations for the calibration of solute transport models.

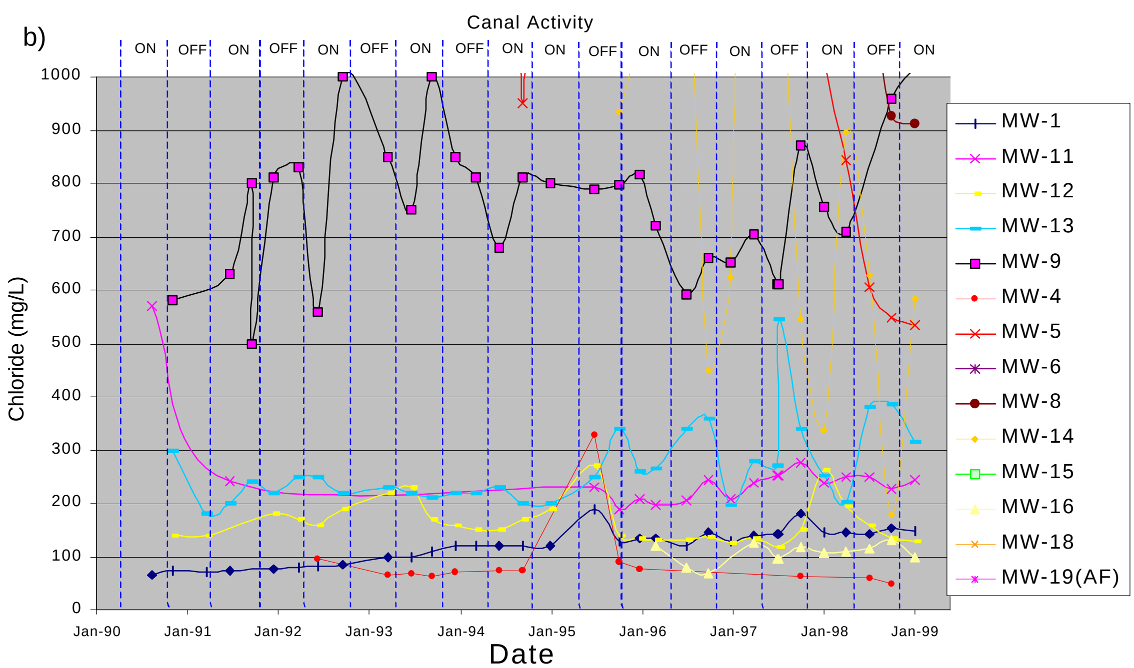
Monitoring well MW-19, which is the only monitoring well completed in the Arapahoe Formation, exhibits chloride concentrations up to 3,000 mg/L, and varies at levels approximately half the concentration measured in adjacent MW-18 which is completed only within the unconsolidated deposits. Produced water has therefore contaminated portions of the Arapahoe to at least that depth (43 ft below the average water table at that location). More data is needed to vertically characterize the distribution of chloride.

Figure16. Chloride concentrations as a function of time in all monitoring wells (a), and for wells with low chloride values (b). Overall, chloride concentrations decrease with time in monitoring wells after the closure of WCWD in May of 1995. Chloride variation is affected by canal activity and produced water concentrations and depth in the disposal ponds.

a)



b)



Chloride concentrations measured in monitoring wells in December of 1998 are manually-contoured in Figure 17. The effect of dilution from canal waters is most apparent in MW-14, which is omitted during contouring. The data show that the greatest chloride concentrations are related to Pond D, which contained produced water until April of 1997, whereas Pond C was empty by December of 1995. The plume illustrates a unique form, appearing to converge down-gradient towards MW-18, rather than disperse as would be expected due to hydrodynamic dispersion. The trends of the data indicate that high chloride concentrations continue east along the same trajectory from MW-18 to the study area boundary and remains focused laterally. This could be indicative of convergent flow caused by a high conductivity zone. Another possibility is that the plume is not converging and the sampling locations are not sufficient to identify the true geometry of the plume. Two possible alternative plume geometries are shown in Figure 18: a plume that 'fingers' down-gradient due to heterogeneous conditions, as shown in Figure 18a; and a plume that descends into the aquifer due to vertical gradients as it disperses laterally, as shown in Figure 18b, which has a football-like shape.

4.6.4 Chloride Transport

The processes controlling solute transport at WCWD are advective transport and hydrodynamic dispersion. The following sub-sections define these processes and present reasonable values for parameters describing these processes.

Advective Transport

Advective transport is the average rate at which a particle moves through the aquifer, and is the primary process causing contaminant migration at the site. Advection is a function of the seepage velocity, *v'*, or the quotient of Darcy velocity and effective porosity:

$$v' = Ki/f$$

Figure 17. Chloride concentrations measured in monitoring wells in December, 1998. Values are manually contoured. The plume is focused as it travels down-gradient indicative of convergent flow.

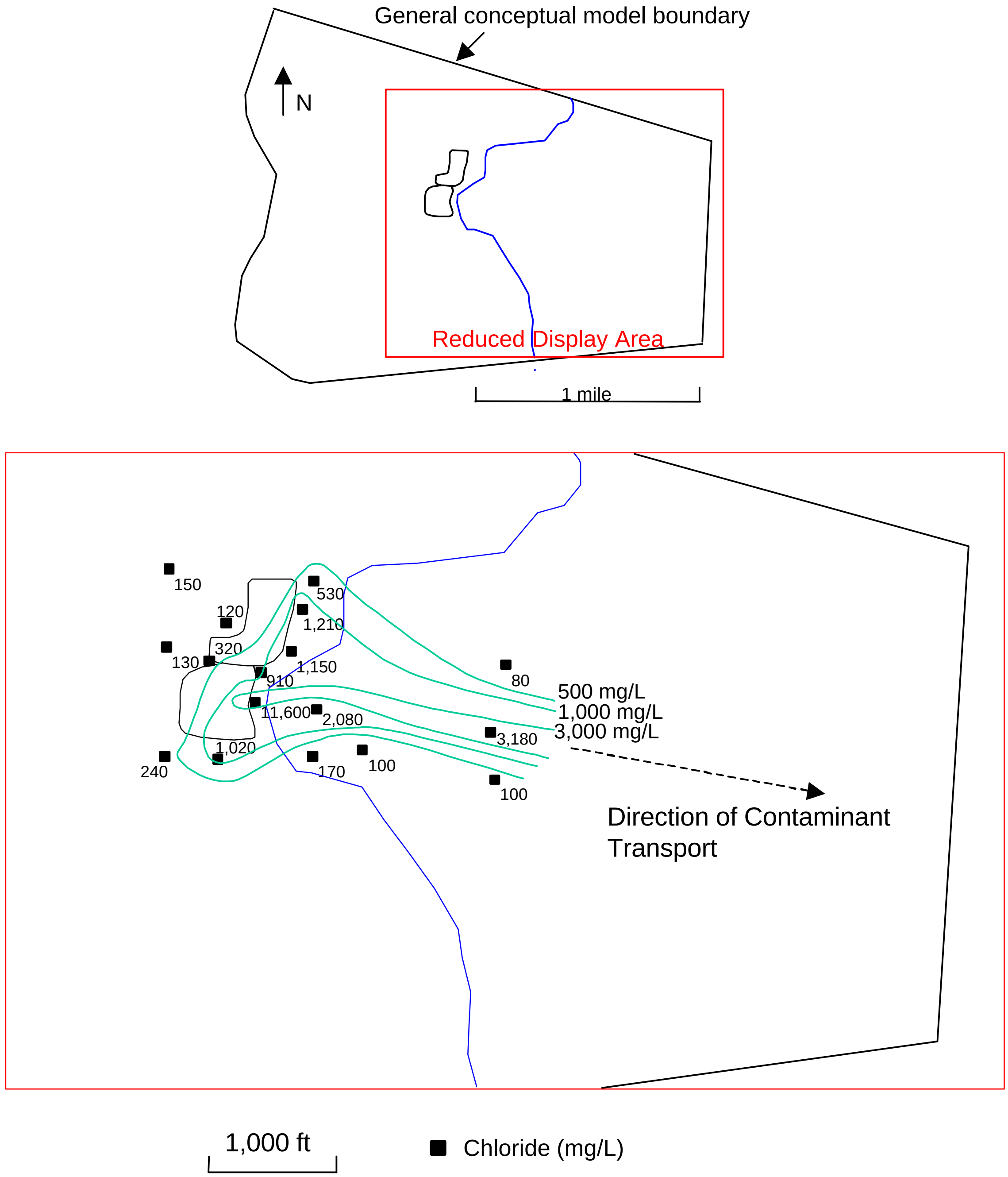
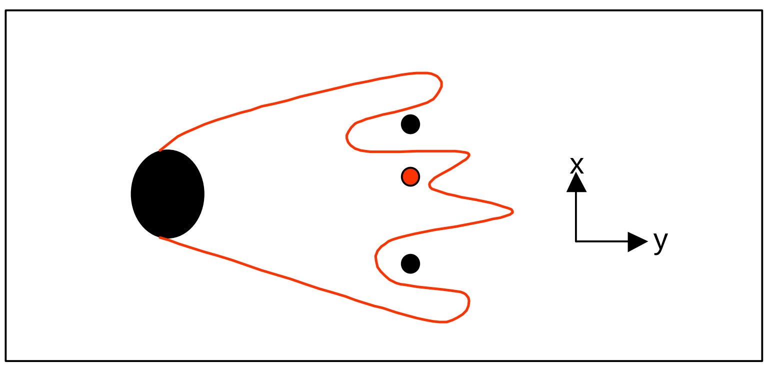
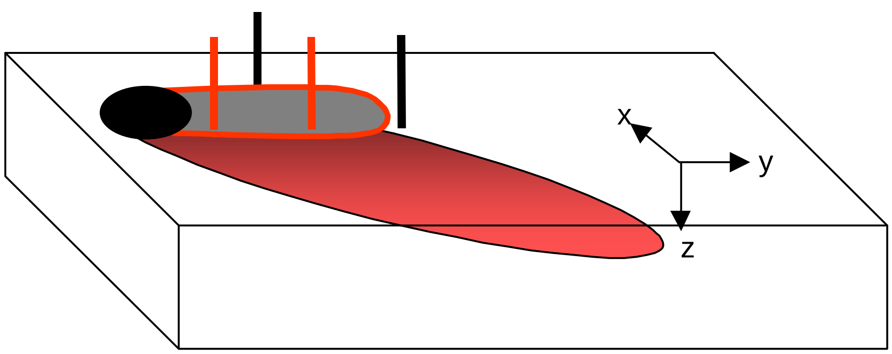


Figure 18. Possible schematic alternative chloride distributions. The source area is shown in black and plume distribution is shown in red. Wells not sampling impacted water are black and those sampling high chloride values are red. a) Horizontal 'fingering' of the plume is caused by aquifer heterogeneity and accurate characterization is dependent upon well placement. b) The descending plume is in the shape of a football, and accurate characterization is dependent upon well placement and screening depth.

a)



b)



Using average values for hydraulic conductivity (3 ft/day), hydraulic gradient (0.016 ft/ft), and effective porosity (0.1), the average value of seepage velocity for the WCWD aquifer is 0.5 ft/day. Another estimate of seepage velocity may be obtained using specific conductance measurements made in May of 1997 in down gradient areas (not shown). Specific conductance is proportional to TDS and elevated specific conductance values measured 4,000 ft down gradient from the ponds in mid 1997 (20.5 years after disposal activity began) may be caused by produced water. In which case, produced water would have traveled at an average rate of 0.5 ft/day, suggesting that the average values used for calculating the rate of advective transport are reasonable.

Hydrodynamic Dispersion

Hydrodynamic dispersion is the combined effect of molecular diffusion and differences in velocity and flow path. The effect of molecular diffusion is insignificant except at very low velocities, thus the coefficient of hydrodynamic dispersion is simplified to:

$$D_i = \mathrm{a}_i v'$$

where:

D_i dispersion coefficient in direction *i*, [L^2/T^{-1}]; and

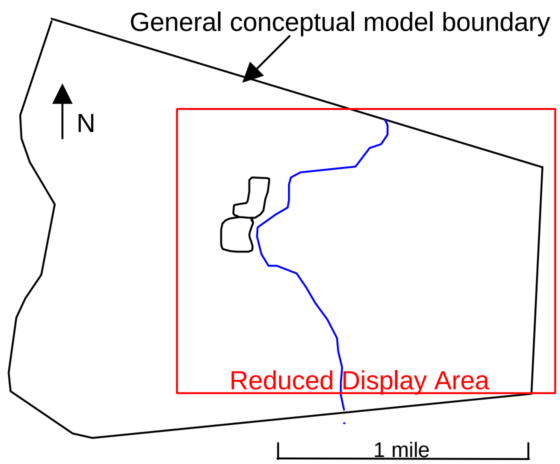
a_i dispersivity of the porous medium in direction *i*, [L].

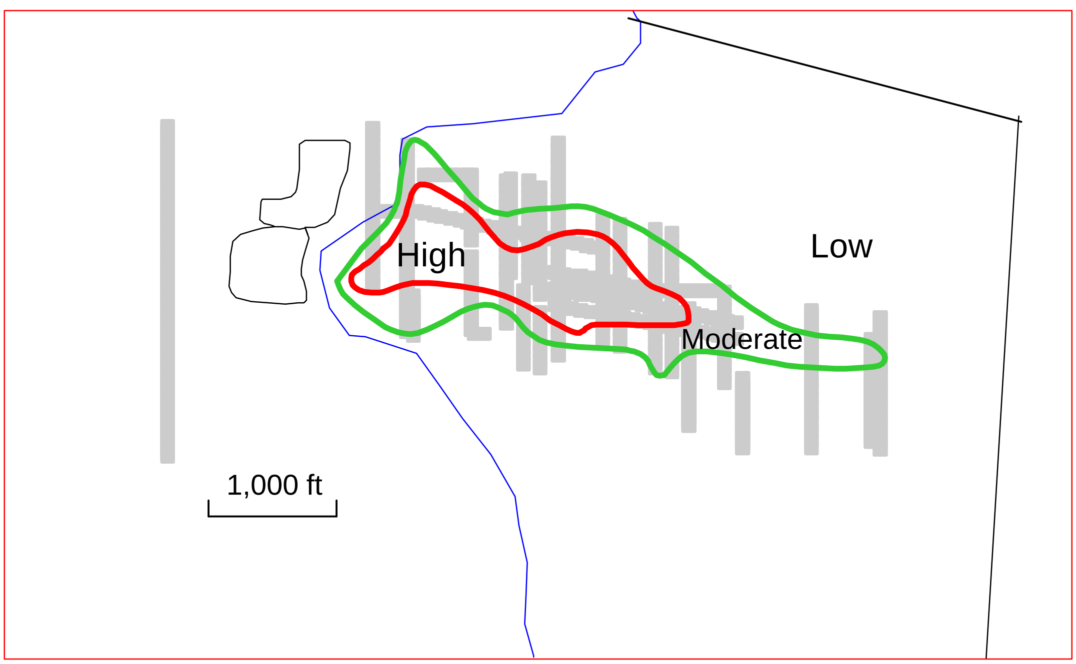
The dispersivity of a material is measured by fitting the dispersion coefficient to field observations of contaminant migration. Dispersivity is related to the scale of the plume. Based on work by Gelhar et al. (1992) a factor of 0.10 is used for a plume that has migrated approximately 4,000 ft (from specific conductance measurements not presented), giving a longitudinal dispersivity of 400 ft. Reasonable values may range by as much as an order of magnitude in either direction. Dispersivity in the lateral transverse direction (orthogonal to flow) is usually considered to be approximately 0.1 to 0.5 times the longitudinal dispersivity (Gelhar et al., 1992). Limited information exists on characteristic vertical dispersivity and values are considered to be about an order of magnitude lower than lateral transverse dispersivity. Initial values of lateral transverse dispersivity and vertical transverse dispersivity are assumed to be 0.2 and 0.04 of longitudinal dispersivity respectively.

4.7 Electrical Conductivity

The electrical conductivity of the unconsolidated units was measured four times during 1998 using geophysical electromagnetic surveys to determine if changes in the cumulative electrical conductivity of the soil and water matrix could be correlated to changes in chloride concentration in ground water. Over 1,200 measurements were made along more than 6 miles of transects (transects are shown in Figure 8). Appendix A presents the sampling procedure used and the data are included on the compact disk. The electromagnetic surveys detected significant changes in the cumulative electrical conductivity of the sediment and water matrix. Contouring the relative magnitude of the more reliable data collected in December 1998 produces the pattern shown in Figure 19. This pattern is similar to the chloride distribution shown in Figure 17, although low conductivity values occur immediately down gradient of the ponds in areas where high chloride concentrations are measured. In order to use electrical conductivity values as additional observations for calibration, a relationship between conductivity and chloride concentrations must be determined. Unfortunately, electrical conductivities are not correlated with chloride levels in nearby monitoring wells. Explanations for this include: geophysical sampling events were not conducted at the same times as water sampling for chloride analysis; the metal collar of monitoring wells may influence conductivity measurements; and conductivity measurements may be reflecting electrical conductance of deeper intervals than those sampled by monitoring wells. Further discussion is

Figure 19. Contour of relative magnitude of reliable electrical conductivity data measured in December 1998. Measurements were made using electromagnetic techniques along transects shown in gray. Measurements are consitent with the high ionic strength of the produced water plume. A discussion of sampling methods and results is included in Appendix A.





included in Appendix A. Given that the data produces a pattern similar to chloride measurements, Figure 19 is used to qualitatively evaluate the calibration of conceptual models later in the study. Additional work using geophysics is recommended for future study.

4.8 Results of Data Analysis

Several types of data contribute to characterizing the properties and parameters of the WCWD aquifer and the distribution and migration of the produced water contamination plume. A summary of the results of data analysis is listed below, grouped according to the required conceptual model data inputs as illustrated in Figure 6.

4.8.1 Hydraulic Boundaries

- The surface of the Arapahoe Formation in the field area identifies a drainage basin consistent with the surface topography, with the exception of a "low" beneath the ponds in the axis of the drainage which may be indicative of an erosion channel.
- The unconsolidated deposits are considered as a single hydrostratigraphic unit. Individual stratigraphic units within the unconsolidated deposits cannot be characterized in three dimensions throughout the field area due to heterogeneity and poor data distribution.
- Portions of the Arapahoe Formation serve as aquifers that may influence chloride migration but aquifers within the Arapahoe Formation cannot be delineated in the study area with the existing data. Bedding in the Arapahoe Formation is horizontal in the study area.
- Hydraulic head near the Beebe Draw aquifer at the eastern boundary of the study area is essentially constant at 4984 above mean sea level (amsl).
- Ground-water flow is towards the east/southeast, with a gradient ranging from 0.008 to 0.016. There appears to be an inflection point in the potentiometric surface,

located approximately 0.5 miles down-gradient from the ponds.

- High chloride concentrations extend at least 0.5 miles down-gradient from the ponds and the contamination appears to be converging rather than dispersing. This may be indicative of a high conductivity zone, or may be a function of data point location.
- High chloride concentrations exist in a saturated interval approximately 30 feet below the surface of the Arapahoe Formation. Therefore, the surface of the Arapahoe Formation may not represent the base of the WCWD aquifer.

4.8.2 Hydraulic Properties

Values for hydraulic properties of the WCWD aquifer are required to model ground-water flow and solute transport. Initial estimates of parameter values are listed in Table 5. During the process of calibration the values are adjusted to obtain the optimal match with field data. It the values fall outside the reasonable ranges then the conceptual model is not a good representation of the site and should be revised or discarded.

Table 5. Initial estimates of parameter values and reasonable ranges.

Parameter	*Estimated Value*	*Reasonable Maximum*	*Reasonable Minimum*
Hydraulic Conductivity (ft/day)	2.3/1.4[1]	$3.0x10^{3}$	$3.0x10^{-2}$
Specific yield	0.10	0.30	0.01
Recharge (ft/day)	$3.5x10^{-3}$	$5.2x10^{-3}$	$1.7x10^{-3}$
Canal seepage, April to October (ft/day)	1.1	2.0	0.5
Pond seepage (ft/day)	$1.5x10^{-3}$	0.15	$1.5x10^{-5}$
Average chloride concentration in ponds (mg/L)	13,000	28,000	3,000
Longitudinal dispersivity (ft)	400	4,000	40
Transverse dispersivity factor	0.2	0.5	0.1
Vertical dispersivity factor	0.04	0.05	0.01

[1]measured in the Arapahoe Formation.

4.8.3 Recharge and Discharge

Several processes recharge and discharge water to and from the aquifer underlying WCWD.

- The Arapahoe Formation may be acting as a source or sink for the WCWD aquifer.
- Ground water from aquifers within the Arapahoe Formation is discharging to Beebe Draw.
- Speer Canal is a major source of recharge to the system and creates seasonal fluctuations in hydraulic head and in chloride levels in the WCWD aquifer.
- Precipitation is a minor source of recharge to the WCWD aquifer and does not have a significant effect on seasonal ground-water levels.
- Pond leakage is a minor source of water recharge to the WCWD aquifer.
- Evapotranspiration is an unknown quantity.
- Ground-water outflow to Beebe Draw is an unknown quantity.

4.8.4 Source of Produced Water

The first goal of the study is to identify an effective tracer of produced water contamination within the WCWD aquifer. Geochemical analyses show that produced water has seeped from the ponds into the WCWD aquifer and can be traced using chloride as a conservative indicator. The concentration of chloride in the ponds is assumed to average 13,000 mg/L. Ambient chloride concentrations in the WCWD aquifer are 85 mg/L.

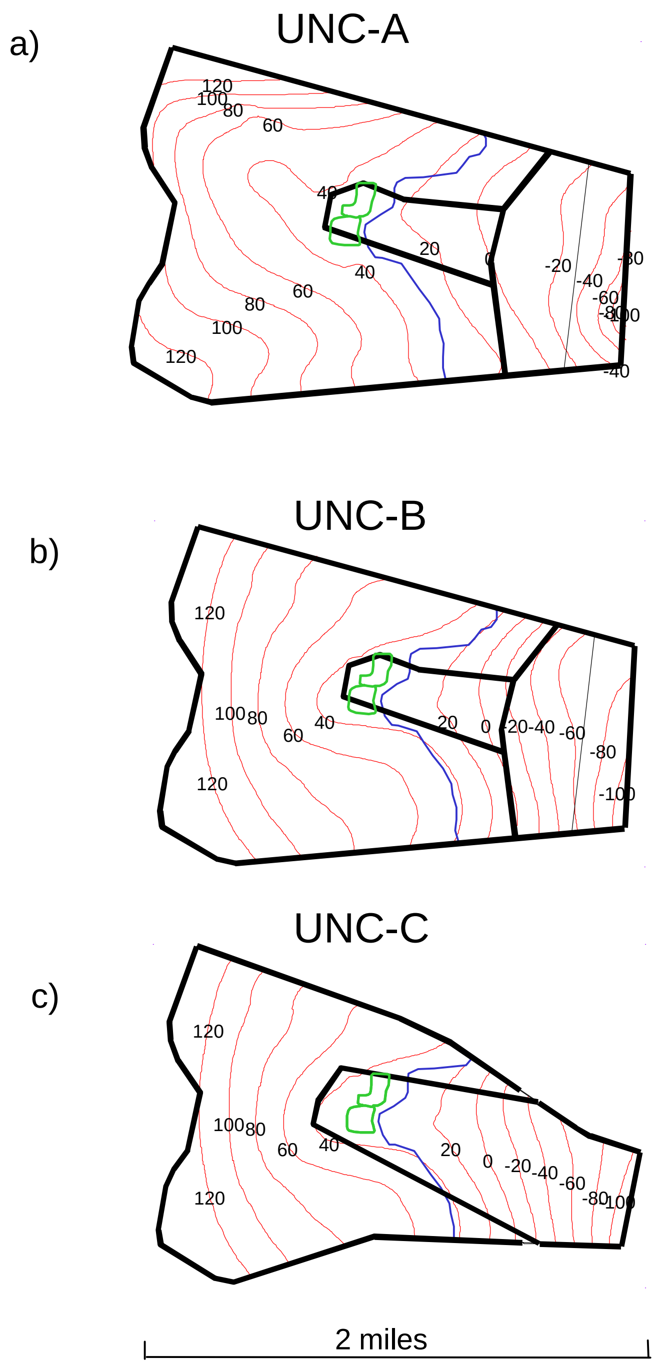
CHAPTER 5. CONCEPTUAL MODELS OF GROUND-WATER FLOW AND CONTAMINANT TRANSPORT

A number of equally plausible conceptual models can be proposed to represent ground-water conditions in the WCWD aquifer. Twelve models are developed and tested. The conceptual models are input to *Groundwater Modeling System* (*GMS*) by delineating model boundaries, aquifer properties, and the locations, rates, and chloride concentrations of sources and sinks. Two fundamentally different types of conceptual models are considered. The first defines the base of the aquifer at the contact between the unconsolidated deposits and the Arapahoe Formation and the second defines the base of the aquifer in the Arapahoe Formation. Variations of the specific configurations of the aquifer base, areal boundaries, hydraulic properties, and sources and sinks, produce additional conceptual models stemming from these two fundamentally different concepts. All twelve conceptual models simulate one-layer systems which assume that hydraulic properties are homogeneous in the vertical dimension and that there are no significant vertical components of flow. Based upon results of model calibration, a multi-layered conceptual model is developed in Chapter 8.

5.1 Unconsolidated-Unit Conceptual Models

The three unconsolidated models presented in this section assume that the Arapahoe Formation is impermeable, thus the base of the aquifer is defined as the top of the Arapahoe Formation. The conceptual models are labeled UNC-A, UNC-B, and UNC-C and are illustrated in Figure 20. Conceptual models UNC-A and UNC-B are based on the assumption that the areal boundaries of the ground-water basin coincide

Figure 20. Unconsolidated-unit conceptual models. Polygons within the boundaries represent different hydraulic conductivity zones. Contours are of aquifer base elevation equal to the top of the Arapahoe Formation referenced to 5,000 ft amsl and inferred from a) all available data, and b) and c) disregarding Geoprobe© data points. Speer canal is shown in blue and the ponds are shown in green.



with surface drainage boundaries and UNC-C represents a basin that is tapered. The aquifer is represented by one layer of variable thickness. Two aquifer bottom configurations were considered, composing the primary difference between UNC-A and UNC-B. UNC-A honored the Geoprobe© data, which identifies the Arapahoe Formation based upon penetration resistance, along with monitoring well and borehole data to infer the base of the aquifer. The result is a surface that gently slopes to the east and then drops steeply into Beebe Draw. Model UNC-B does not use the Geoprobe© data and the overall slope of the aquifer bottom is steeper and more constant. Both surfaces contain an erosional scour, trending from the northwest, underneath the ponds, and continuing east. Model UNC-C uses the basement configuration of UNC-B. Recharge from precipitation for all models is spatially and temporally uniform. To represent possible combinations of gravel and loess distributions and possible channel orientations, up to four individual zones of hydraulic conductivity are defined.

5.2 Mixed-Unit Conceptual Models

Mixed-unit conceptual models consider the WCWD aquifer to consist of both unconsolidated material and material of the upper Arapahoe Formation. This is supported by data from only one monitoring well, MW-19, completed 30 feet below the top of the Arapahoe Formation, which exhibits significant chloride levels (up to 3,000 mg/L as described in Chapter 4, section six). A five foot thick shale was detected beginning just below the screened interval within the Arapahoe Formation. For these models this shale is considered to be the base of the WCWD aquifer at the well location. This shale is located 43 ft below the average water table elevation measured at this location. Away from MW-19, the base of the aquifer varies among models. Nine distinct conceptual models of this type are considered.

5.2.1 BOX Conceptual Model

The BOX conceptual model is shown in Figure 21. The areal boundaries define a rectangle, roughly encompassing the drainage basin. The base of the aquifer is 43 feet below the average potentiometric surface, and sloped to the east at 0.016 ft/ft in up-gradient areas and 0.002 ft/ft in down-gradient areas. Two zones of hydraulic conductivity are defined as K1 and K2, with the division determined by the approximate change in slope of the hydraulic gradient. Two zones of recharge are defined as RCH1 in up-gradient areas and RCH2 in down-gradient areas. The rationale for this is that recharge incorporates ground-water inflow from zones within the Arapahoe Formation, which may differ between up-gradient and down-gradient areas.

5.2.2 CHANNEL Conceptual Model

The CHANNEL conceptual model, shown in Figure 22, incorporates a channel-shaped zone of hydraulic conductivity (K3) into the previous BOX conceptual model. The purpose of this feature is to generate convergent flow should K3 be estimated at a larger value than surrounding hydraulic conductivity.

5.2.3 FLATBOT Conceptual Model

The FLATBOT conceptual model, also shown in Figure 22, has a different aquifer base configuration than the BOX conceptual model. This model assumes that up-gradient of MW-19 the base of the aquifer is the black shale layer detected within the Arapahoe Formation at a constant elevation of –24 ft (referenced to 5,000 ft above mean sea level [amsl]). Down-gradient of MW-19 the base of the aquifer is 43 feet below the average water table (as in the previous models) to represent fluvial scouring on the Arapahoe surface near Beebe Draw. This conceptual model has only two zones of hydraulic conductivity as in the BOX conceptual model. The two recharge zones used by previous models are unchanged.

Figure 21. BOX conceptual model. (a) Plan view displaying the base of the aquifer as red contours referenced to 5,000 feet amsl, and two zones of hydraulic conductivity and recharge. (b) Cross section.

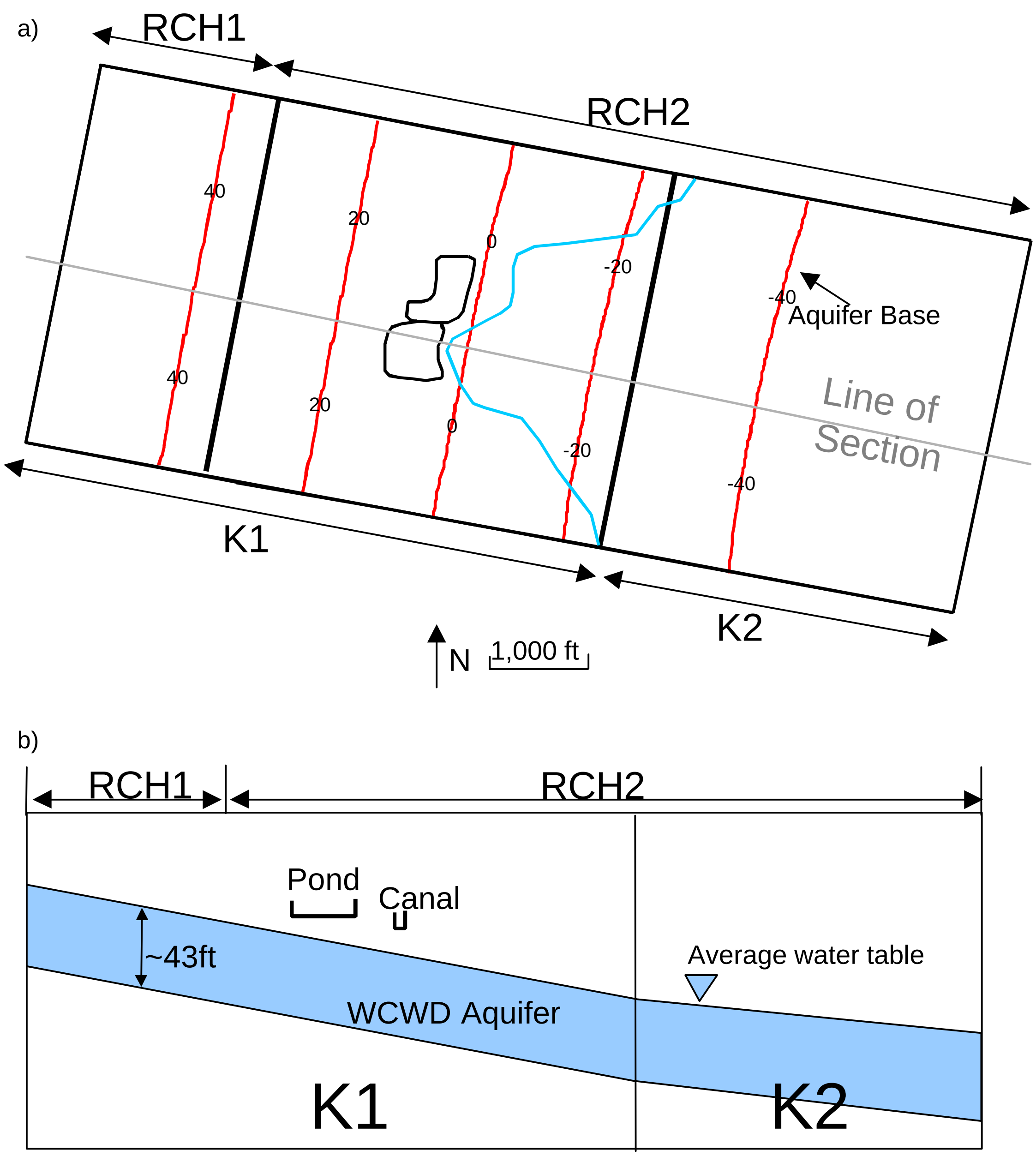
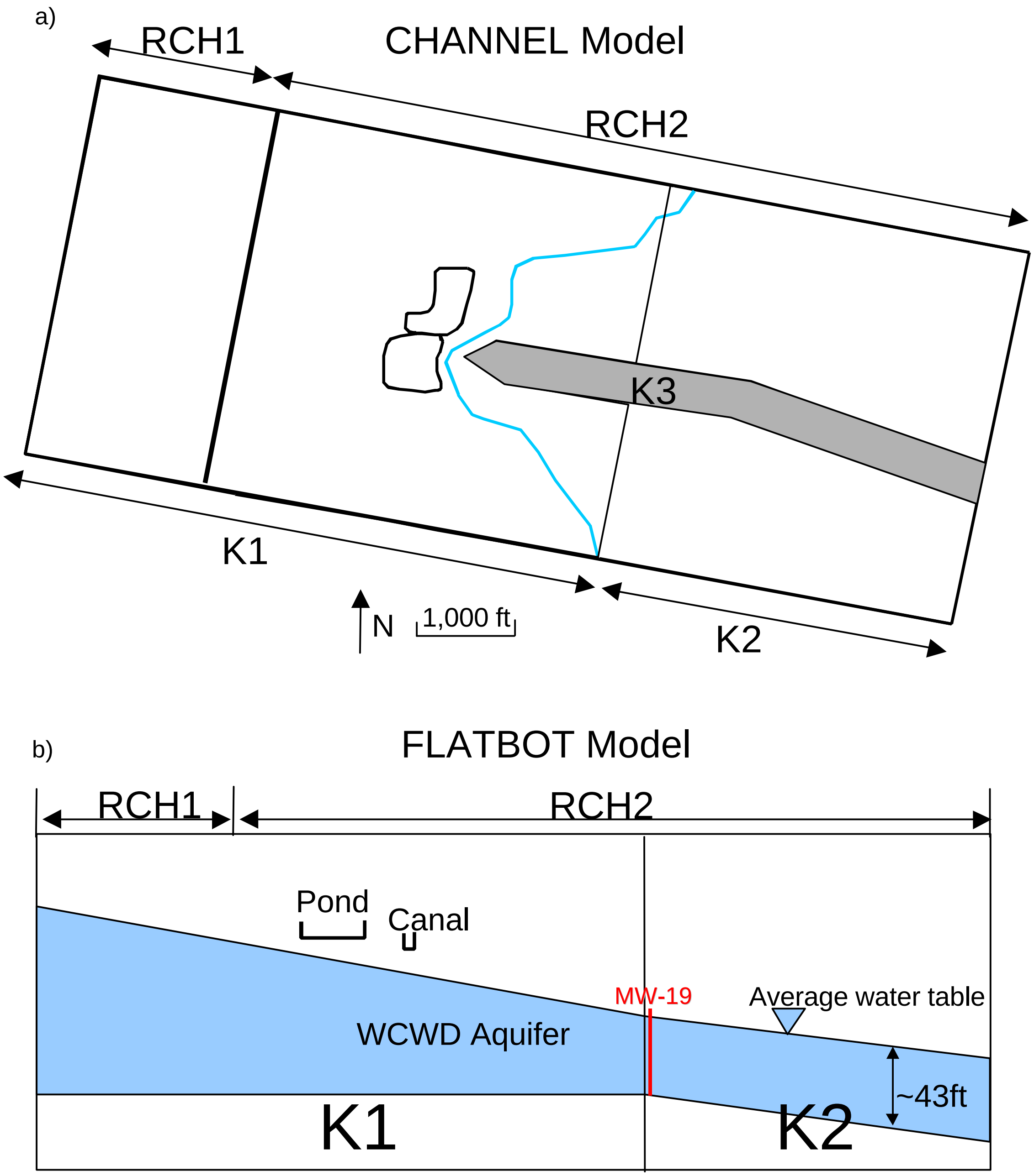


Figure 22. (a) CHANNEL conceptual model in plan view illustrating three zones of hydraulic conductivity and two zones of recharge. In cross section view (not shown), the model resembles the BOX model shown in Figure 21. (b) FLATBOT conceptual model in cross section view illustrating the flat aquifer base up-gradient of MW-19 and two zones of hydraulic conductivity and recharge. In plan view the model is the same as the BOX model shown in Figure 21.



5.2.4 ISLAND-K Conceptual Model

The ISLAND-K conceptual model uses a unique hydraulic conductivity zonation. Data are not available north and south of MW-18 and MW-19, and it is possible that rather than convergent flow focusing the plume, a stagnation zone up-gradient of a low hydraulic conductivity zone immediately down-gradient of MW-18 and MW-19 causes an accumulation of chloride. The ISLANDK conceptual model, shown in Figure 23, uses the standard K1 and K2 zones of other models and places a third, island-like, zone of hydraulic conductivity immediately down-gradient of MW-18 and MW-19 that may be estimated at a low value by regression. The recharge zonation and aquifer bottom are the same as in the BOX conceptual model.

5.2.5 ET Conceptual Models

Two evapotranspiration (ET) models were simulated: 1) ETNO, with two hydraulic conductivity zones as in the BOX model and; 2) ETCHAN with a third hydraulic conductivity zone as in the CHANNEL model. The base of the aquifer has a constant slope as in the BOX model.

5.2.6 CONE Model

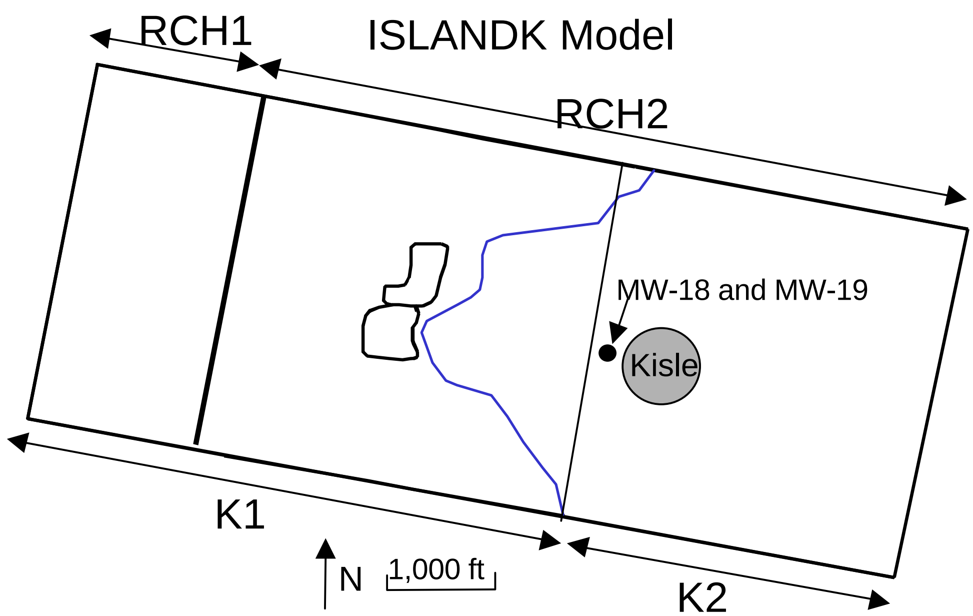
The CONE model has a different areal geometry from the other models. This model uses a tapering boundaries to facilitate convergent flow. The CONE conceptual model is shown in Figure 23 and uses the recharge and aquifer base configuration of the BOX conceptual model.

5.2.7 RECHARGE Conceptual Models

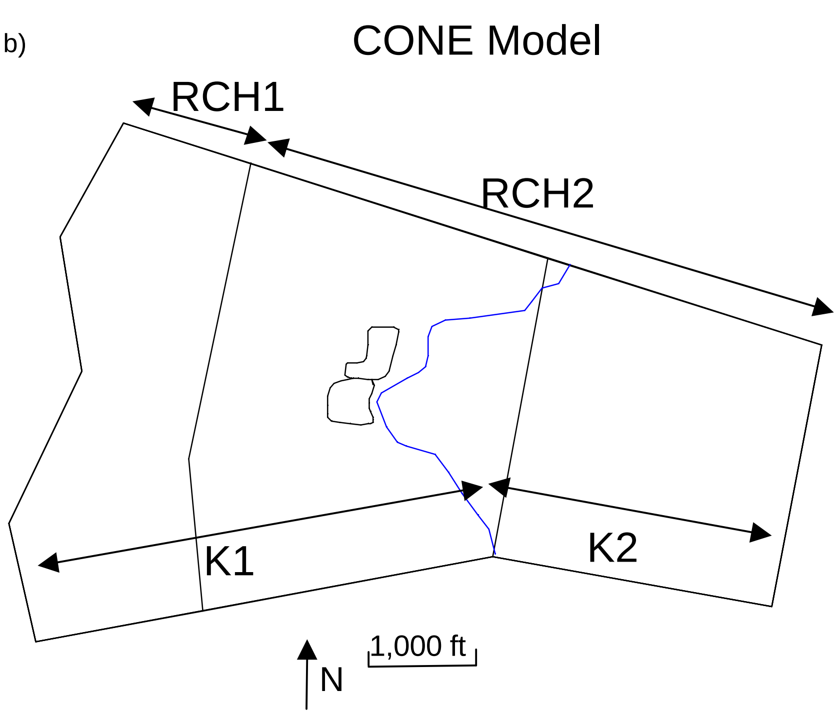
RECHARGE conceptual models represent seepage from Speer Canal and from the ponds differently than previous models by using the recharge package in MODFLOW

Figure 23. (a) ISLAND-K conceptual model in plan view illustrating the use of a island-like third zone of hydraulic conductivity. (b) CONE conceptual model illustrating a tapering geometry similar to the surface drainage basin. In cross section view both model are similar to the BOX model shown in Figure21.

a)



b)



instead of the River and General Head Packages. The reasons for this relate to problems experienced with models described previously where the ponds and canal acted as ground-water sinks when simulated heads were excessively high. Two RECHARGE conceptual models were simulated, RCH and RCHFLAT. The RCH model uses the constant thickness and slope of the aquifer from the BOX model, and RCHFLAT uses the varying aquifer bottom of the FLATBOT model. In all other respects the RECHARGE conceptual models are the same as the CHANNEL model, with a third, channel-shaped, zone of hydraulic conductivity and two recharge zones.

CHAPTER 6. NUMERICAL MODELING AND CALIBRATION

Each of the conceptual models is constructed as a MODFLOW and MT3D^{PD} numerical model using GMS with initial values listed in Table 5. The constructed models are executed and calibrated using UCODE. Statistics produced by UCODE were used to discriminate between conceptual models. This chapter discusses the numerical modeling procedure and outlines the protocol for calibrating the models. Numerical modeling issues discussed here include: grid design; mathematical representation of boundary conditions; temporal discretization; parameterization; initial conditions; solution controls; and model calibration.

A compact disk is provided in the back cover of this report which includes input files for selected numerical models, UCODE input files used to estimate parameters for these models, and the applications needed to conduct a regression.

6.1 Grid Design

The model area is spatially divided into block-centered grids. The grid domain is oriented 11 degrees south of east in the primary direction of flow as determined by the average potentiometric surface. The grid domain includes the entire surface drainage basin, however, some models utilize only portions of the entire domain. The entire grid area is defined by 107 cells in the x-dimension and 72 cells in the y-dimension. Grid dimensions for the rectangular boundary used by most conceptual models consists of 97 cells in the x-dimension and 40 cells in the y-dimension. Cell dimensions are uniformly 100 feet in both the x and y directions which places each observation point within a unique cell. With a maximum hydraulic gradient of 0.016, the maximum hydraulic head difference between cells is 1.6 ft.

The Peclet number gives an indication of appropriate grid spacing that will limit numerical errors in the $MT3D^{PD}$ solution. The Peclet number is the ratio of the cell length divided by dispersivity, and should be less than or equal to one (Anderson and Woessner, 1992). Using the assumed value of 400 ft for dispersivity, a grid cell size of 100 ft is appropriate. Experimentation with finer grid spacing did not significantly change simulation results.

Models of different areal geometry activate different cells for simulation. Figure 24 features the two grids used most frequently: that which is used for Unconsolidated-type models UNC-A and UNC-B, and that which is used for all the Mixed-type models except for the CONE model.

6.2 Boundary Conditions

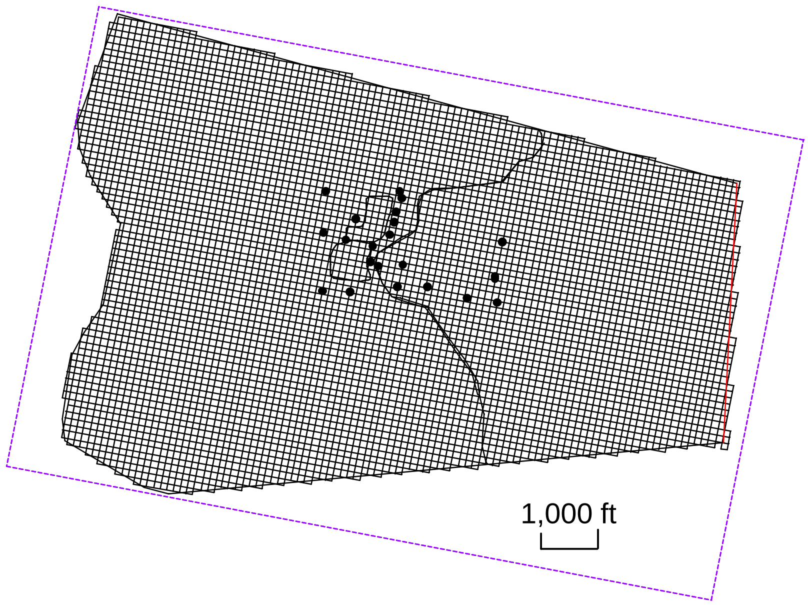
The aerial extent of the modeled area and sources and sinks that are dependent upon ground water flow such as canal and pond seepage are treated as boundaries in MODFLOW. This section discusses how information presented in Chapter 4 is used to simulate the behavior of these boundaries.

Boundaries on the north, west, and south are specified in numerical models as no flow boundaries. The eastern boundary is a constant head, equal to the average water level measured in the Supple wells (4983.5 ft above mean sea level [amsl]). The WCWD Aquifer is unconfined and is represented in MODFLOW as a type one layer so that the transmissivity (calculated as hydraulic conductivity multiplied by the saturated thickness) varies depending upon the saturated thickness of the aquifer (McDonald and Harbaugh, 1988).

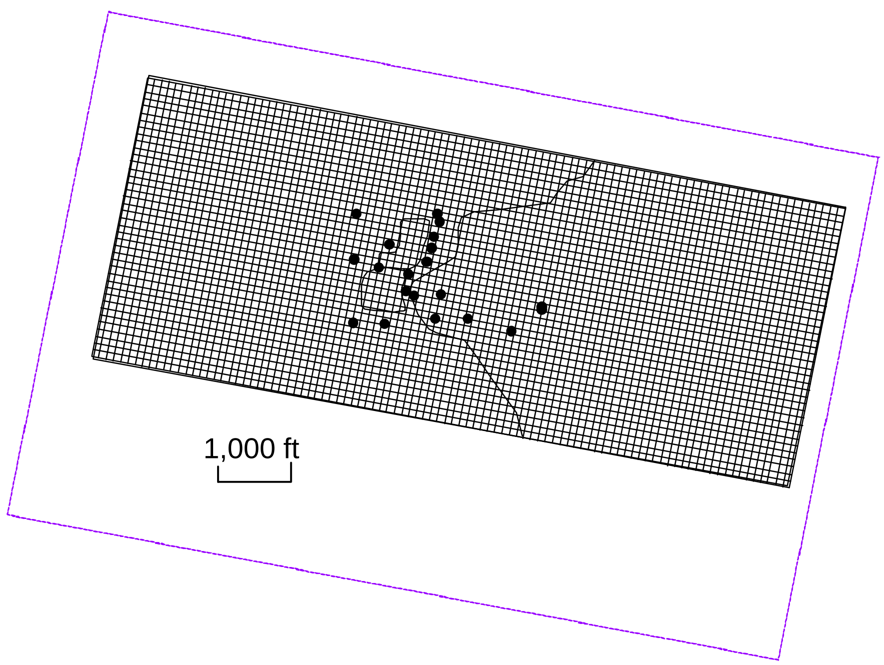
The base of the aquifer is a no flow boundary. Although deeper aquifers may be hydraulically connected to the WCWD aquifer, data delineating such connections are not available. The effect of deeper aquifers is accounted for indirectly through source/sink

Figure 24. Grids used for Unconsolidated-unit (a) and Mixed-unit(b) models. Grid cells are 100 feet long in the 'x' and 'y' dimensions. The black dots identify monitoring well locations.

a)



b)



behavior within the WCWD aquifer. For example, a model that has a high recharge value, but is valid otherwise, may indicate discharge from deeper aquifers into the WCWD aquifer.

Additional boundary conditions include the canal, ponds, and evapotranspiration. The mechanism for representing these features and initial values for parameters describing the features are presented in the remainder of this section. These values are adjusted during model calibration.

The canal is represented using the river package in MODFLOW. The canal bottom is at an elevation of 5053 ft (estimated from USGS Hudson Quadrangle, 1994). The water depth is 2 ft, giving a stage elevation of 5055 ft (an average of four field measurements). Based on average water table elevations shown in Figure 12, the aquifer head beneath the canal is, on average, 13 feet below the base of the canal. The thickness of the streambed material is assumed to be 2 feet. The width of the canal was measured to be 10 feet. The conductance of a river bottom is calculated as (McDonald and Harbaugh, 1988):

$$CRIV = \frac{K\ L\ W}{M}$$

where:

CRIV	conductance of the material separating the stream and aquifer [L^2T^{-1}].
K	vertical hydraulic conductivity of the canal-bed material [LT^{-1}];
L	length of the stream segment (or cell) [L];
W	stream width [L]; and
M	thickness of the streambed material [L].

The seepage rate is calculated as (McDonald and Harbaugh, 1988):

$$QRIV = CRIV\ (HRIV - HCELL)$$

or, if the head in the aquifer is below the bottom of the canal-bed material:

$$QRIV = CRIV\ (HRIV - HBOT)$$

where:

QRIV	flow between the river (canal) and the aquifer [L^3T^{-1}];
HRIV	head (stage) in the river (canal) [L];
HCELL	head in aquifer cell [L]; and
HBOT	elevation of the base of the canal-bed material [L].

When the canal is flowing, the seepage rate is estimated to be 193,000 ft^3/day during its time of operation over a length of 7,523 ft, and the seepage per unit length is 25.7 ft^2/day. Given that the hydraulic conductivity of the canal bottom is not known, and that the canal is always perched above the water table, the conductance per unit length is calculated to be 6.4 ft/day. This is the initial conductance value input into GMS. GMS automatically multiplies the length of each reach in each cell by this number and assigns that conductance value to the river package in MODFLOW.

Seepage from the ponds is represented by a general head boundary in MODFLOW. Unlike the river package, the general head boundary package assumes that there is always hydraulic connection between the two features that are simulated (the ponds and the aquifer). The base elevation of the ponds averages 5053 ft (LTE, 1997). The average depth of the pond water is assumed to be 3 ft at a stage of 5056 feet. The thickness of the material separating the pond bottom from the aquifer is, on average, 7 feet. MODFLOW calculates the flow between a general head cell and an aquifer cell as:

$$QGHB = \frac{K\ A\ (HPOND\text{-}RCELL)}{M}$$

or

$$QGHB = CGHB\ (HPOND - HCELL)$$

where:

QGHB	flow between the ponds and the aquifer, [L^3T^{-1}];
K	vertical hydraulic conductivity of the pond liner material, [LT^{-1}];

A	area of the ponds within a cell, [L];
M	thickness of the liner material, [L];
HPOND	head (stage) in the pond, [L];
HCELL	head in the cell below the ponds [L];
CGHB	conductance of the material separating the pond and aquifer;

GMS automatically calculates the conductance of the pond for each cell as the product of the pond area and the unit conductance. The unit conductance entered into GMS is the quotient of the hydraulic conductivity of the pond liner (8.4×10^{-4} ft/day) and the thickness of the material separating the pond from the aquifer (7 ft), or 1.2×10^{-4} ft^{-1}.

In some models canal and pond seepage are simulated using the recharge package in MODFLOW. This is done by specifying the seepage rate directly. Because cells contain different amounts of canal and pond areas, the percentage of the area containing the canal or pond in each cell is multiplied by a factor, which is then added to the recharge from precipitation and input to MODFLOW as the recharge rate for that cell. One factor is used to describe the magnitude of the canal seepage and one to describe the magnitude of pond seepage. This substitution is performed using UCODE and is described later in this chapter.

The evapotranspiration package of MODFLOW is used in the ET models to simulate ground-water discharge that removes only water and not chloride. Evapotranspiration is calculated in MODFLOW as:

$$RET = RETM \qquad HCELL > HS$$

$$RET = 0 \qquad HCELL < (HS-D)$$

$$RET = RETM * \frac{(HCELL - (HS - D))}{D} \qquad (HS-D) \;\; HCELL \;\; HS$$

where:

RET	rate of water loss in a cell per unit surface, [LT^{-1}];

RETM	maximum rate of loss, $[LT^{-1}]$;
HCELL	head in the cell, [L];
HS	elevation at which the maximum rate of loss occurs, [L]; and
D	cutoff, or extinction depth, where evapotranspiration does not occur if the head in a cell is lower, [L].

The maximum rate of loss in the ET models likely varies seasonally from May to October and from November to April. Initially, a uniform maximum rate is set to 8.6×10^{-4} ft/day, but this may be adjusted to vary seasonally during calibration. The value of HS is equal to the surface elevation of the model area. Anderson and Woessner (1992) consider the normal range for extinction depth, D, to be 6 to 8 feet below the land surface, so lacking site specific data, a value of 7 feet is assumed here.

6.3 Temporal Discretization

The time period of interest begins in April of 1978 when pond operation commenced and ends in December 1998 with the last head and chloride observations, for a total of 7552 days. Transient simulations in MODFLOW are divided into stress periods, during which stresses, such as canal and pond stage, are held constant. To simplify the process of extracting simulated values at the times when observations are available, additional stress periods are defined to end at those times. Consequently, 88 stress periods are defined for transient simulations.

In MODFLOW, stress periods are divided into time steps to attain numerical accuracy as the system adjusts to a new stress. The appropriate length of the first time step after a new stress is introduced can be calculated according to de Marsily (*in* Anderson and Woessner, 1992) as:

$$\Delta t_c = \frac{Sa^2}{4T}$$

where:

Δt_c the initial time step of a new stress period, [T];
S the specific yield of the aquifer, [dimensionless];
a the average grid dimension, [L]; and
T the transmissivity of the aquifer, [L^2T].

Using an average estimated specific yield of 0.10, a cell length of 100 ft, an average hydraulic conductivity of 3 ft/day, and assuming an average aquifer thickness of 60 ft, the first time step of a stress period is set to 1.4 days. Because the effect of the stress on the numerical solution dissipates with time, a time step multiplier is used to increase subsequent time steps of the stress period, minimizing computational time. As recommended by de Marsily (*in* Anderson and Woessner, 1992) a time step multiplier of 1.4 is used.

$MT3D^{PD}$ uses a constant flow field for the entire length of each MODFLOW time step, but further discretizes time steps for the transport calculation to limit numerical errors. Transport steps are determined automatically by $MT3D^{PD}$ based on the grid definition, aquifer properties, plume configuration, and solution controls.

6.4 Parameters

The conceptual models define areas of uniform parameter values (such as K1 and K2 illustrated in Figures 21, 22, and 23). Because the initial values for parameters presented in Table 5 are uncertain, UCODE is used to estimate optimal parameter values that best simulate field observed conditions for each conceptual model. UCODE implementation is discussed in section 8 in this chapter. Parameter values to be estimated by UCODE are listed in Table 6 with a description and rationale for including the parameter in the estimation. The constant head at the eastern model boundary is not estimated in any of the models and is held constant at 4983.5 ft.

Table 6. Parameters estimated by conceptual models

Parameter	*Description*	*Rationale*	*BOX*	*CHANBOX*	*FLATBOX*	*ETBOX*	*ETCHAN*	*ISLANDK*	*CONE*	*RCH*	*FLATRCH*
K1	up-gradient hydraulic conductivity zone	up-gradient areas exhibit a steep potentiometric surface	X	X	X	X	X	X	X	X	X
K2	down-gradient hydraulic conductivity zone	down-gradient areas exhibit a less steep potentiometric surface	X	X	X	X	X	X	X	X	X
K3(CH)	channel shaped hydraulic conductivity zone	high chloride concentrations may be caused by a high conductivity channel in an eroded area of the Arapahoe Formation		X	X		X			X	X
K3(Isle)	island shaped conductivity zone	high chloride concentrations may be caused by a stagnation point.						X			
RCH1	up-gradient recharge zone	recharge may indirectly simulate flux from underlying aquifers, ET, and infiltration which may vary from the upper reaches of the model area to the lower	X	X	X	X	X	X	X		
RCH2	down-gradient recharge zone		X	X	X	X	X	X	X		
RCHall	constant areal recharge	recharge may be uniform								X	X
CP	pond conductance factor	uncertain value	X	X	X	X	X	X	X		
CR	canal conductance factor	uncertain value	X	X	X	X	X	X	X		
PRCH	pond recharge factor	uncertain value								X	X
CRCH	canal recharge factor	uncertain value								X	X
ETS	summer ET maximum	evapotranspiration is likely greater in the summer months than winter months				X	X				
ETW	winter ET maximum					X	X				
STO	specific yield	uncertain value	X	X	X	X	X	X	X	X	X
SS	chloride source strength of pond water	uncertain value	X	X	X	X	X	X	X	X	X
DL	longitudinal dispersivity	uncertain value	X	X	X	X	X	X	X	X	X
DT	transverse dispersivity factor	uncertain value	X	X	X	X	X	X	X	X	X

6.5 Initial Conditions

The simulation begins in April of 1978. In early simulations all heads were set at 5,100 feet at the start of the simulation. For the results presented in this report, initial heads were derived from the results of these early simulations, using the flow field simulated for April of 1998.

To decrease the computational time for solute transport modeling, the ambient chloride concentration is adjusted to be zero so that chloride concentration is only calculated in cells that are impacted by chloride that issued from the ponds. Initial chloride concentrations are set to zero and the source strength of the ponds is reduced by the average ambient chloride concentration (85 mg/L). The measured chloride levels used to calibrate models are also reduced by this amount. Recharge from precipitation and seepage from the canal are assumed to contain zero chloride concentrations.

6.6 Numerical Model Solution Controls

Heads are solved by MODFLOW using the Strongly Implicit Procedure, with a head change tolerance of 0.01 ft for convergence, 125 maximum iterations, and no relaxation. The advective portion of the transport equation is solved using the Hybrid Method of Characteristics, HMOC. The relative concentration gradient determining the use of Method of Characteristics (MOC) and Modified Method of Characteristics (MMOC) is 1×10^{-5} mg/L. Particles representing chloride are placed randomly, with a maximum of 16 particles per cell. The First-order Euler tracking algorithm is used with a concentration weighting factor of 0.5.

6.7 Observations for Calibration

Time varying hydraulic head and chloride concentrations measured in the monitoring wells compose the majority of the observation data for calibration (locations shown in Figure 9). MODFLOW and MT3D numerical models are simulated sequentially and calibrated to a total of 650 observations of hydraulic head and chloride concentration using UCODE. Observations include 359 hydraulic head observations measured in monitoring wells beginning in June 1995 and ending December of 1998. Additional flow observations include hydraulic head measurements in MP-3 and MP-8 in October 1995, hydraulic head measured in the Old Piezometer in June 1997 and August 1997, and canal leakage rates measured in June 1997 and August 1997 (locations are shown in Figures 8 and 9). All head data are referenced to a 5,000 ft datum so that computed heads have the greatest possible number of significant figures to increase the accuracy of statistics calculated by UCODE. Chloride observations include 283 measurements made on samples collected from monitoring wells beginning in August of 1990 and ending in December of 1998. Additional chloride measurements are available for MP-3 and MP-8 in October 1995. Weights are used by UCODE to reflect the confidence associated with each observation. Table 7 summarizes the observations and the associated 95% confidence level.

Table 7. Summary of Observation and weighting data used

Observation Type	*Number of Observations*	*95% Confidence Interval*
Head in monitoring wells	359	+/- 0.2 ft [1]
Head in monitoring points	2	+/- 5.0 ft [2]
Old piezometer	2	+/- 5.0 ft [2]
Seepage from Speer Canal	2	+/- 20% of value
Chloride in monitoring wells	283	+/- 20% of value [3]
Chloride in monitoring points	2	+/- 20% of value [3]

[1] wells are surveyed and measured with a digital depth sounder
[2] ground surface estimated from topographic map
[3] minimum interval of 2.0 mg/L is used

6.8 UCODE Implementation

This study uses four UCODE input files: the Universal File where solution controls are defined and measured observations and associated weights are specified; the Prepare File where parameter substitutions are specified, the Function File where functions of the parameter values are used as input to the application models, and the Extract File where the extraction of simulated values at observation locations are specified.

In the Universal File the user specifies control parameters for the regression, the names of application models, MODFLOW and $MT3D^{PD}$, and observation information. The convergence criteria used is that the maximum parameter change must be less than or equal to 5% of the parameter value before the regression completes (1% is recommended by Poeter and Hill (1998) and the use of a larger tolerance is discussed in the following chapter). Each observation value is entered with variance associated with that measurement. The variance is calculated as the square of the quotient of the value that is believed to represent the magnitude of possible deviation with a 95% certainty and 1.96 (the normal deviate for two standard deviations), as expressed below (Hill, 1998):

$$\text{variance} = [(\text{magnitude of deviation with 95\% certainty})/1.96]^2$$

The Prepare File is used to specify how parameters are substituted into application input files and specifies starting values for those parameters. This is done by creating template files from numerical model input files where the value to be estimated is replaced by a character string. During regression, UCODE manipulates these template files to create numerical model input files with estimates of parameter values. The parameters that are estimated and those that are held constant by the nine conceptual models are defined and explained earlier in Table 6.

All models estimate multiplication factors that are used to describe seepage rates for the canal and ponds using the UCODE Function File. For RECHARGE models the

UCODE Function File is used to multiply these factors by the portion of each cell that is acting as a canal or pond source, and then add recharge from precipitation to this value. For all other models the canal and pond factors are multiplied by the GMS calculated conductance of each cell that is acting as a canal or pond source. These computed values are then substituted into the MODFLOW Recharge Package for RECHARGE models or River and General Head Boundary packages for all other models.

The Extract File describes how to extract values from the output, and how those values shall be used to calculate simulated equivalents of the observations. After a simulation is executed, UCODE extracts values for the four cells surrounding each observation from the MODFLOW and MT3D^{PD} output files. Weights calculated manually using bilinear interpolation are used by UCODE to compute a simulated value at the observation location. UCODE files and the applications needed to run UCODE are included in the compact disk in the back cover of this report.

CHAPTER 7. MODEL EVALUATION

The conceptual models are evaluated based upon MODFLOW and MT3D^{PD} output from optimized simulations and regression results from UCODE. Regressions were performed using the initial values listed in Table 5. Models are evaluated using four criteria: 1) convergence and numerical validity; 2) realistic optimized parameter values; 3) non-correlated optimized parameters; 4) acceptable overall model fit; and 5) randomly distributed residuals throughout time and space. All twelve models do not satisfy all criteria and are therefore are not capable of providing valid predictions. However, some models are better representations of the aquifer system than others, and the analyses presented in this chapter identify several important characteristics of the system. The results of these analyses are used to develop a multi-layered model presented in the following chapter. A summary of the evaluation of all twelve single-layered conceptual models is provided in Table 8.

7.1 Convergence and Numerical Validity

All models must converge to an optimal set of parameter values and the results of the numerical simulations must be valid for a model to be retained as a viable representation of the ground-water system. The Unconsolidated-type models would not converge. Numerous cells would “go dry” early in the simulation due to the oscillating canal activity. Successful simulations were only obtained for parameter sets that increased the recharge to unreasonable levels, resulting in heads well above the elevation of the average potentiometric surface. Parameter estimation by UCODE quickly resulted in parameter sets that caused the models to “go dry” and MODFLOW would fail to

Table 8. Summary of model evaluation.

Model	*Convergence and numerical validity*	*Parameter values*	*Parameter uniqueness*	*Overall Fit*	*Residual Distribution*	*Rank/ Discard*
FLATBOT	acceptable	realistic	unique	**poor**	**not random**	DISCARD
RCH	acceptable	realistic	unique	**poor**	**not random**	DISCARD
FLATRCH	acceptable	realistic	unique	**poor**	**not random**	DISCARD
BOX	acceptable	realistic	unique	**poor**	**not random**	DISCARD
ISLAND-K	acceptable	**unrealistic**	na	na	na	DISCARD
CHANNEL	acceptable	**unrealistic**	na	na	na	DISCARD
ETBOX	acceptable	**unrealistic**	na	na	na	DISCARD
ETCHAN	acceptable	**unrealistic**	na	na	na	DISCARD
CONE	acceptable	**unrealistic**	na	na	na	DISCARD
Unconsolidated -type models	**FAIL**	**unrealistic**	na	na	na	DISCARD

Models are listed in order of increasing error.
Failure criteria for each model is shown in bold.
na = not applicable.

converge. Despite considerable effort in exploring various alternative aquifer geometries, parameterizations, and initial parameter values, no models were derived that allowed for successful regression or that produced hydraulic head distributions that were reasonable representations of the system. Therefore, all Unconsolidated-type models are discarded as non-representative of the system.

All regressions for the Mixed-type models converge to optimal parameter values using a criteria of a maximum fractional parameter change of 5% in generally less than 10 iterations, but not for the suggested criteria of a maximum fractional parameter change of 1% (Poeter and Hill, 1998). Regressions that were allowed to proceed for additional iterations exhibited oscillating parameter values (generally oscillating less than 5%) without significantly decreasing the sum of squared weighted residual value. Because convergence is attained for a higher criterion than recommended, regression results require thorough analysis to ensure that optimal calibrations are attained and that conceptual model errors are not present. However, because all models fail to satisfy the criteria defining a viable conceptual model, only results that have implications for the development of future conceptual models are presented.

Cumulative mass balance of total flows and total chloride flux is a good measure of the reliability of MODFLOW and $MT3D^{PD}$ simulations respectively. The acceptable percent discrepancy of cumulative flow volumes is less than 1% (Anderson and Woessner, 1992). At optimized parameter values, all of the models exhibit acceptable mass balance for MODFLOW simulations. The same criteria is used to evaluate $MT3D^{PD}$ simulations, and all models simulate cumulative mass balance discrepancies less than 1%.

7.2 Analysis of Optimized Parameter Values

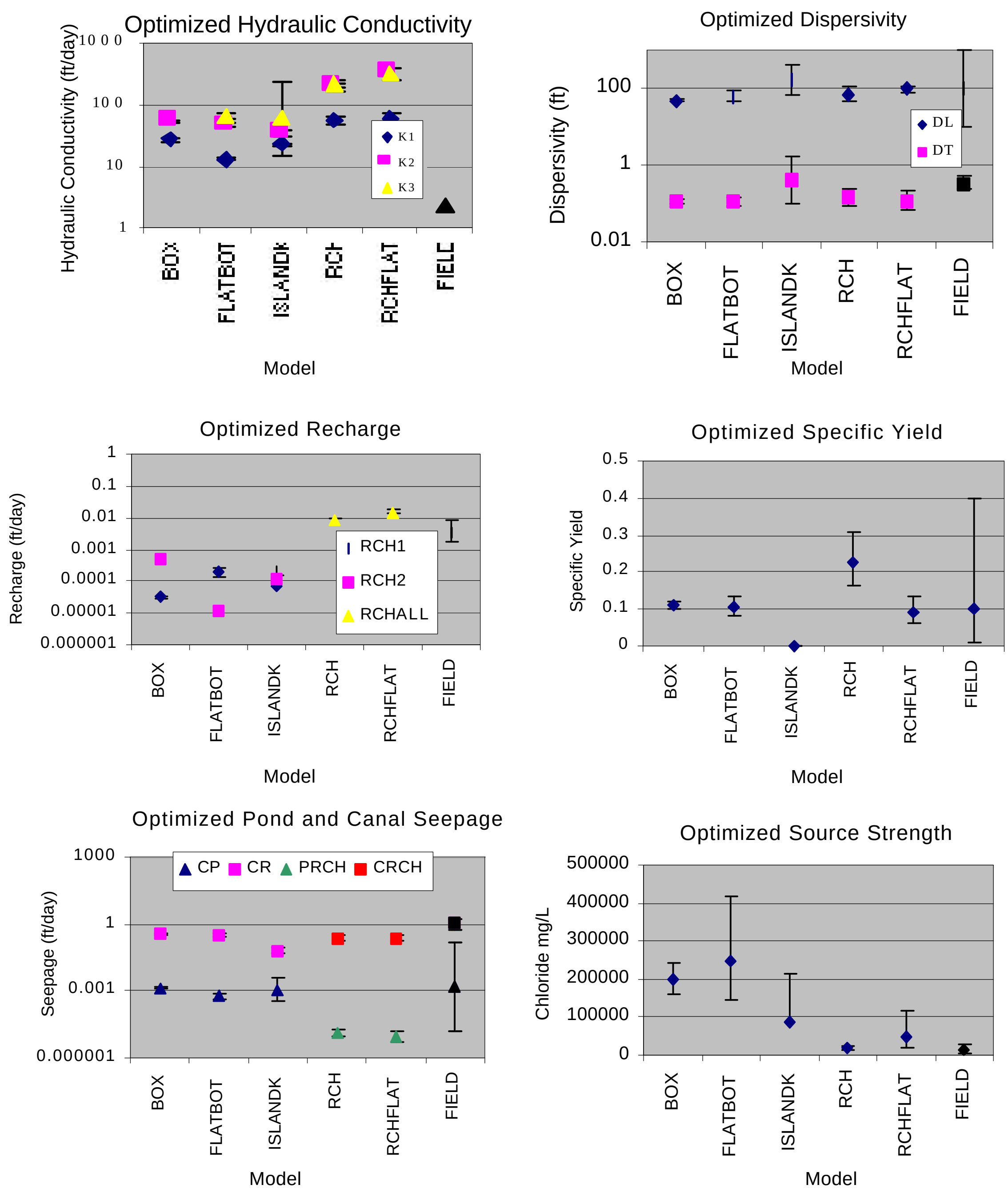
Qualitative analysis of the optimal parameter values identifies significant problems with four of the nine models. Optimized parameters for the CHANNEL model include a negative value for RCH2. Because this results in chloride leaving the system during the $MT3D^{PD}$ simulation, this model must be discarded (although the presence of a channel-shaped zone of hydraulic conductivity is not ruled out for other models). The rationale for creating the ET models was in part due to this development, because evapotranspiration in $MT3D^{PD}$ only removes water from the system, not chloride. However, optimized parameter values for both of the ET Models yielded flow fields where the hydraulic heads were higher than the stage in the ponds and canal. The same occurred for the CONE Model. Regression by UCODE treated the canal and pond as sinks and increased conductance parameters in an effort to lower the water table. These models are also discarded as non-representative of the system. Evaluation of these models resulted in the creation of the RCH and RCHFLAT models, in which the seepage from the ponds and canal is represented as a specified flux rather than a head dependent boundary.

Optimized parameter values for the remaining 5 models and 95% confidence intervals (as error bars) are shown in Figure 25. Generally, all parameters are estimated with low uncertainty. Also posted are ranges and average parameter values calculated from field measurements and literature values identified in Table 5. All models contain at least one optimized parameter value that lies outside of the estimated range. The graphs shown in Figure 25 are discussed in the following paragraphs.

Hydraulic Conductivity

All models estimate hydraulic conductivity values that are high compared to field measurements but they are within the broad range of reasonably possible values. RCH and RCHFLAT models estimate hydraulic conductivity values that are two orders of magnitude greater than the highest measured in the field. Up-gradient hydraulic conductivity (K1) is less than down-gradient hydraulic conductivity (K2) for all models and the channel-shaped zone of hydraulic conductivity (K3) is greater than or equal to the K2 value for all models. This is consistent with an expected increase in gravel deposits

Figure 25. Optimized parameter values for 5 retained models. Parameters are defined in Table 6. 95% confidence intervals are shown as error bars. FIELD signifies a field or literature derived average value (in black) and range of reasonable values.



near Beebe Draw and in erosional channel areas.

In the ISLAND-K model the island-shaped zone of hydraulic conductivity (Kisle) is estimated to be slightly higher than the down-gradient (K2) value rather than lower than the surrounding hydraulic conductivity as is needed to simulate a stagnation zone. This suggests that a high conductivity zone is more conducive to simulating high chloride values in MW-18 than a stagnation zone and models that include a channel shaped zone of hydraulic conductivity may be more realistic.

Recharge

All models estimate at least one recharge parameter that is more than an order of magnitude different than the recharge rate estimated from precipitation data. Because the RCH parameters may include inflows from deeper or up-gradient aquifers, and may incorporate evapotranspiration, optimized values outside the estimated range are not considered unreasonable. In models that simulate two zones of recharge, estimated values are below field estimated values. The FLATBOT model estimates up-gradient recharge to be an order of magnitude greater than estimated down-gradient recharge, due to increased discharge associated with the inclusion of the channel-shaped zone of hydraulic conductivity. Models that simulate a single zone of recharge (RCH and FLATRCH) have optimized recharge values that are much greater than field estimated values.

Pond and Canal Seepage

All estimated values of seepage from the ponds and the canal are less than those estimated from field measurements. The BOX and ISLAND-K models estimate seepage rates from the ponds to be approximately 80% of estimated. All other models estimate canal and pond seepage rates less than 50% of estimated and may be unrealistic. Analyses in Chapter 4 identified canal seepage as a major component of total recharge to the aquifer. Temporal residual analysis, discussed later in this chapter, is needed to fully evaluate which canal seepage rates are reasonable.

Dispersivity

Longitudinal dispersivity values estimated by BOX, FLATBOT, and ISLANDK model are all within expected ranges. Models RCH and RCHFLAT estimate dispersivity values slightly below the reasonable range.

Specific Yield and Source Strength

Values of specific yield are within estimated limits for all models except for ISLANDK which is estimated to be 0.001, an order of magnitude below the expected value. This estimated value is unrealistic for unconfined aquifers (Driscoll, 1986). Because of this unrealistic value, and because the island shaped hydraulic conductivity parameter (Kisle) is estimated to be similar to the channel-shaped zone of hydraulic conductivity in other models, the ISLAND-K model is discarded.

Source strength optimized values are significantly higher than the average value measured in Pond D of 13,000 mg/L. This is because all conceptual models only simulate one-layer systems. In the models, the total chloride concentration is mixed throughout the entire thickness of the aquifer, and very high source strengths are needed to simulate field observed conditions in areas of large aquifer thickness. There are two significant problems associated with this model short-coming. Vertical chloride concentration gradients that are shown to exist between monitoring wells MW-18 and MW-19 and likely exist elsewhere in the study area are not simulated. This prohibits the simulation of an alternative explanation of plume distribution shown in Figure 18 and realistic prediction in wells that are not screened through the entire thickness. The second problem is that calculations of the total amount of chloride entering and leaving the study area are not meaningful. From a regulation or remediation viewpoint such mass balance computations are essential. Consequently, a multi-layered model is presented in the following chapter to address this issue.

7.3 Parameter Sensitivity and Uniqueness

Sensitivities are used to determine if a parameter can be effectively estimated by the regression given the available data. The sensitivity of each optimized parameter to each observation is calculated by UCODE using central differences for a 1% perturbation of parameter values. Composite scaled sensitivities are good measures of overall parameter sensitivity. The magnitude of the composite scaled sensitivity indicates if the field observations contain enough information to estimate a parameter. Values estimated for parameters that have composite scaled sensitivities two orders of magnitude less than the largest composite scaled sensitivity may not be valid because the lager sensitivity parameter(s) may dominate the regression, inhibiting accurate estimation of the lower sensitivity parameter(s) (Poeter and Hill, 1998).

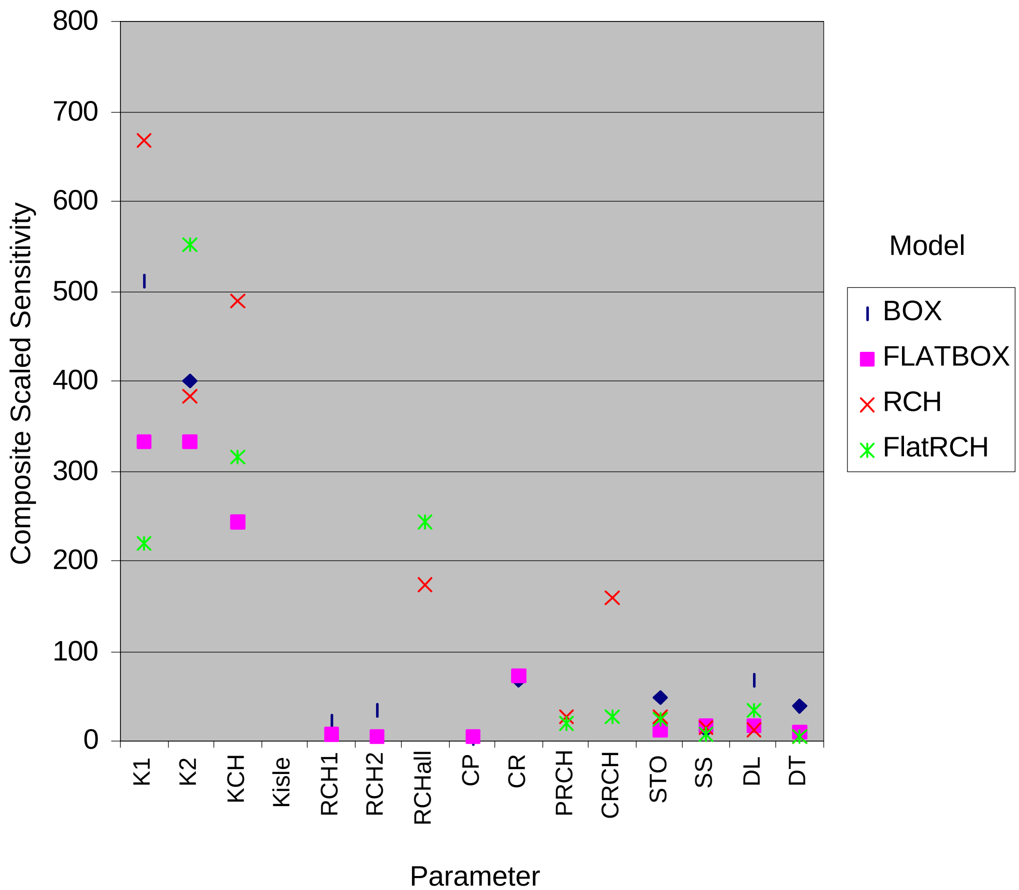
Composite scaled sensitivities for the four retained conceptual models which remain valid representations of the system at this point in the analysis are presented in Figure 26. Parameter sensitivities are similar for all models, although models BOX, RCH, and FLATRCH produce the most uniformly high composite scaled sensitivities and therefore produce the most reliable optimized parameter values.

Hydraulic conductivity is the most sensitive parameter for all models. This suggests that the observations contain information most applicable to the estimation of hydraulic conductivity.

Parameters with significantly low composite scaled sensitivity are the chloride strength of the ponds (SS), and longitudinal and transverse dispersivity. Increasing the amount by which parameter values are perturbed to 5% did not significantly change the sensitivities of these parameters.

Parameter sets for the RCH and RCHFLAT models exhibit the most uniformly high composite scaled sensitivities. This indicates that these models are calibrated with the most certainty.

Figure 26. Composite scaled sensitivities for the 4 retained models at optimized parameter values. Parameters are defined in Table 6. The large composite scaled sensitivity for hydraulic conductivity in all models may inhibit accurate estimation of the remaining parameters.



A measure of the potential for the regression to independently estimate a parameter is the correlation between parameters. Correlation coefficients greater than 0.95 suggest that the parameters may not be estimated uniquely (Poeter and Hill, 1998). Parameter correlation coefficients for models BOX and FLATBOT are below 0.95. For models RCH and FLATRCH the parameters K1, K2, RCH have correlation coefficients greater than 0.95. To determine if the parameters for these models were independently estimated, additional regressions were undertaken with significantly different initial parameter values. The regressions arrived at similar optimized parameter values indicating that the solutions are unique and the RCH and RCHFLAT models remain valid at this point in the analysis.

7.4 Overall Model Fit

A measure of overall model fit is the sum of the weighted squared residuals (SWSR). Because the number of observations is large, this value can also be large. Another measure of model fit that has more physical meaning is the standard error of the regression (SER). The SER can be thought of as an average weighted residual and is calculated as:

$$SER = \sqrt{\frac{SWSR}{(\#\,observations - \#\,paramerters)}}$$

The SWSR and SER are presented for all models in Figure 27. It appears that all models fit the observed data with approximately the same accuracy, although the BOX model has slightly higher values of SWSR and SER. The RCH model produces the lowest SWSR value of 1.3×10^5 and SER of 14.2. Ideally, the SER is equal to zero. Therefore, all of the four retained models simulate observed conditions poorly. The percentage of hydraulic head and chloride weighted residuals is presented in Table 9. Chloride weighted residuals comprise less than 8% of the SWSR (and SER) value, while

Figure 27. SWSR and SER for the 5 retained models at optimized parameter values. The SER is derived from the SWSR and can be thought of as an average weighted residual. Ideally, SER values should be close to one, and the four retained models are not capable of simulating field observed conditions with acceptable accuracy.

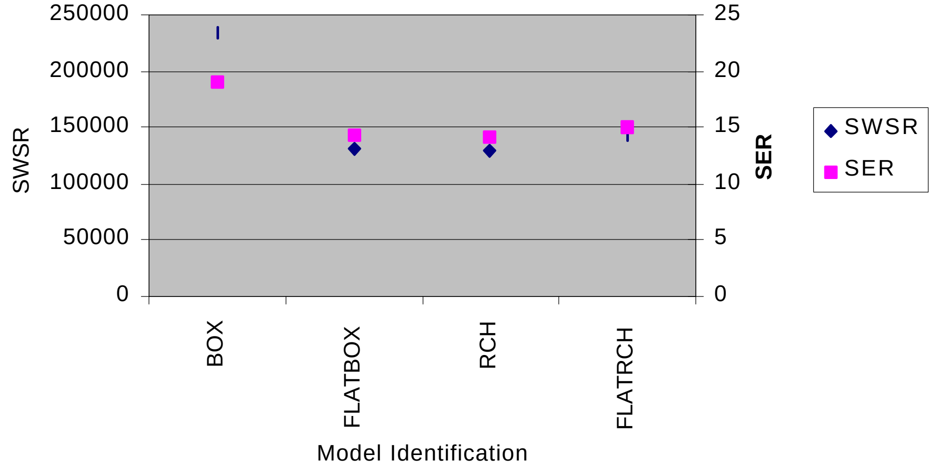


Table 9. Percentage SWSR value by observation type for the 4 retained models

Model	*Hydraulic Head*	*Chloride*
BOX	92.4	7.4
FLATBOT	96.2	3.6
RCH	94.4	5.6
RCHFLAT	94.9	5.1
No. of observations	363	285

hydraulic head residuals comprise more than 92%. This does not mean that chloride observations are not important in the regression. Parameters are estimated according to sensitivities of all observations. The high contribution of hydraulic head weighted residuals to the SWSR implies that the main source of model error is the inability to accurately simulate hydraulic head at the measured locations. While this is cause to reject all 4 of the retained models as viable representations of the system, analysis of the weighted residuals reveals model strengths that are incorporated into the multi-layer model presented in the following chapter.

Because hydraulic head observations are all weighted the same, dividing the SER by the square root of the weight used for hydraulic head gives an indication of the average difference between simulated and measured hydraulic head. The same can be done for chloride using an average weight. These values discussed later in Section 5.2.

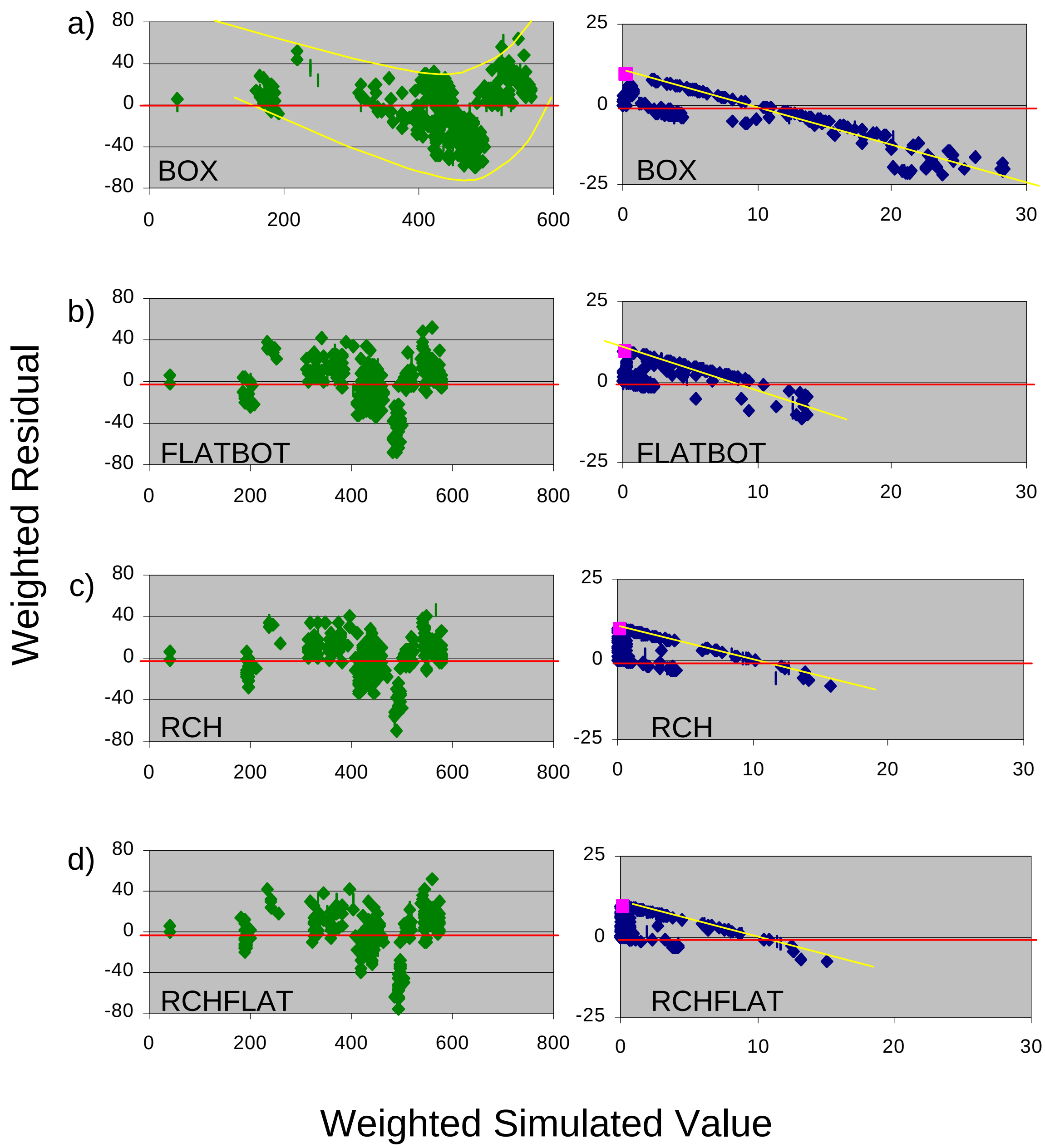
7.5 Residual Analysis

For a model to be considered valid, weighted residuals must be independent from weighted simulated values (Hill, 1998). Correlation between weighted residuals and weighted simulated values indicate model bias and that the conceptual model does not adequately represent the aquifer system (e.g. hydraulic heads in up-gradient areas are uniformly over-estimated due to a problem with the conceptual model). Weighted residuals are calculated as the measured value minus the simulated value, multiplied by the square root of the weight resulting in a dimensionless value. This section analyzes weighted residuals for the four retained models.

7.5.1 Weighted Residuals and Weighted Simulated Values

Weighted residual versus weighted simulated values are plotted for all 4 four retained models in Figure 28. Weighted residuals that are not biased must be randomly distributed above and below the “x” axis.

Figure 28. Plots of weighted simulated values versus weighted residuals for a) BOX Model, b) FLATBOT model, c) RCH model, and d) FLATRCH model. Green = hydraulic head, blue = chloride, magenta = canal seepage. Residuals should be randomly distributed above and below the ‘x’ axis, shown in red, for models to be valid. Yellow lines identify trends that are indicative of model bias.



Hydraulic head weighted residuals for all retained models are slightly more positive than negative because simulated hydraulic head is generally greater than measured values (Figure 28). In the BOX model, hydraulic head weighted residuals define a trend indicative of conceptual model bias, where yellow lines identify weighted residuals that are high in up and down-gradient areas, and low in the middle range of simulated hydraulic head. Other models do not exhibit this correlation, likely due to the inclusion of a channel-shaped zone of high hydraulic conductivity, and the BOX model is therefore discarded.

Vertical clusters of hydraulic head weighted residuals result due to simulated values not matching the oscillations of measured hydraulic head in individual monitoring wells. The maximum vertical difference for these clusters is approximately 40 (dimensionless). The square root of the weight for all hydraulic head measurements is 9.8, and the maximum error between simulated and measured heads at a monitoring well is calculated to be approximately 4 ft (the maximum oscillation observed in monitoring wells is 5 ft.). Therefore, in some wells the seasonal oscillation of hydraulic head is not simulated with sufficient magnitude. Overall, the vertical clusters are centered near zero and the difference between the maximum and minimum value is less than 40, indicating that average hydraulic heads are matched approximately and that seasonal hydraulic head fluctuations in many of the monitoring wells is being simulated within 4 ft.

Chloride weighted residual distribution for all models exhibit inverse correlations identified by red lines. This is particularly evident for the BOX model. However, the linear trend of this correlation is exaggerated due to larger chloride observations having lower weights than lower chloride concentrations (recall 95% confidence intervals for chloride measurements are 2% of the measured value and that weights are inversely proportional to the 95% confidence interval). It is possible that the method of weighting chloride residuals is contributing to model error. This is discussed further in Chapter 8, Section 2.2 *Residual Analysis*.

Chloride weighted residual for RCH and FLATRCH models are mostly positive, and chloride concentrations in these models is being simulated lower than observed concentrations for most observations. Of the three remaining viable conceptual models, the FLATBOT model simulates chloride concentration most accurately, with approximately an equal amount of positive and negative chloride weighted residuals.

7.5.2 Un-Weighted Residuals

The magnitude of hydraulic head weighted residual is as much as 8 times greater than the magnitude of chloride weighted residuals, indicating that chloride is being simulated much more accurately than hydraulic head given the uncertainty in the measured values. Calculating the average un-weighted hydraulic head and chloride residuals for the FLATBOT model reveals a significant limitation of the modeling effort. The average magnitude of the un-weighted hydraulic head residual for the FLATBOT model is 1.5 ft, which considering the large fluctuation observed in monitoring wells is an acceptable margin of error. In contrast, the average magnitude of the un-weighted chloride residual for the FLATBOT model is 500 mg/L. Chloride concentrations in almost half of the monitoring wells are below 500 mg/L, and monitoring wells with higher chloride concentrations exhibit chloride concentration oscillations that are generally less than 1,000 mg/L. Therefore, simulated chloride concentrations can significantly differ from measured values and still comprise a small portion of model error as viewed by UCODE. This is a result of the large uncertainty associated with measuring chloride concentrations in ground water and the correspondingly small weights assigned to these observations. This discrepancy is discussed further in the following chapter.

7.5.2 Spatial and Temporal Weighted Residuals

When plotted spatially and temporally, weighted residuals must have no discernable pattern (Hill, 1998). Weighted residuals for the three retained conceptual models, FLATBOX, RCH and FLATRCH, are plotted in Figure 29. Generally the magnitude of the residuals is constant throughout the area of data coverage. Positive and negative weighted residuals identify slight spatial trends in the study area. The majority of the residuals are positive, except the area immediately down-gradient from Pond D and at the most down-gradient sampling location (MW-18 and MW-19) where weighted residuals are mostly negative.

Temporal variations in weighted residuals in monitoring wells MW-6, MW-14, MW-16, and MW-18 are presented in Figure 30. Monitoring wells MW-6 and MW-16 are locations where weighted residuals are mostly positive, and monitoring wells MW-14 and MW-18 are locations where weighted residuals are mostly negative (Figure 29). All models have similar weighted residuals over time. The spatial trend apparent in Figure 29 is due to hydraulic head weighted residuals and not chloride weighed residuals. Two possible explanations for this spatial correlation that 1) optimized seepage from Pond D is too great, or 2) that the hydraulic conductivity in this area is too low. Simulated pond seepage is a minor contributor to ground-water recharge as is expected and it is more likely that the channel-shaped zone of hydraulic conductivity should extend into this area.

Measured hydraulic head in all four wells oscillates over time (Figure 13). This is not simulated accurately by any of the three models, illustrated by the oscillation of hydraulic head weighted residuals in Figure 30. Measured chloride concentrations oscillate only for MW-14 and MW-18 (Figure 16), and these oscillations are also not simulated accurately by any of the three retained models. For MW-14, the chloride weighted residuals calculated by the FLATBOT model are less than, and oscillate with greater magnitude, than in other models. However, because the FLATBOT model has chloride weighted residuals that are lower in magnitude than other models, the

Figure 29. Spatial distribution of weighted residuals for all times for a) FLATBOT model, b) RCH model, and c) FLATRCH model. The magnitude of the weighted residual is proportional to the size of the circle. Positive weighted residuals are black and negative weighted residuals are red.

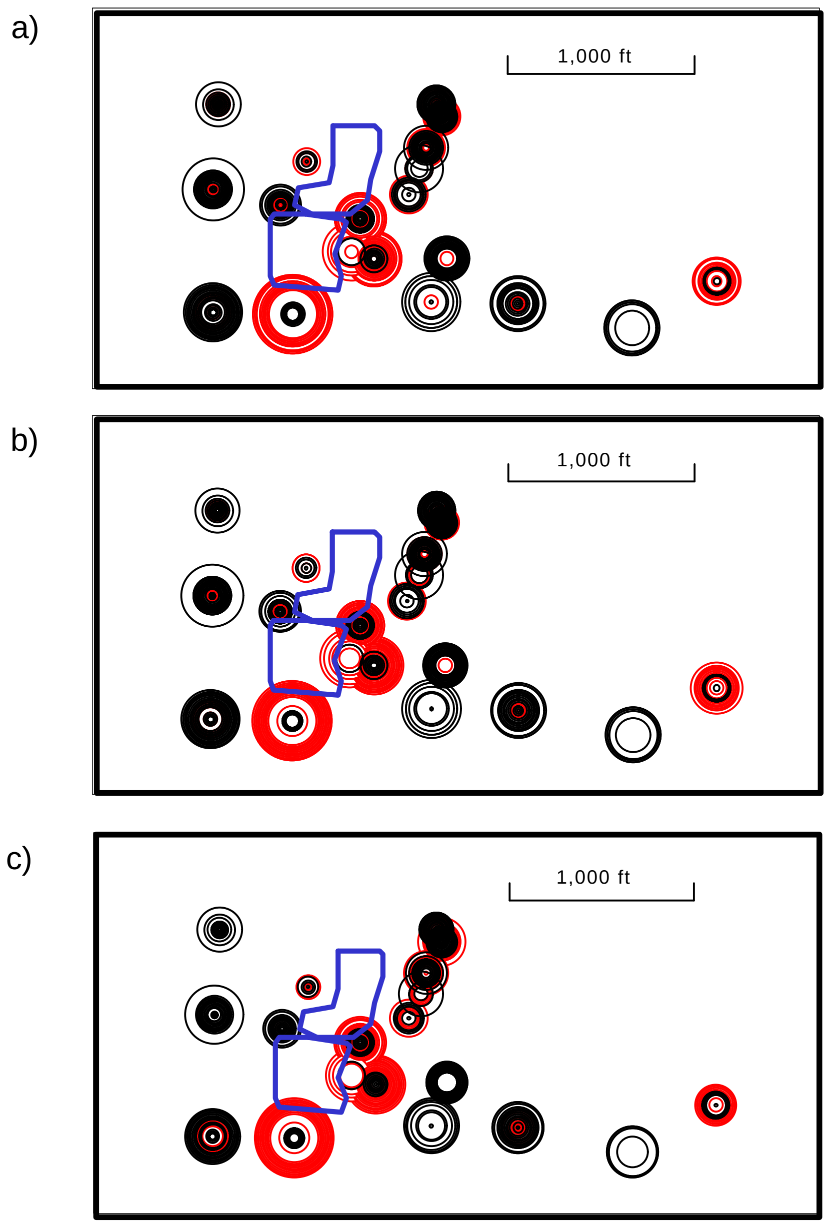
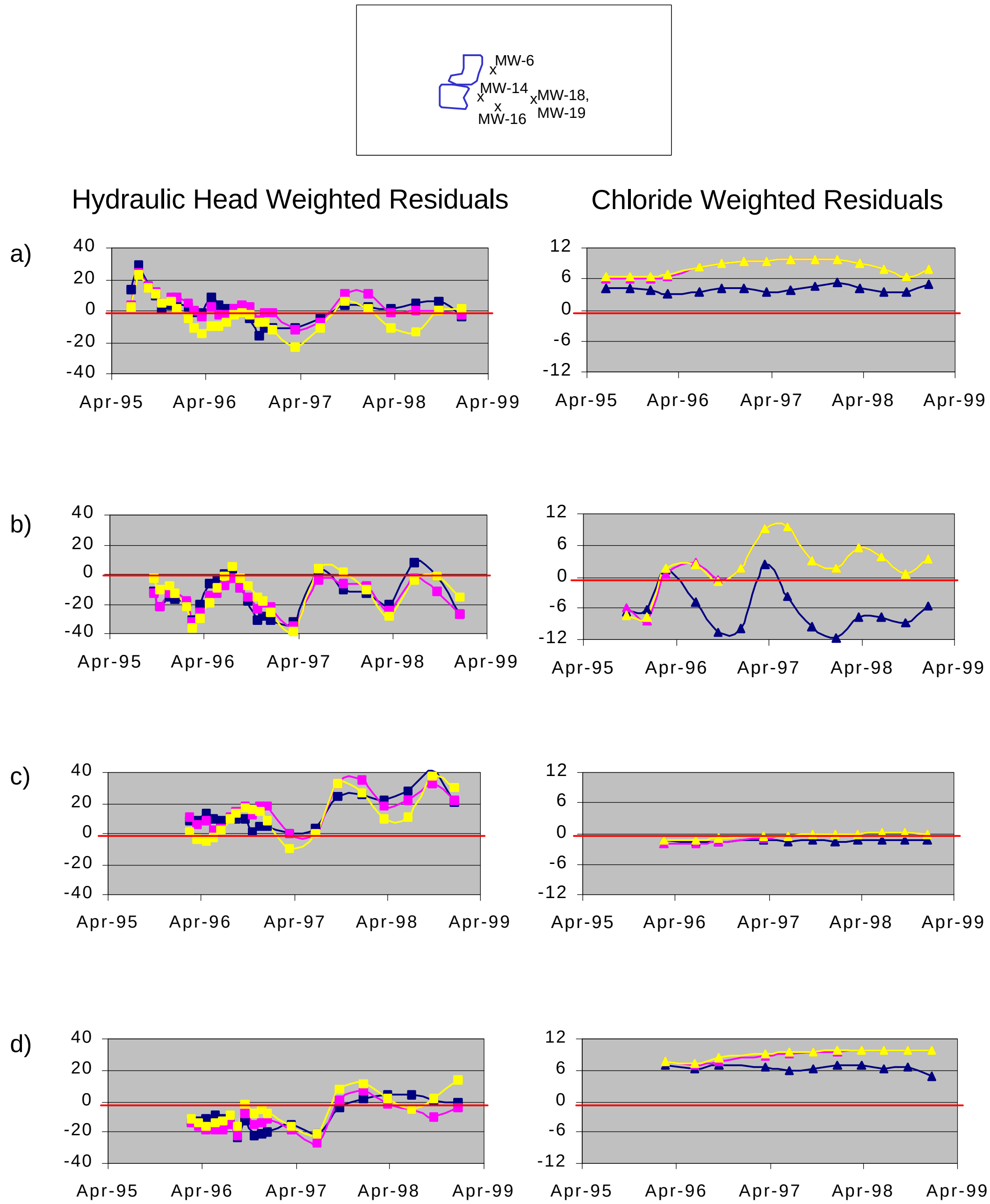


Figure 30. Temporal variation of weighted residuals at a) MW-6, b) MW-14, c) MW-16, and d) MW-18. Hydraulic head weighted residuals are plotted in the left column as squares and chloride weighted residuals are plotted in the right column as triangles. Blue = FLATBOT model; Magenta = RCH model; Yellow = FLATRCH model.



FLATBOT model is the most favorable model of the three.

It is encouraging that there is not a significant increase or decrease of chloride weighted residuals over time. This indicates that the decrease of measured chloride concentrations associated with the migration of the produced water plume down-gradient is being simulated with some accuracy.

7.6 Simulated Chloride Distribution

The simulated distribution of chloride concentration in December, 1998 is shown for the FLATBOT model in Figure 31. For comparison, manually contoured chloride concentrations and relative electrical conductivity data measured in December 1998 are shown as well as. The simulated chloride distribution is significantly different from distributions measured in the field. The majority of the chloride is simulated to have left the study area by this time. Models RCH and FLATRCH simulate all chloride having left the study area at this time and are not shown.

All models simulate advective transport to be too rapid. A typical conclusion is that effective porosity is too low. However, effective porosity is estimated and also used as specific yield, thus the resulting plume is a “compromise” between matching heads and chloride concentration data. Simulated chloride concentration distributions for all models are therefore unrealistic and additional conceptual models are needed.

Chloride distributions simulated for December, 1995 when the ponds are still active are shown in Figure 32. The simulated chloride distribution for the RCHFLAT model (c) is the most similar to measured concentrations in December 1998 (shown in Figure 31), although all models simulate the plume to extend to the model boundary which is not indicated by the geophysical field data shown in Figure 31.

Analysis of the character of the simulated chloride distributions produced by the three retained models identifies conceptual model strengths that are useful in guiding the development of additional conceptual models. The models, FLATBOT, RCH, and

Figure 31. (a) Simulated chloride distribution for the FLATBOT model at final simulation time (December, 1998). Contour interval is 250 mg/L. (b) Manually-contoured chloride distribution measured in monitoring wells in December, 1998). (c) Contours of relative magnitude of reliable geophysical data collected in December 1998. The majority of the chloride is simulated to have left the study area at this time.

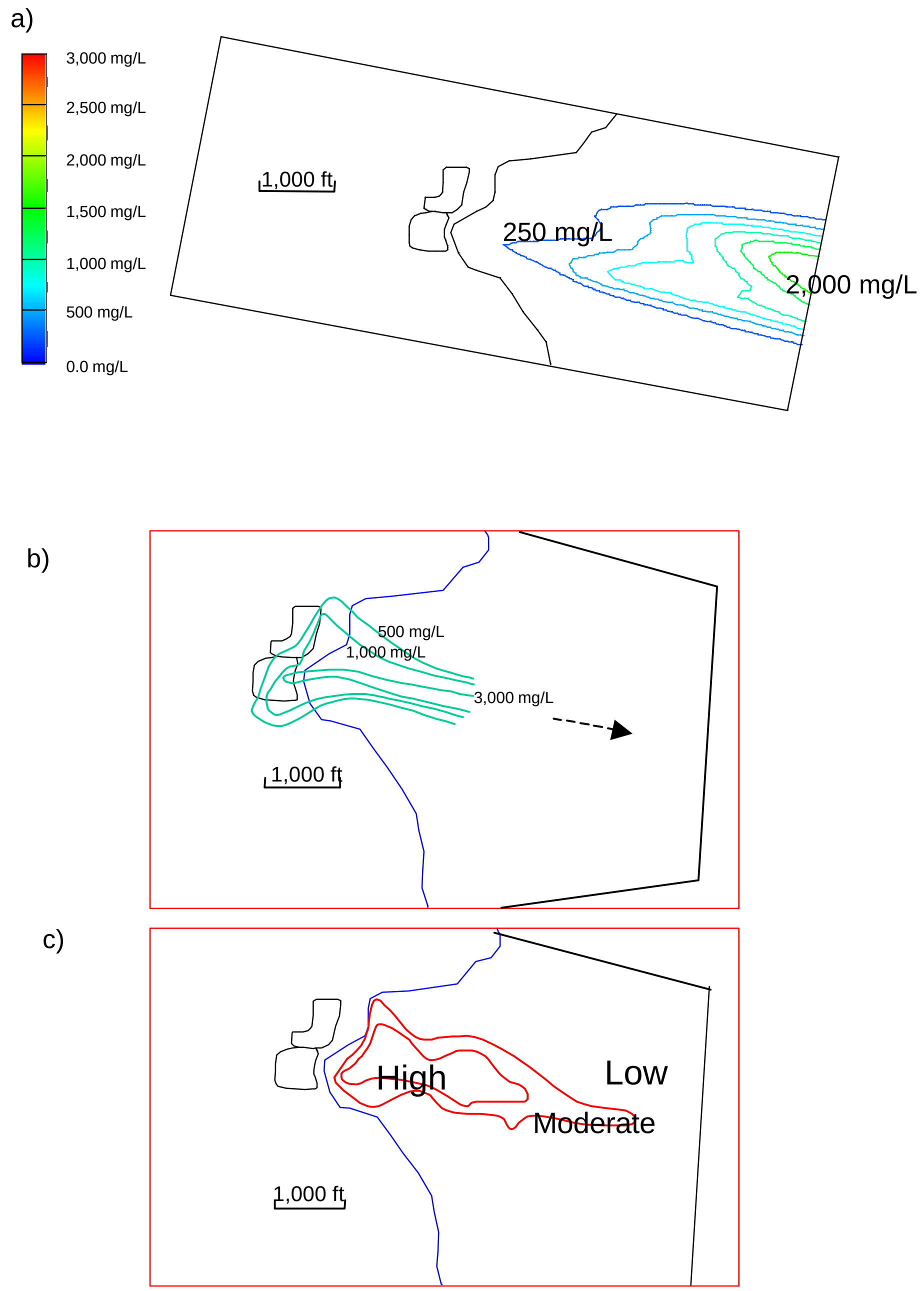
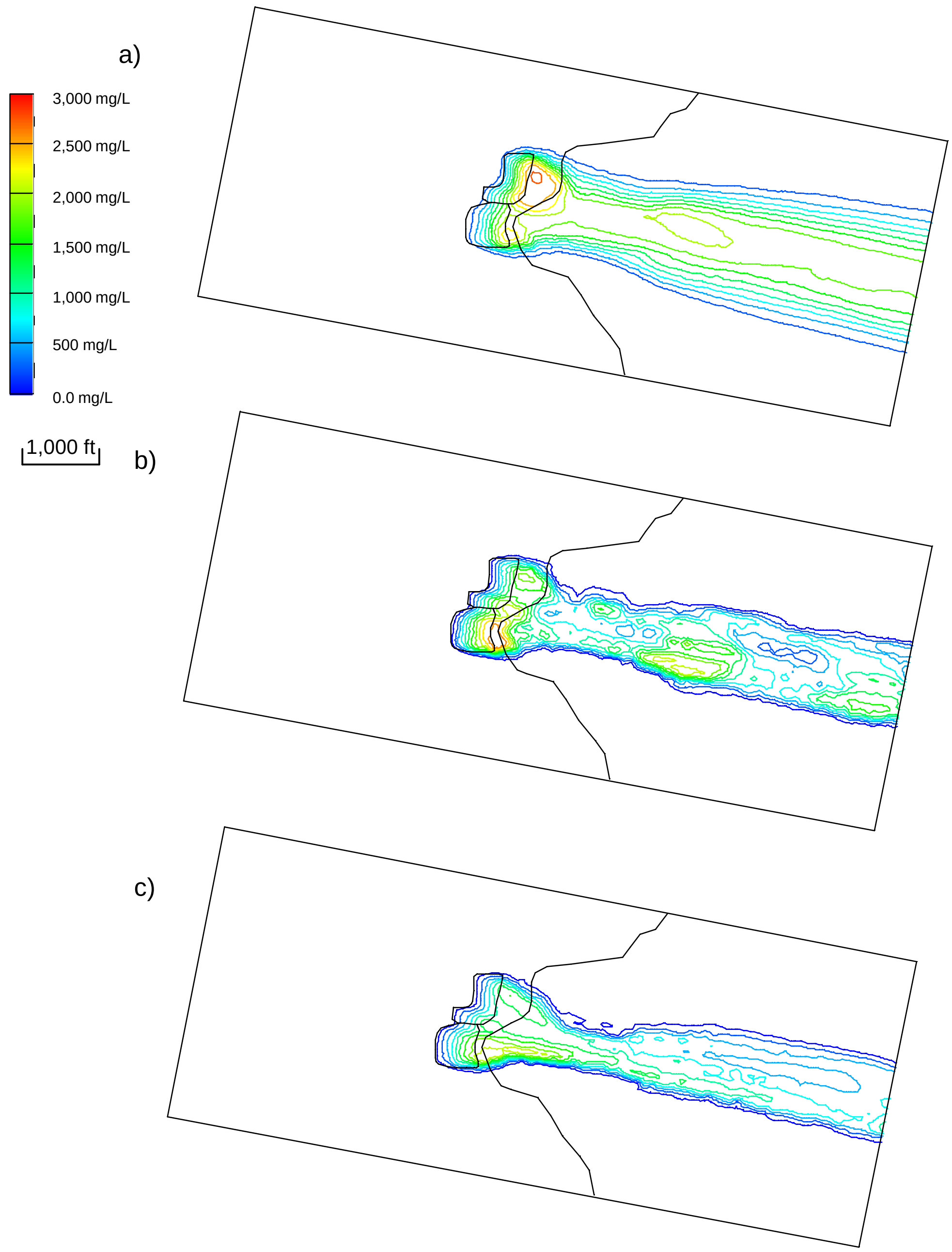


Figure 32. Simulated chloride distribution on December, 1995 for a) FLATBOT model, b) RCH model, and c) RCHFLAT model. Contour interval is 250 mg/L. The simulated chloride distribution for the FLATRCH model (c) is the most similar to measured concentrations in December 1998 (shown in Figure 31). All models erroneously simulate the plume to extend to the model boundary at this time.



FLATRCH, contain a channel-shaped zone of high hydraulic conductivity that acts to limit the amount of lateral spreading of the plume immediately down gradient of the ponds, although the plume is not focused to the degree observed in the field. While it is possible that the inclusion of additional zones of hydraulic conductivity may simulate increased focusing of the plume, it is more likely that chloride is migrating vertically downward and that monitoring wells are sampling only the top portion of the plume. This concept was presented earlier in Figure 18. A multi-layered model is needed to simulate this process.

A significant difference between chloride distributions simulated by the three models is the location of the highest chloride concentrations. The FLATBOT model simulates seepage from the ponds as head-dependent, and the northern pond (Pond C) is contributing more chloride to the ground-water than the southern pond (Pond D). The reverse is true for models RCH and FLATRCH, which simulate seepage from the ponds as specified flux, and the southern pond appears to be contributing more chloride than the northern pond. This may be the cause of additional plume spreading observed in the FLATBOT model relative to the RCH and FLATRCH models. Pond D has greater areal extent than Pond C and it is more likely that Pond D is the major source of chloride to ground water. Therefore, the simulation of pond seepage is more accurate using a specified flux value.

7.7 Summary of Single Layer Modeling

All twelve single layer conceptual models fail to simulate field observed conditions with acceptable accuracy and predictive simulation is not warranted. Analysis of statistics provided by UCODE provides valuable insights into conceptual model deficiencies that point to the need for a multi-layered model for accurate predictive simulation. A summary of the results of single-layered modeling used in the development of a multi-layered model are listed below.

Boundary Definition

- Models that simulate only the unconsolidated units are not valid. The aquifer underlying WCWD Aquifer extends below the unconsolidated units into the Arapahoe Formation.
- The areal boundaries are best represented by a rectangle rather than tapering down-gradient as in the CONE model.
- The aquifer base used in the FLATBOT and FLATRCH models produced the lowest SWSR and is the most representative of the geohydrologic conditions in the study area. This configuration defines the base of the aquifer as constant elevation up-gradient of MW-19 and sloping according to the average measured potentiometric surface down-gradient of MW-19.
- The specified head of 4983.5 ft amsl at the outflow boundary is reasonable.
- Seepage from the canal and ponds is best simulated as specified flux boundaries. This avoids problems associated with the ponds and canal acting as ground-water sinks when estimated parameters raise the potentiometric surface above the land surface elevation and is shown to simulate a narrow plume.

Parameterization

- Hydraulic conductivity is the most sensitive parameter and therefore can be estimated with the greatest confidence by UCODE.
- Low sensitivity parameters include the conductance factor for pond seepage, specific yield, source strength, and longitudinal and transverse dispersivity. With the exception of the pond conductance, it is reasonable to fix these parameters at measured or published values to improve calibration and reduce computational time required for regression.

- When seepage from the pond is simulated as specified flux, the sensitivity of the seepage factor increased.
- Independently estimating hydraulic conductivity in up-gradient and down-gradient zones resulted in acceptable calibration to hydraulic heads.
- The inclusion of a channel-shaped hydraulic conductivity zone limited the lateral migration of chloride and improved the calibration of hydraulic head.

CHAPTER 8. MULIT-LAYERED MODEL

A twelve layer model, MULTI, was developed to simulate chloride migration in three dimensions. While several viable conceptual models exist, only one model is presented and recommendations for future conceptual models are presented based upon simulation results. This chapter presents the multi-layered model, evaluates the accuracy of model calibration, presents results of predictive simulations made using the multi-layered model, and quantifies the error associated with those predictions. Calibration statistics identify limitations of the twelve-layer model similar to those observed for single-layer models, but the overall distribution and migration of the chloride plume simulated by the twelve-layer model replicates field conditions with reasonable accuracy.

8.1 Definition of the MULTI Model

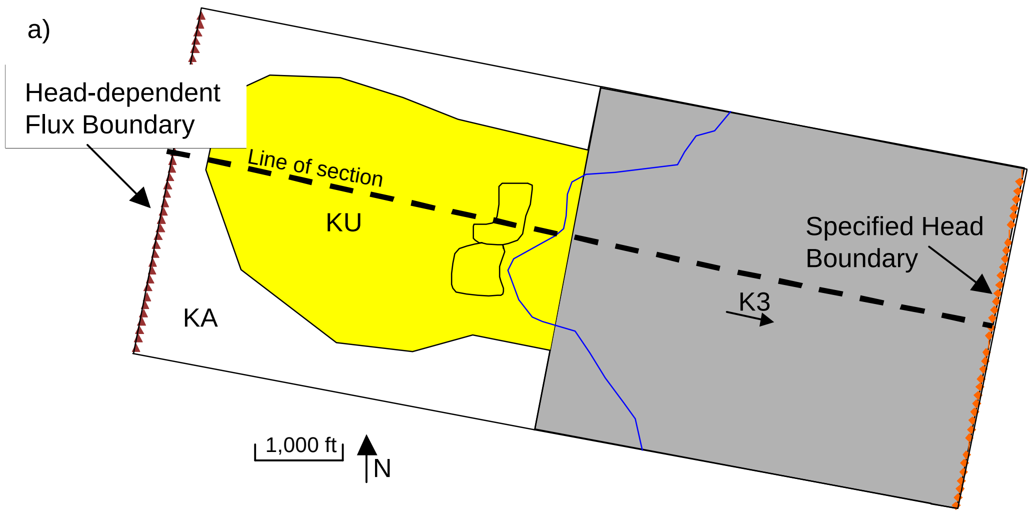
Results of analyses of single-layer model calibration are used to develop the twelve-layer model, MULTI. The primary objectives of a multi-layered model are 1) to simulate accurate source strength chloride concentrations so that analysis of total chloride mass transport is meaningful, 2) to simulate vertical concentration gradients observed in monitoring wells MW-18 and MW-19 and likely present throughout the plume area, and 3) to apply insights gained from single-layered models to generate a more accurate conceptual model of the study area so that plume migration can be predicted accurately.

8.1.1 Multi-layer Conceptual Model

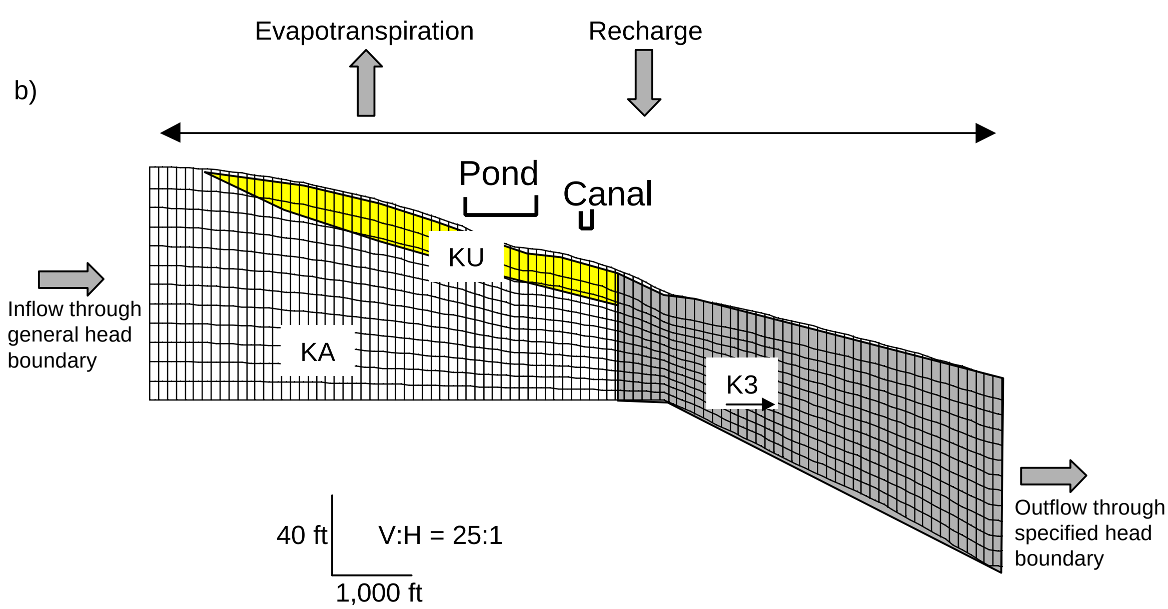
The MULTI conceptual model is presented in Figure 33. Initially, the MULTI model was constructed using the same aquifer geometry as the FLATBOT and

Figure 33. Multi-layer conceptual model, MULTI. (a) Plan view. The model area is divided in to three zones of hydraulic conductivity: unconsolidated deposits (KU) = yellow, Arapahoe Formation (KA) = no color, and unconsolidated deposits with increasing amount of coarse gravel (K3) = gray. A head-dependent flux boundary is specified at the up-gradient boundary to simulate ground water recharge from up-gradient aquifers. (b) Cross section. Recharge is constant throughout the model area and evapotranspiration occurs as a function of water table depth throughout the model area.

a)



b)



FLATRCH models, however, preliminary simulations resulted in steep hydraulic gradients near the model outflow boundary that are not observed in the field. To generate a more uniform gradient in this area, the base of the aquifer down-gradient of MW-18 and MW-19 in the MULTI model slopes at a angle steeper than in the FLATBOT and FLATRCH models, to a maximum thickness of 83 ft at the eastern boundary.

Hydraulic conductivity in the MULTI model is divided into three zones, KU, KA, and K3. KU encompasses the areal and vertical extent of the unconsolidated deposits up-gradient of MW-18 and MW-19 defined by the aquifer base in the unconsolidated-type models. The area below KU and up-gradient of MW-18 and MW-19 is represented by KA (Arapahoe Formation). A third zone, K3, extends down-gradient of MW-18 and MW-19 throughout the thickness of the aquifer. Based upon steep gradients near the outflow boundary simulated by preliminary simulations, K3 is calculated to increase linearly from MW-18 and MW-19 to the out-flow boundary where it is 1.2 times greater using the function file in UCODE. When viewed in terms of transmissivity (hydraulic conductivity times thickness) the resulting parameterization of hydraulic conductivity and aquifer geometry resembles that of the single-layered models that include a channel-shaped zone.

Seepage from the ponds and canal is simulated as a specified flux boundary, where conductance factors are estimated as in the RCH and FLATRCH models.

Recharge (from precipitation) is estimated as a uniform value over the study area. Preliminary simulations estimated areal recharge values near zero. To allow for more flexible optimization of recharge, the evapotranspiration used in ET models is included with the MULTI model.

Vertically, the aquifer is divided into 12 layers of equal thickness. Vertical hydraulic conductivity and specific yield are constant for all layers throughout the model.

The up-gradient boundary of the MULTI model is a general head boundary intended to simulate recharge from aquifers up-gradient of the study area. If up-gradient recharge was simulated using areal recharge applied to only the top layer (as in single-layered models), unrealistically large vertical gradients may develop between model layers. The general head boundary is used to simulate horizontal flow into the aquifer so that vertical flow may be simulated realistically.

8.1.2 Numerical Simulation

The rectangular, single-layer grid used in most of the single-layer models (97 cells in the x-dimension and 40 cells in the y-dimension) is divided into 12 layers of equal thickness, resulting in a total of 46,560 cells. Vertical cell thickness increases from a minimum of 4 ft in the area of MW-18 and MW-19, to 9 ft at the up-gradient boundary, and to 7 ft at the down-gradient boundary.

All layers are simulated in MODFLOW as unconfined by specifying each layer as type 3 in the BCF package (except the top layer which is type 1) and using specific yield as the primary and secondary storage coefficient value. All other MODFLOW settings are as in previous models.

The twelve-fold increase in cell number caused forward simulations to run too slowly for effective regression (approximately one day) and several changes are made to model settings to minimze MODFLOW and MT3D computational time. When comparing flow fields and calculated residuals, it was determined that the number of time steps for the 88 stress periods could be decreased to half as many without sacrificing numerical accuracy. To limit MT3D computation, cells 1,000 ft up-gradient of the ponds are inactive. To further decrease MT3D computational time, the pure finite difference method is used to calculate advection. The use of the pure finite difference method can lead to significant numerical dispersion in areas of large concentration gradients (Zeng, 1990). Therefore, the estimation of optimized parameter values is performed using the pure finite difference method, and once the optimal parameters are obtained, simulations are conducted using the more accurate HMOC method for the calculation of results.

All monitoring wells are screened through the top layer of the model and partially into the second layer except for MW-19, which is completed in the bottom layer only. To reduce model simulation time and output file size it is necessary to extract heads from only one layer of the model. The second layer was chosen because in some simulations cells in the top layer went “dry”. Preliminary simulations showed that vertical gradients in the top two layers are less than 0.005 and this does not introduce significant error into the regression. Simulated chloride in monitoring wells is computed between layers as the weighted average of the screened interval in each layer.

8.1.3 Parameterization

Parameters estimated and specified in the MULTI model and initial values are listed in Table 10. Optimized values for hydraulic conductivity from the FLATBOT model are used as initial values for horizontal hydraulic conductivity in the MULTI model because these values resulted in the best calibration of single-layer models. Vertical hydraulic conductivity is uniform throughout the aquifer and an initial value is presented in the final paragraph of this section.

The hydraulic head at the up-gradient head-dependent flux boundary is initially set to 81 ft, which is the value simulated in those cells by the optimized FLATRCH model on April 1998. The conductance of the head dependent boundary cells is calculated using the function file in UCODE as the hydraulic conductivity of the cells, KA, multiplied by the thickness of the cell (cell length and width are equal so they cancel out).

The initial value of the maximum evapotranspiration rate is derived from optimized ET models, and the initial value for RCHALL is derived from the optimized value from the FLATRCH model. Field measured and analytically calculated canal and pond seepage rates are used as initial values. The chloride concentration (SS) of the ponds is fixed at 13,000 mg/L based upon an average of three measurements.

The most significant factor limiting MT3D simulation time is the maximum allowable transport step size. The maximum allowable transport step size is calculated by MT3D to ensure numerical stability for equations used to solve advection and dispersion processes. For the MULTI model, the dispersion term is controlling the maximum transport step size, which is proportional to specific yield and inversely proportional to dispersivity and vertical hydraulic conductivity. Therefore, these parameters were not estimated during regression for the MULTI model. To yield a reasonable maximum transport step size it was necessary to specify specific yield at 0.30, which is more than twice the optimized value of single layer regressions, but within the reasonable parameter range. This large value of specific yield may inhibit the simulation of oscillating hydraulic head values. To yield a reasonable maximum transport step size it is also necessary to specify a low value of longitudinal dispersivity of 10 ft, which is approximately 17% of the optimized value in single-layer models. This is potentially a significant error in the conceptual model. The factors used to calculate transverse and vertical dispersivity is specified at published values.

Vertical hydraulic conductivity is also held constant to limit MT3D simulation time and is specified in MODFLOW as VCONT, the vertical hydraulic conductivity divided by the layer thickness. To account for vertical stratification of fine-grained units within the unconsolidated deposits and Arapahoe Formation, vertical hydraulic conductivity is assumed to be 2 orders of magnitude less than KU, the horizontal hydraulic conductivity of the unconsolidated deposits (46 ft/day initially). Using an average layer thickness of 6 feet the value for VCONT specified in MODFLOW is 0.08 day^{-1}. In preliminary regressions which estimated VCONT, this value did not change significantly in 3 iterations, indicating that this is a reasonable estimate for parameter values near the initial values listed in Table 10.

Table 10. Parameter summary for the MULTI model.

Parameter	*Description*	*Estimate (E) or Specify (S)*	*Initial Value*
KU	unconsolidated hydraulic conductivity	E	46 ft/day
KA	Arapahoe Formation hydraulic conductivity	E	13 ft/day
K3	linear increasing hydraulic conductivity	E	64 ft/day
VCONT	two orders of magnitude less the quotient of hydraulic conductivity KU and the average cell layer thickness (6ft)	S	0.08 day^{-1}
HGHB	hydraulic head at the up-gradient head dependent boundary	E	81 ft
CGHB	conductance factor for cells at the up-gradient head dependent boundary	S	8 ft
ET	maximum rate of evapotranspiration	E	0.0012 ft/day
RCHALL	constant areal recharge rate	E	0.012 ft/day
CRCH	recharge from Speer Canal	E	1.1 ft/day
PRCH	recharge from the ponds	E	1.5×10^{-3} ft/day
SS	chloride concentration of pond water	S	13,000 mg/L
DL, DT, DV	longitudinal dispersivity, transverse dispersivity factor, vertical dispersivity factor	S	10 ft, 0.2, 0.04

8.2 Evaluation of MULTI Model Calibration

At optimized parameter values, numerical simulations using MODFLOW and MT3D (using HMOC) converge with acceptable mass balance errors less than 1% and numerical results are considered to be valid. When parameters are estimated using UCODE, regressions fail to converge using the criteria of a 5% maximum fractional parameter change. After 12 iterations the SWSR no longer decreases although parameter estimates continue to change by as much as 15%. After 14 iterations estimated parameters produce MT3D simulations that do not converge. Therefore, parameters estimated at the twelfth iteration are considered to be the optimal parameters for the MULTI model.

Calibration statistics for optimized parameter values illustrate similar problems that were identified for single-layer models: a poor overall fit to measured data. However, the simulated spatial distribution of chloride is similar to the observed distribution in the field and reveals additional information about system.

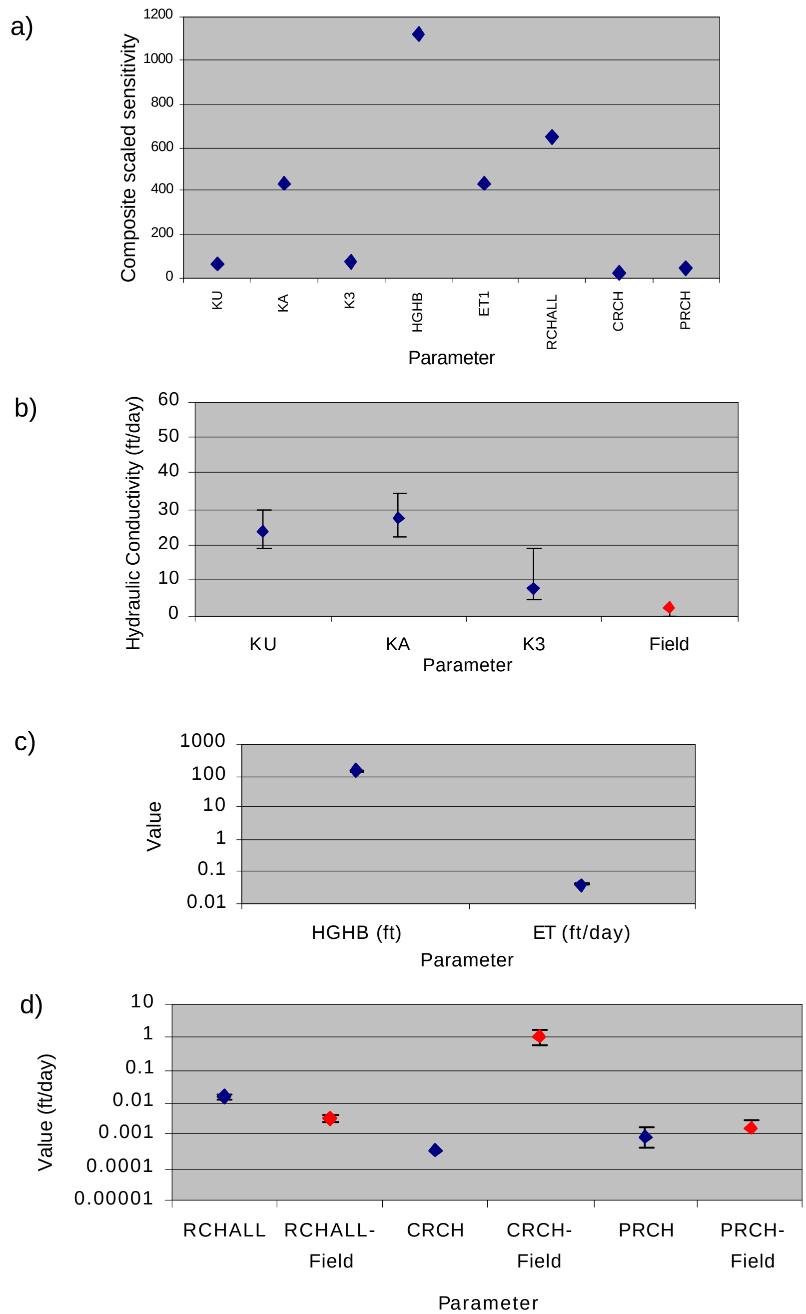
8.2.1 Optimized Parameter Values

This section discusses optimized parameter statistics. Parameter correlations do not exist for any of the estimated parameters.

Composite scaled sensitivities

Composite scaled sensitivities calculated at optimized parameter values using central differences are presented in Figure 34(a). The composite scaled sensitivities for all parameters are within two orders of magnitude of the most sensitive parameter, except for the canal seepage (CRCH), which is zero. Several actions were taken to increase the sensitivity of canal seepage (and consequently its ability to be accurately estimated): 1) beginning regressions with significantly different initial values arrives at similar

Figure 34. Optimized parameter statistics for the MULTI model. Parameters are defined in Table 10. (a) Composite scaled sensitivities calculated at optimized parameters. (b)-(d) Optimized parameter values and 95% confidence intervals (as error bars). FIELD indicates analytically calculated value and ranges and these values are posted in red where available.



optimized parameters and sensitivities; 2) increasing the perturbation amount that is used to calculate sensitivities results in MT3D simulations that do not converge; and 3) specifying a value for canal seepage results in poorer model calibration. Therefore, the seepage from the canal is not estimated accurately by this conceptual model.

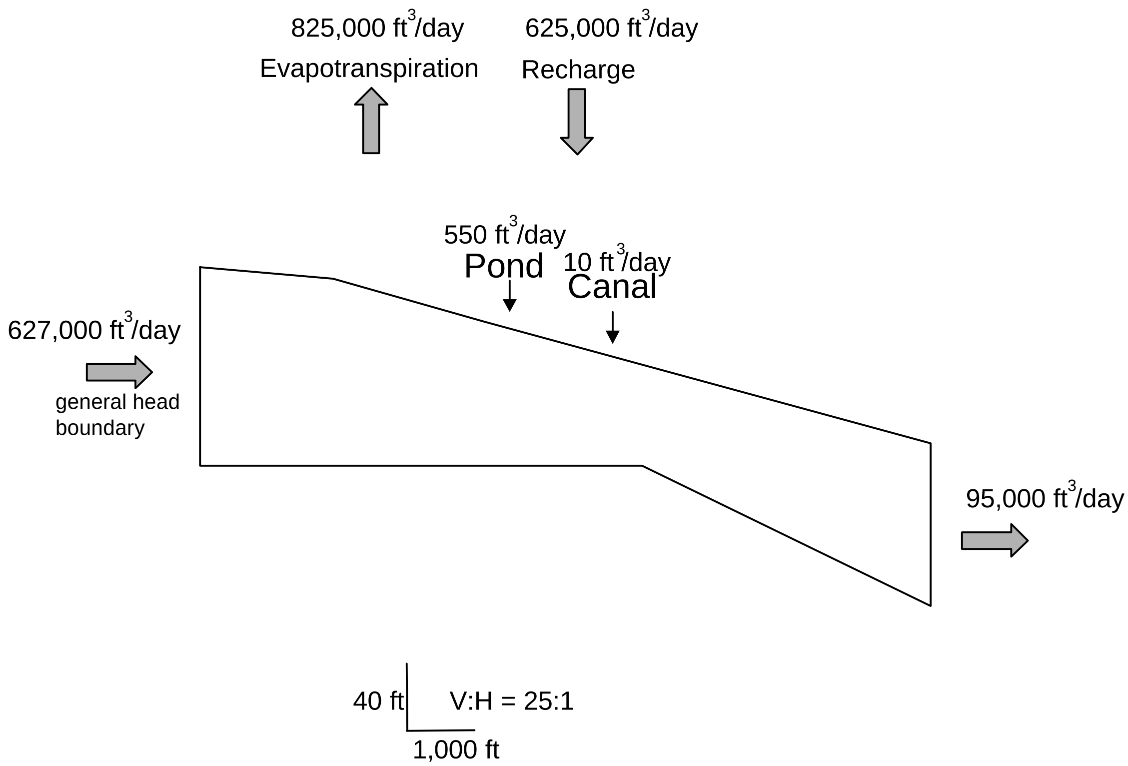
Parameter Values and Confidence Intervals

The optimized parameter values and 95% confidence intervals are presented with initial and reasonable values (when applicable) in Figure 34(b-d). All parameters are estimated with narrow 95% confidence intervals except for canal seepage (due to zero sensitivity). Hydraulic conductivity values are all within measured ranges. Values for KU and KA are similar, 24 ft/day and 27 ft/day respectively. The third zone of hydraulic conductivity, K3, is estimated to be 8 ft/day in up-gradient areas, increasing to 9.6 ft/day at the eastern boundary. It is geologically reasonable to expect hydraulic conductivity to increase in the direction of Beebe Draw as a result of coarser grained sedimentation, and the low value of K3 indicates the aquifer may be too thick in the eastern area.

A water budget is presented in Figure 35 to illustrate the flows simulated by optimized source and sink parameters. The estimated hydraulic head at the western head dependent boundary is 5140 ft above mean sea level (amsl), 60 feet higher than the initial value, simulating large amounts of ground-water inflow. The hydraulic head at this location in the Arapahoe Formation is estimated to be approximately 5120 ft amsl (Robson, 1991). The difference in values is likely due to the lack of heterogeneities being represented and is not thought to be indicative of model error.

A similarly high recharge volume is estimated, two orders of magnitude greater than what is analytically determined reasonable. This large amount of recharge is offset by an equally large amount of evapotranspiration. However, correlations between these parameters do not exist and the sensitivity of both parameters is significantly large. Therefore, these values may be reasonable. Seepage from the canal is simulated to be a minor contributor to system, contrary to what is inferred from hydrographs in

Figure 35. Conceptual water budget for optimized parameter values in the MULTI model shown in cross section view. Recharge from canal seepage is estimated by the regression to be too low.



monitoring wells. Further analysis in later sections identifies this low estimate to be a significant source of error in the MULTI conceptual model. Seepage from the pond is estimated to be roughly equal to the analytically calculated seepage rate.

Model Linearity

Model linearity is calculated using the modified Beale's measure of linearity. For the 95% confidence intervals to be valid, the model must be approximately linear in the vicinity of the optimized parameter values. A discussion of the modified Beale's measure is provided in Hill (1994). Model linearity could not be calculated for the entire parameter set due to problems associated with the zero sensitivity of canal seepage. Beale's measure calculated at optimized parameter values excluding canal recharge is two orders of magnitude greater than the number that would indicate model linearity. Therefore, 95% confidence intervals are not calculated accurately and are approximate values that are useful for only for comparison and qualitative analysis.

8.2.2 Residual Analysis

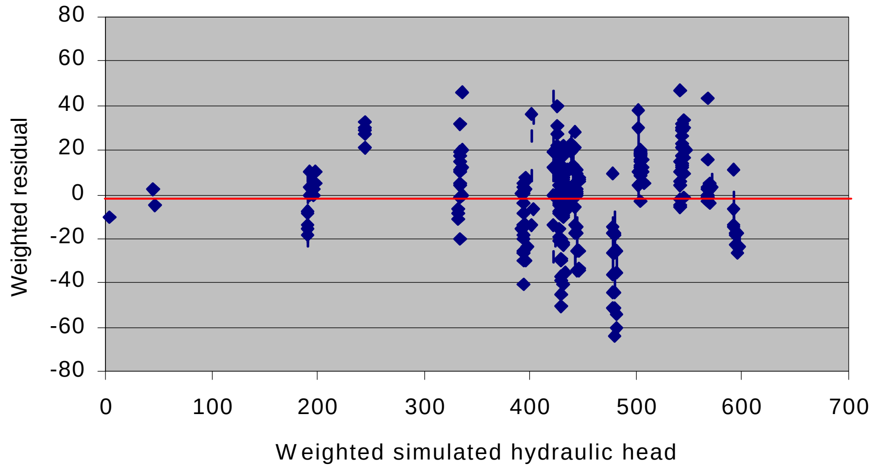
The sum of the weighted squared residuals (SWSR) calculated in the MULTI model is 1.4×10^5 and the standard error of the regression (SER) is 14.6. For comparison, the FLABOT model has the lowest SER of single-layer models of 14.2, indicating that the MULTI model simulates field observed conditions with less accuracy than the FLATBOT model. However, the analyses of simulated chloride distribution presented in a later section demonstrates that the multi-layer conceptual model is considerably more accurate than single-layered models.

Weighted Residuals and Weighted Simulated Values

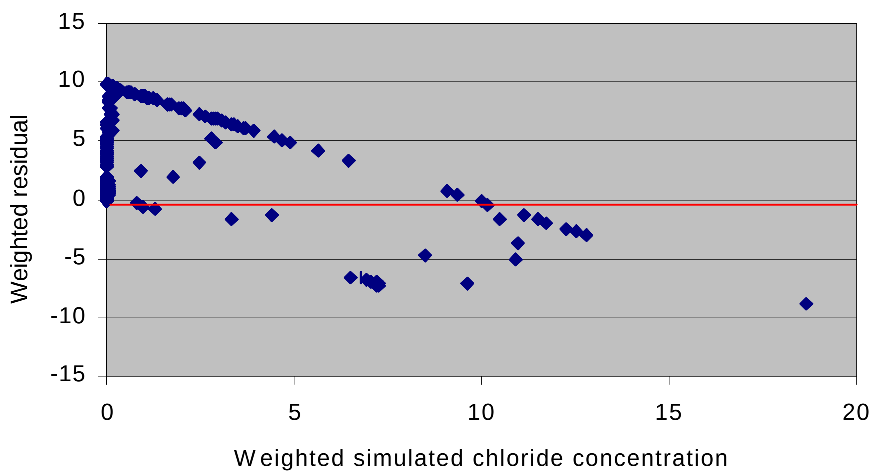
Weighted residuals calculated for the MULTI model display correlations to weighted simulated values (shown in Figure 36) that are similar to those identified in

Figure 36. Weighted residuals versus weighted simulated values for the MULTI model for (a) hydraulic head and (b) chloride concentration. Hydraulic head weighted residuals are evenly distributed above and below the 'x' axis, but are correlated in vertical clusters because the seasonal fluctuation is not simulated. Chloride weighted residuals are correlated to the weighted simulated value.

a)



b)



single-layer models. When plotted versus weighted simulated values, hydraulic head weighted residuals in Figure 36(a) are evenly distributed above and below the x axis, but are clustered vertically indicating that the seasonal oscillation of hydraulic head is not simulated accurately. Chloride weighted residuals versus weighted simulated values, shown in Figure 36(b), are inversely correlated. The majority of the chloride weighted residuals are positive, and the magnitude of the residual decreases as the weighted simulated value increases, indicating that generally simulated chloride concentrations are too high and that larger measured chloride concentrations are simulated with greater accuracy.

Discussion of the Effect of Different Data Types on Regression

A possible explanation for the bias in the chloride concentration residuals is that hydraulic head and chloride concentration are fundamentally different types of data. Hydraulic head is an interval scale data type, where data values have no limits and can range above and below zero (Swan and Sandilands, 1995). Weighting assigned to hydraulic head measurements is also done using interval type data, where there is an 95% certainty that the measurement is accurate to plus or minus 0.2 feet. Chloride concentration is closed data type where concentrations are essentially percentage chloride measurements, and values are restricted between 0% chloride and values where chloride salts begin to precipitate (Swan and Sandilands, 1995). Weights assigned to chloride measurements are also closed form data types, or 2% of the measured value. Therefore, there is a correlation between the measured chloride value and the weight assigned to that measurement that does not exist between hydraulic head measurements and weights.

It is not clear how these fundamentally different types of data affect the regression. Experimental regressions that use interval scale data to weight chloride measurements (95% confidence interval of plus or minus 200 mg/L) resulted in worse overall model fit and similar un-weighted residual distributions. Similar results occur when the weighting for chloride observations is reversed, so that lower chloride concentrations are weighted less than large concentration values.

A highly controlled and calibrated model is needed to properly analyze the effect of using different data types on regression. Future work in this area should investigate the effect of using a normalization scheme to convert hydraulic head data to a closed form data type.

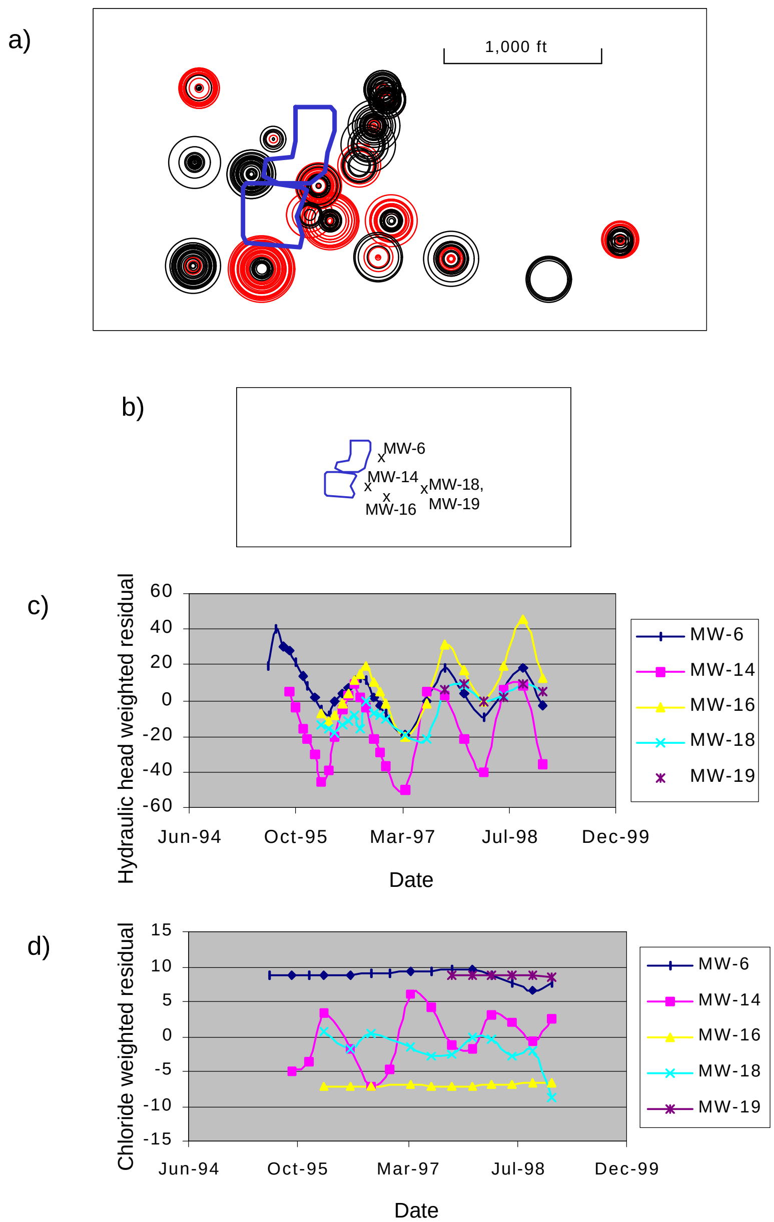
Spatial and Temporal Distribution of Weighted Residuals

The spatial and temporal distribution of weighted residuals for the MULTI model is displayed in Figure 37. Spatial bias is not evident in the conceptual model. The spatial distribution of all weighted residuals is more evenly distributed with respect to magnitude and sign (positive or negative) than in previous single-layer models indicating that the MULTI model is more representative of the system.

The temporal distribution of hydraulic head weighted residuals (Figure 37c) and chloride weighted residuals (Figure 37d) is plotted for monitoring wells MW-6, MW-14, MW-16, MW-18, and MW-19. Hydraulic head weighted residuals oscillate over time and seasonal water table fluctuations are not simulated. Measured chloride concentrations for monitoring wells MW-6, MW-16, and MW-19 do not oscillate significantly over time, whereas measured chloride concentrations in monitoring wells MW-14 and MW-18 oscillate by as much as 1,000 mg/L. Chloride weighted residuals plotted over time indicate that these oscillations are not simulated by the model. Additional simulations were conducted to determine if a lower value of specific yield would simulate hydraulic head and chloride oscillation observed in the field. Reducing specific yield by half (0.30 to 0.10) did not produce a detectable increase in simulated value oscillation (MODFLOW simulations using specific yield values less than 0.10 did not converge). Therefore, the low contribution of canal seepage to total flow in the aquifer is the suspected cause of temporal residual bias and is a major deficiency of the MULTI model.

The MULTI model appears to be simulating plume migration too slowly.

Figure 37. Spatial and temporal distribution of weighted residuals for the MULTI model. (a) Weighted residuals are plotted in plan view. The size of the bubble is proportional to the magnitude of the weighted residual. Positive weighted residuals are black and negative weighted residuals are red. (b) The location of the monitoring wells plotted in (c) and (d). (c) Hydraulic head weighted residuals over time in selected monitoring wells. (d) Chloride weighted residuals over time in selected monitoring wells.



Measured chloride concentrations in wells shown in 37d decrease over time at significantly different rates as the chloride plume migrates down-gradient (Figure 16). When a straight line is fitted to the chloride weighted residuals in these wells (not shown), the slope is horizontal for all wells except for the most recent weighted residuals in MW-18. This indicates that the rate of overall chloride decrease associated with plume migration is being simulated accurately in all wells but MW-18, where the simulated plume is migrating too slowly.

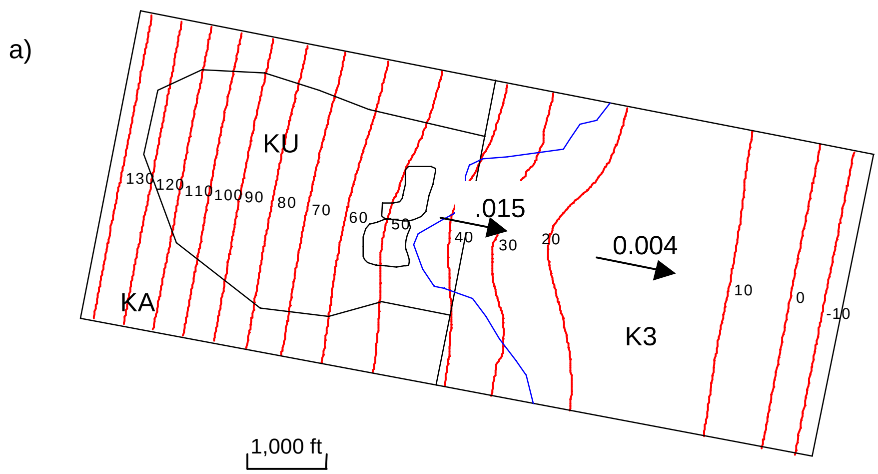
8.2.3 Simulated Flow Field

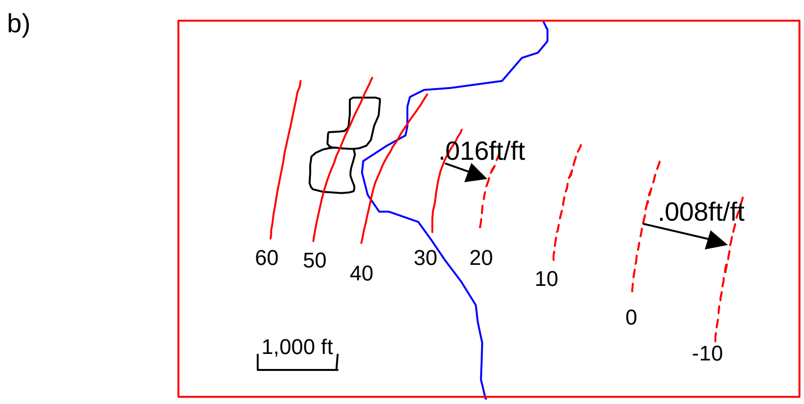
No significant vertical hydraulic gradients are simulated. Hydraulic head simulated in the top layer by the MULTI model and hydraulic head measured in December, 1998, are contoured in Figure 38. The simulated flow reproduces field conditions with reasonable accuracy in the pond area, but underestimates the hydraulic gradient in the eastern portion of the study area by 50%. This is an area of poor data coverage, and the simulated flow field cannot be ruled as invalid based upon inferred hydraulic head values. However, the steep gradient simulated at the model out-flow boundary is clearly controlled by the specified head at that boundary and future conceptual models should evaluate alternative parameterization of hydraulic conductivity in this area.

8.2.3 Simulated Chloride Distribution

The total amount of chloride simulated to enter the aquifer over the period of pond activity from April, 1978 to April, 1997 is 2,486,700 lb (1,128,000 kg). At the final simulation time (December, 1998) all of this amount remains in the study area. One unexpected aspect of the chloride distribution simulated by the MULTI model for December, 1995 is discussed, followed by a complete analysis of the simulated chloride distribution for December, 1998.

Figure 38. Simulated and measured hydraulic head distribution in December, 1998. (a) Simulated hydraulic head and (b) measured hydraulic head distribution referenced to 5,000 ft above mean sea level. Maximum and minimum hydraulic gradients are posted next to the arrows where calculated. Dashed contours are areas of inferred hydraulic head.





Simulated Chloride Distribution in December, 1995

In plan view, simulated chloride concentration in December, 1995, shown in Figure 39, identifies a distinct plume that is high in concentration strength. The limited areal extent of the simulated plume reflects convergent flow that is apparent in Figure 38, but is also due to the low dispersivity values.

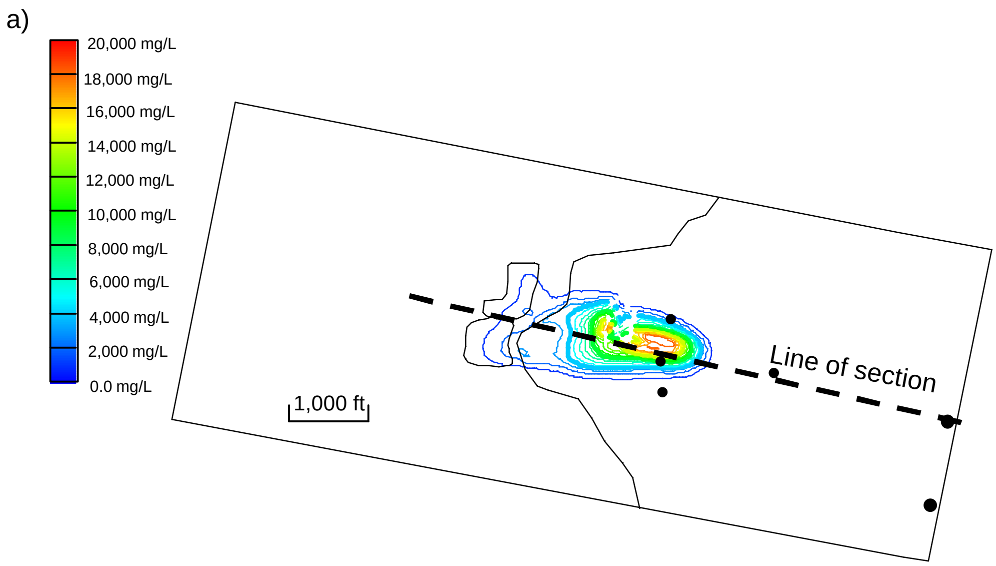
It is unusual that chloride concentration is simulated to increase down-gradient in December 1995, while ponds are actively contributing chloride to ground-water at this time. The area of greatest chloride concentration (20,000 mg/L) occurs where the simulated water table is nearest the surface, and this increase is attributed to large amounts of evapotranspiration removing fresh water in this area. This is a viable process that was not anticipated during model conceptualization.

Simulated Chloride Distribution on December, 1998

The chloride distribution simulated for December, 1998 (final simulation time) is shown in Figure 40. The simulated plume matches contours of measured chloride concentration with acceptable accuracy. Measured electrical conductivity is matched with greater accuracy, including the increase in plume contamination down-gradient due to evapotranspiration. The plume is not simulated to extend down-gradient at high concentrations as measured data indicates, possibly due to the low value of longitudinal dispersivity used in the model.

The effect of evapotranspiration yields maximum simulated chloride concentrations of 20,000 mg/L in the center of the plume which is approximately twice the highest chloride concentration measured in monitoring wells. The areal extent of the plume is small; chloride concentrations greater than 2,000 mg/L occupy an area of 350,000 ft^2 (0.012 $miles^2$) in December, 1998. The effect of evapotranspiration does not increase plume strength until the plume has migrated down-gradient of the majority of the monitoring wells. Therefore, high chloride concentrations may exist in the field that are not reflected in the monitoring well data.

Figure 39. Simulated chloride distribution for December, 1995.
(a) Plan view distribution in the top layer. Contour interval is 250 mg/L. (b) Cross section. The six black data points identify locations where chloride concentration is predicted. At this time the ponds are actively contributing chloride to the ground water. Chloride concentrations increase down-gradient due to evapotranspiration.



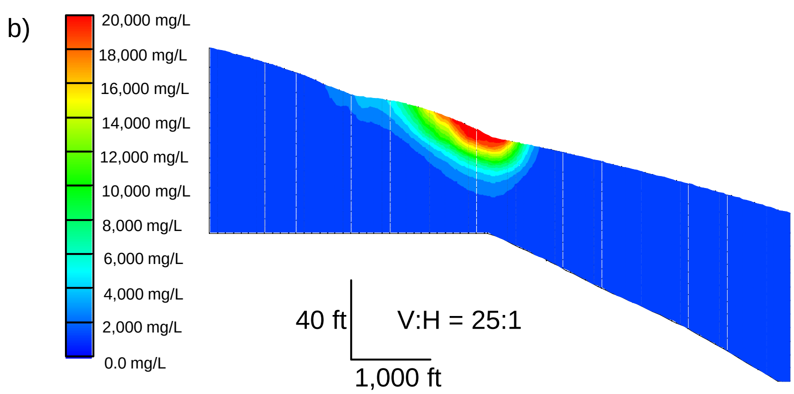
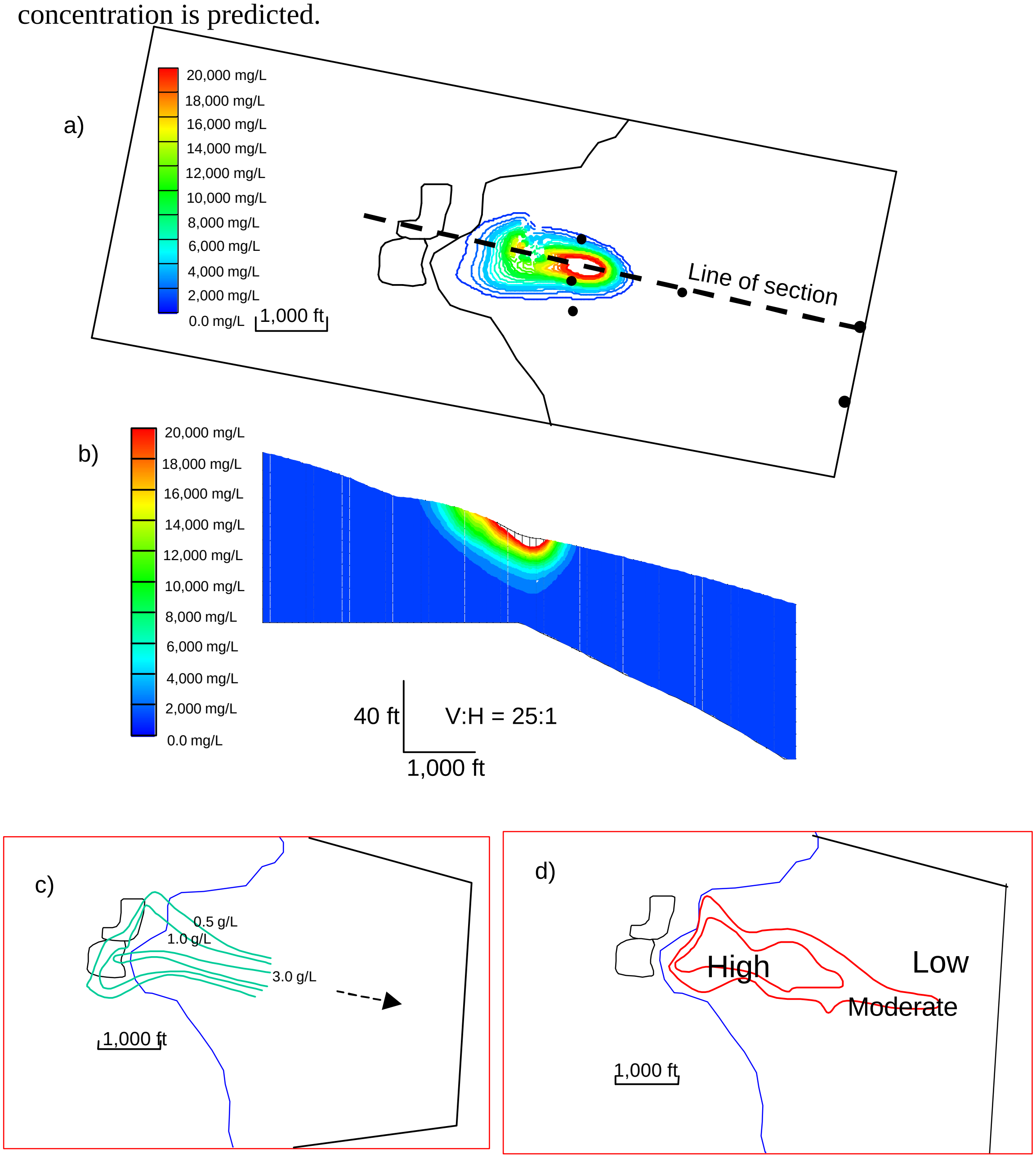


Figure 40. Simulated chloride distribution for December, 1998. Values are in mg/L. (a) Plan view distribution in the top layer and (b) in cross section. Chloride concentrations increase to 27,000 mg/L in the center of the plume and the scale is set at a maximum of 20,00 mg/L to facilitate comparison with Figures 39 and 41. (c) Inferred chloride and (d) electrical conductivity distribution from measurements made December, 1998. The six black data points in (a) identify locations where chloride concentration is predicted.



The areal extent of the plume decreases with depth in the aquifer. Vertically, the simulated plume extends to the base of the aquifer at concentrations up to 500 mg/L at the exact location of MW-19 (although not apparent in Figures 39 and 40 due to the scale used). Measured chloride concentration in MW-19 averages 2,500 mg/L. This discrepancy could be due to the specification of either vertical hydraulic conductivity or vertical dispersivity at too low a value for significant vertical hydraulic flow to be simulated. However, considering the lack of data at depth in the aquifer, the simulated vertical distribution of chloride is encouraging.

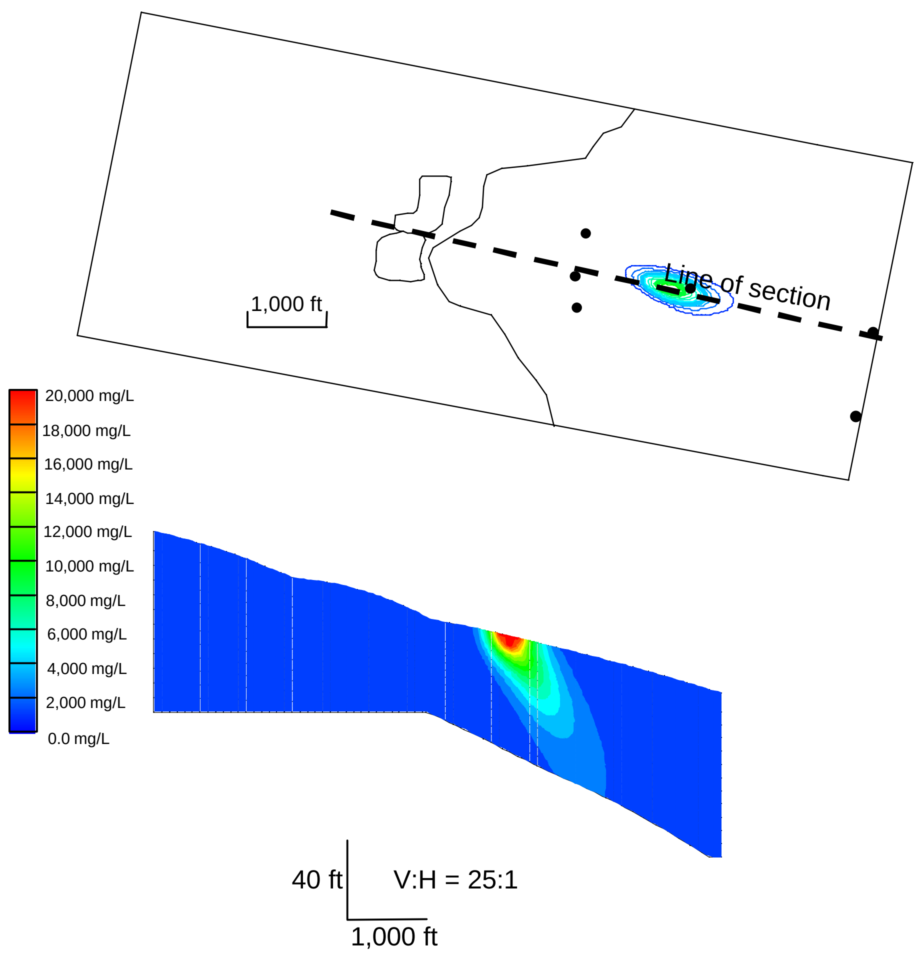
Chloride concentrations greater than 5,000 mg/L are simulated to extend downward to approximately the middle of the aquifer thickness and then migrate down-gradient. Down-gradient of the plume center, vertical migration is not apparent and ground-water flow is horizontal to the discharge zone at the model boundary.

The simulated plume moves slowly due to the low simulated gradient below the pond area. One and a half years after pond seepage stopped, the plume has traveled less than 0.5 miles from the source at an average rate of 0.4 ft/day. Calculations of plume movement in Chapter 4 report a minimum average advective velocity of 0.5 ft/day using specific conductance values measured in down-gradient sampling points. Considering that these measurements may be sampling portions of the plume that are dispersed in front of the center of the plume, the simulated rate of plume migration is reasonable.

8.3 Predictive Simulation Using the MULTI Model

Predictive simulation cannot accurately represent the seasonal effect of canal seepage, but may be used to forecast general migration and dilution rates. The MULTI conceptual model is used to simulate chloride migration for seventy years after the facility begins operation in April, 1978, to December, 2048. At final simulation time, 82% of the total amount of chloride has left the study area. The chloride concentration distribution shown in Figure 41 has not changed significantly other than decreasing in

Figure 41. Simulated chloride distribution for December, 2048.
Values are in mg/L. (a) Plan view distribution in the top layer and (b) cross section. The six black data points in (a) identify locations where chloride concentration is predicted.



magnitude. The plume migration has slowed to an average rate of 0.07 ft/day and is projected to have left the model area by the third millennia. By this time it will likely have been diluted to near ambient conditions. The cause for the slowdown in migration is that the simulated hydraulic gradient is only 0.004 in the region immediately down-gradient of MW-18 and MW-19, one half the gradient inferred from monitoring wells. Therefore, the simulated plume migration may be too slow by as much as a factor of two. Vertically, chloride concentration extends further down-gradient at greater depths. This is a result of the aquifer geometry used and cannot be supported or refuted with the existing data.

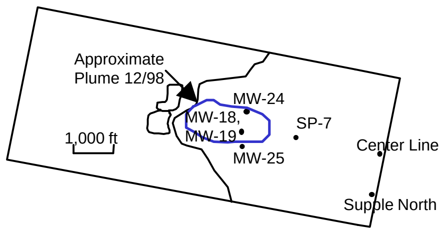
Simulated chloride concentration is plotted versus time at seven locations from December, 1978 through December, 2048 in Figure 42. The locations selected are four monitoring wells (MW-18, MW-19, MW-24, and MW-25); a piezometer, SP-7; the northern Supple private water well; and an arbitrary location at the out-flow boundary along the plume migration axis (Center Line). Six of the locations are shown in Figures 39, 40, and 41, with the seventh location being MW-19 adjacent to MW-18. Monitoring wells MW-24 and MW-25 were installed in late 1998 and SP-7 is a piezometer that is sampled infrequently and chloride data are not available for these locations. All locations sample only the top two layers of the model except MW-19 which is screened in the bottom layer, and Supple North which is screened throughout the entire aquifer.

The plume is clearly detected in MW-18, SP-7 and MW-25 for approximately 30 years. The Center Line monitoring location shows increasing chloride concentration for the final 20 years of predictive simulation, but at very low levels.

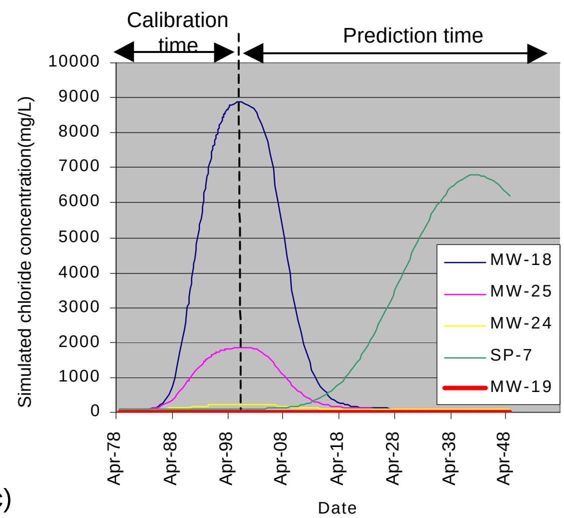
Monitoring wells MW-19 and MW-24 and the Supple North well do not show significant chloride concentrations, indicating that only wells that are shallow, and directly in the path of plume migration are predicted to be affected. Therefore, this model predicts that no water supply wells in the study area are likely to be impacted, although there is significant error in this prediction which is addressed in the following section.

Figure 42. Simulated chloride concentration at seven locations from December, 1978 to December, 2048. (a) Simulated locations. (b) Up-gradient locations. (c) Down-gradient locations.

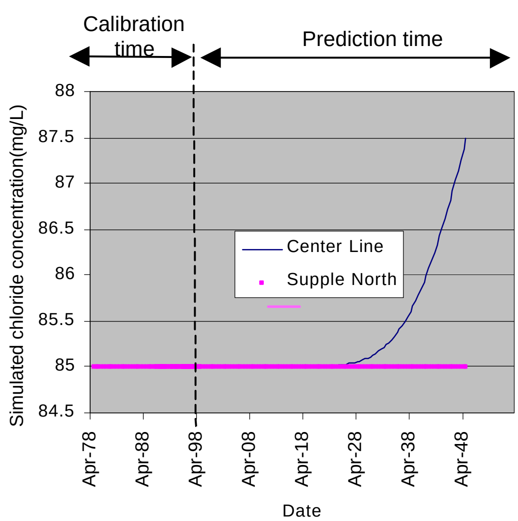
a)



b)



c)



The chloride concentrations leaving the study area as ground-water discharge to Beebe Draw are predicted to be near ambient levels (85 mg/L). The chloride plume front is detected in the year 2022 at the Center Line location, but at very low levels. An estimate of the maximum chloride concentration that will be detected at the Center Line location may be calculated using the simulated decrease in maximum chloride concentration from MW-18 to SP-7, a decrease of 22%. Projecting this decrease to the Center Line location, the maximum chloride concentration reached at this location will be 4,300 mg/L assuming linear decay of the plume strength.

Chloride leaving the study area will likely be diluted rapidly by large amounts of ground-water flow in Beebe Draw as it is carried north towards the Platte River 20 miles to the north near Greeley. The average simulated ground-water flux leaving the study area is 100,000 ft^3/day. The simulated chloride distribution in the year 2048 (Figure 41) indicates that a maximum of one fourth of the ground-water leaving the study area, or 25,000 ft^3/day, has significant chloride concentrations. Ground water in Beebe Draw is flowing at a much greater rate, approximately 3,300,000 ft^3/day (Smith et. al. 1964). The simulated plume is therefore diluted at a ratio of 1:132. The maximum plume chloride strength of 4,300 mg/L acts to raise chloride concentrations in Beebe Draw by a maximum of only 33 mg/L, from 90 mg/L (Table 3, Schneider, 1931) to 123 mg/L.

8.4 Analysis of Model Error

Two main error sources limit the accuracy of simulated chloride concentrations: the lack of vertically distributed sampling locations and measurements of canal seepage or data that would facilitate its estimation, and assumptions made about aquifers system parameters that are specified during regression. UCODE calculates 95% prediction intervals for simulated chloride concentrations that incorporate the first error source. The parameters that are not estimated by regression are not included in UCODE prediction statistics.

Prediction intervals calculated by UCODE use parameter sensitivity information and error associated with the measurement of chloride concentration to calculate 95% confidence intervals on model predictions. The calculated Beale's measure of model linearity identified that the MULTI model is non-linear in the vicinity of optimized parameter values, therefore, 95% confidence intervals are not accurate, but are useful for comparison and qualitative analysis. UCODE is unable to calculate 95% confidence intervals on predictions for the Supple North well, likely due to computational problems associated with the zero values of chloride simulated in that location.

Because canal seepage is not sensitive to simulated values, 95% confidence intervals on predictions are very large, indicating that chloride concentrations cannot be accurately simulated at any of the locations (excepting the Supple North well). The narrowest 95% confidence interval on predictions (most confidence in simulated value) occurs for the Center Line location and is plus or minus 27 mg/L. The second smallest 95% confidence interval on predictions is calculated for MW-19 and is plus or minus 10,000 mg/L. At other locations 95% prediction intervals are generally twice as large.

This large error precludes the MULTI model from being used as an accurate predictive tool. Canal seepage is a major influence in chloride migration and the unrealistic value estimated by the MULTI model is reflected in this high prediction uncertainty.

Error not incorporated into the calculation of 95% prediction intervals are associated with parameters that are not estimated. These parameters are source strength, specific yield, and dispersivity. Quantifying the error associated with these assumptions can only be done through the comparison of alternative conceptual models. Generally, it can be said that the specified value of source strength produces a reasonable amount of chloride in the system. Specific yield is specified at the high range of measured and published values and the resultantly low advective velocity limits chloride migration rates and the simulated plume migration may be conservatively low. Besides generating a low advective transport velocity, the high value of specific yield also acts to limit the amount of water held in storage in the aquifer. This may be contributing to the inability of the model to accurately simulate the oscillation of hydraulic head and chloride concentrations. Experimental simulations at low values of specific yield failed to converge for forward MODFLOW simulations. Dispersivity is specified at a low range of measured and published values, resulting in simulated plume dispersion rates that may be conservatively low, contributing to the perceived slow rate of simulated plume migration.

Given additional time and computing power, the three parameters not estimated in this study (source strength, specific yield, and dispersivity) should be included in the regression so that their associated error may be incorporated into 95% prediction interval calculations.

8.5 Implications for Other Similar Investigations

While there exists a large amount of data describing conditions at WCWD, the use of numerical modeling and parameter estimation identified that the data does not describe certain aspects of the system that are needed for the development of representative models that can accurately simulate the migration of produced water. Investigations of other similar produced water contamination sites should use these tools to guide data collection. As conceptual models are derived and revised according to characterization data collected, additional data that are needed to improve parameter sensitivity and break correlation will be identified. This process will limit expenditures, maximize the understanding of the system, and lead to accurate numerical model predictions.

CHAPTER 9. SUMMARY AND CONCLUSIONS

Dissolved chloride can distinguish between ground-water impacted from produced water and ground-water impacted by other saline sources in the study area and is used as a tracer to simulate solute fate and transport in the study area. Geophysical electromagnetic surveys are capable of identifying relative levels of produced water contamination, but are not clearly related to chloride concentration.

At optimized parameter values, single layer models are not capable of representing field conditions with acceptable accuracy. A twelve-layer model, constructed based upon interpretation of UCODE calibration statistics from single-layer models, incorporates portions of the Arapahoe Formation and simulates discharge from up-gradient aquifers into the study area. When calibrated, the multi-layered model does not accurately simulate measured seasonal oscillation of hydraulic head and chloride concentration because canal seepage is estimated as an unrealistically low value. However, the multi-layered model does accurately simulate the overall distribution, migration rate, and migration direction observed in the field base on chloride concentration and electrical conductivity.

The fate of chloride concentration is simulated for a total of 70 years using the multi-layered model, from the date of the disposal facility inception (December, 1978), to the year 2048. Predictions indicate that the plume does not disperse significantly as it migrates slowly down-gradient. In areas where the water table is near the land surface, evapotranspiration significantly increases chloride concentrations. As it migrates, the plume is slowly diluted by large amounts of ground water entering the modeled area from up-gradient aquifers in the Arapahoe Formation. Monitoring locations in the path of plume migration are impacted for a period of 30 years at chloride concentrations greater than 1,000 mg/L. No water supply wells are in the direct path of plume transport in the study area and chloride concentration levels exiting the study area are low. Organic contaminants present in ground water were not studied in this project and may pose a threat to ground-water users.

Qualitative error analysis indicates that the plume may disperse and migrate more rapidly than simulated. Quantitative error analysis indicates that the model simulates chloride concentration with large uncertainty due to the lack of data to allow accurate estimation of canal seepage and a lack of vertically distributed data. Therefore, the twelve-layer model is not an accurate predictive tool.

Several implications of this study may be applied to other similar produced water contamination sites. The use of geophysical electromagnetic surveys provides rapid, inexpensive characterization of the distribution of produced water and could potentially be used as observations for model calibration with appropriate weighting. The use of numerical modeling and parameter estimation enhances understanding of parameters controlling the transport and distribution of produced water. UCODE discriminates between alternative models, but cannot identify representative models if field data are insufficient. Data collection programs will be most economical and effective if modeling is used to determined the type and location of data that are most useful to defining the system. UCODE can be used to make such determinations.

CHAPTER 10. FUTURE WORK

Future effort should focus on three areas: generating additional conceptual models to be tested, determining the field data that would be most useful to improving model calibration, and the investigation of bias in chloride concentration residuals.

Alternative conceptual models should focus on improving model sensitivity to canal seepage to capture oscillations in hydraulic head, and to a lesser extent, simulating more realistic gradients in the eastern portion of the model. These problems are best addressed through experimentation with alternative representations of model boundaries. Possible alternative conceptual models include: the inclusion of a low permeability layer separating the unconsolidated unit from the Arapahoe Formation; specifying the aquifer base as a general head boundary to more accurately represent regional discharge of the Arapahoe Formation; limiting the vertical extent of the up-gradient general head boundary; and reducing aquifer thickness in down-gradient areas. Modifications to parameterization should include: seasonal fluctuation of evapotranspiration rates and inclusion of additional hydraulic conductivity zones in down-gradient areas. The continued analysis of UCODE statistics should guide the development of additional conceptual models.

Improved model accuracy can be obtained most effectively via additional data acquisition. Geophysical electromagnetic surveys have proven effective at detecting high electrical conductivity associated with produced water and can be conducted quickly and at low cost. Additional geophysical work coupled with sampling and analysis of produced water contaminant concentrations may identify a relationship between electrical conductivity and chloride concentration so that survey locations may be used as calibration observations in the regression.

Data describing the hydrostratigraphy, hydraulic head, and chloride concentration of the Arapahoe Formation are also needed. Ideally, nested piezometers would be installed over an interval to a depth where chloride concentrations are at ambient levels and a continuous low hydraulic conductivity zone is identified. To maximize the benefit of installation and monitoring costs, UCODE can be used to identify locations where additional monitoring locations would provide the most useful information. This is done by analyzing sensitivities to, and correlations of parameters given, hypothetical observations for a range of possible data types and monitoring locations. Ultimately, numerical modeling and parameter estimation should be used from the start of the investigation to guide data collection.

Use of both hydraulic head and chloride concentrations to calibrate a model proved problematic. A test model should be constructed to analyze this problem.

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APPENDIX A. GEOPHYSICS REPORT

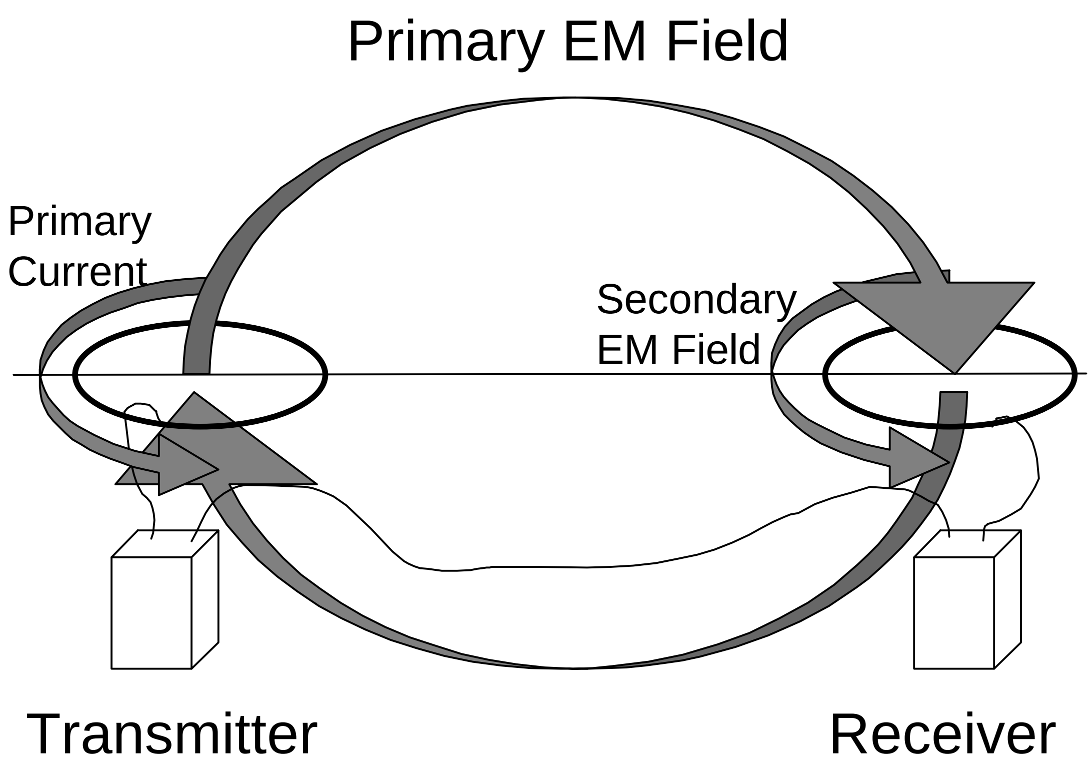
Introduction

The electrical conductivity of aquifer material is usually controlled by porosity, clay content, and the conductivity of the pore fluid (Thamke, 1998). Geophysical electromagnetic (EM) surveys were used at the study site to determine if changes in the cumulative electrical conductivity of the soil and water matrix could be correlated to changes in chloride concentrations indicative of produced water contamination.

Methods

EM surveys were conducted using a Geonics EM34 Non-Contacting Terrain Conductivity Meter which consists of a transmitting loop and receiving loop shown in Figure A-1. The transmitting loop carries an alternating current at an audio frequency which induces an electromagnetic field in the earth which, in turn, induces an electromagnetic current in the receiving loop proportional to the conductivity of the earth material between the two loops. Increasing the spacing between the loops incorporates more earth in the electromagnetic field and at a greater depth. By changing the orientation of the loops from on end (horizontal dipole) to lying flat (vertical dipole), electromagnetic fields of orthogonal orientation are created. Measurements with the horizontal-dipole orientation as in Figure A-1, samples a shallow (approximately 75% of spacing) amount of material, and vertical-dipole measurements increase the depth of electromagnetic penetration to approximately 150% of the spacing distance (McNeill, 1980). Due to the nature of the electromagnetic fields created, the horizontal dipole orientation is generally more sensitive to near surface conductive materials such as

Figure A-1. Schematic Diagram of Geonics© EM-34



fences, while the vertical dipole orientation is more sensitive to vertical conductors such as well casings (although the opposite effect was observed in this study).

A grid composed of five lines of 20m spacings was surveyed at the locations shown in Figure 8. The survey lines were directed north/south and east/west and were oriented near monitoring wells MW-16 and MW-18 so that EM conductivity could be related to chloride content of ground waters measured in those wells (access to all other wells is restricted). Generally, chloride levels in MW-16 are equal to ambient conditions, averaging 100 mg/L, and MW-18 chloride levels average 5,000 mg/L. Vertical and horizontal dipole measurements were made at each sampling point.

Results

EM conductivities varied from 31-110 mmhos/meter, with horizontal dipole measurements values generally 30% larger than vertical dipole measurements. Measured vertical dipole conductivities did not identify any discernable pattern and were highly sensitive to the many fences in the study area, contrary to theory, whereas, horizontal dipole conductivities seemed to identify systematic subsurface trends. These trends are manually contoured in Figure 19 where values greater than 100 mmhos/meter are “high”, values between 85 and 100 mmhos/meter are “moderate”, and values less than 85 mmhos/meter are “low”. These trends are similar to chloride distribution trends shown in Figure 17.

Measured vertical dipole EM conductivity and chloride concentration near MW-16 and MW-18 is displayed in Figure A-2 and does not exhibit a clear correlation that is needed to directly relate electrical conductivity to chloride concentration. Therefore, the data presented in Figure 19 is only useful for qualitative calibration purposes. However, because EM and Cl sampling events are not coincident, it is possible that trends may exist, although not identifiable with the data gathered. Additional error sources include material heterogeneities, cultural effects, lack of correction for topographic variation, and possibly improper coil spacing. However, the conductivity pattern identified may warrant additional geophysical surveying because data collection is relatively easy and low-cost. These surveys should be conducted coincident with geochemical sampling events and should cover more comprehensive areas than current land access allowed. Additionally, significant effort should be put into designing the appropriate coil spacing and orientation.

Figure A-2. Measured chloride concentration and vertical magnetic loop (VML) measurements. The lack of correlation limits the use of geophysical data as additional observations to calibrate numerical models.