Inter-Code Comparison of Variably Saturated Fluid Flow and
Prediction of Percolation through a Tailings Impoundment
in Southeast Nevada, USA.

A thesis submitted in partial fulfillment of the
Requirements for the degree of Master in Science in
Hydrogeology

by
Spencer K. Whitman
Dr. Ronald J. Breitmeyer, Thesis Advisor
December, 2016
We recommend that the thesis prepared under our supervision by

SPENCER K. WHITMAN

Entitled

Inter-Code Comparison Of Variably Saturated Fluid Flow And Prediction Of Percolation Through A Tailings Impoundment In Southeast Nevada, USA.

be accepted in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

Dr. Ronald J. Breitmeyer, Advisor

Dr. Scott Tyler, Committee Member

Dr. Adrian Harpold, Graduate School Representative

David W. Zeh, Ph.D., Dean, Graduate School

December, 2016
Abstract

Hypothetical infiltration columns were simulated to evaluate the performance of 6 different modeling codes (HYDRUS 1D, HYDRUS 2D/3D, HELP, SV FLUX, UNSAT-H, and VS2D) at simulating near ground surface water balance processes occurring at mine process components (e.g. tailings pile or heap leach pile) under a simplistic scenario. Model results suggest that various codes for unsaturated flow arrive at similar solutions for identical models of well-defined problems. A literature review of several previous model comparison studies was conducted in order to provide insight into considerations for more complicated and realistic modeling scenarios. Unsaturated zone hydrologic modeling, field investigations, and laboratory analysis were conducted for a legacy tailings impoundment in Caselton, Lincoln County, Nevada to assess the potential for percolation of meteoric water through the tailings material. Field investigations consisted of field-saturated hydraulic conductivity testing, in-situ density measurement, and collection of tailings samples for laboratory analysis. Laboratory analysis included determination of field moisture content, bulk (dry) density, and water retention curve measurement by hanging column, pressure plate, and chilled mirror hygrometer methods. Hydrologic models of the tailings were performed using a variety of conceptual models, hydraulic property models, finite element discretization, temporal boundary condition data resolutions, tailings hydraulic property descriptions, and lower boundary conditions. Numerical, mechanistic hydrologic flow models predict percolation rates ranging from 51 - 0 mm/yr. through the tailings, while previous efforts utilizing non-mechanistic water balance models predict a rate of 3.2 mm/yr., suggesting that significant variability exists in the model results depending on model approach and assumptions. Some simulations utilizing more complex and physically representative models resulted in higher percolation rates than the HELP simulation, which is counter to common assumptions of over prediction of drainage for simple water balance approaches.
Acknowledgements

I would like to extend my gratefulness to the many people who have provided support to me during my work towards completing this thesis.

First, I would like to thank Dr. Ronald J. Breitmeyer, for selecting me as his student, and bringing me to the University of Nevada, Reno to study under his guidance. I feel fortunate to have found an advisor whose interests and expertise align strongly with my goals, and to work on a project that I had a high level of interest in. I am grateful for his financial support, as well as his sincere willingness to spend time discussing project goals, and career development.

I would like to thank the Nevada Mining Association for their financial support and interest in the project.

I would also like to recognize Dr. Scott Tyler and Dr. Adrian Harpol for serving as advisory committee members, and providing valuable feedback throughout the process of completing my thesis.

I would like to thank Jeryl Gardner at NDEP for involving UNR, myself, and Dr. Breitmeyer in the important work progressing at the Caselton Tailings impoundment.

I would like to thank my office mates Rowan Gaffney and John Volk for their help in teaching me Python, without which, this project would have been much more difficult.

I would also like to thank my parents for their love and support, and for making sure that I had the childhood educational foundation to achieve a graduate degree.

Finally, I would like to thank my partner, Annelia Tinklenberg, for her constant loving support during the highs and lows that inevitably come as a part of completing a years long project.
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Introduction

The management of solution from mine process components (e.g. waste rock pile, tailings retention facilities) in post-closure operations is a primary long-term environmental concern when regulatory agencies evaluate the closure and ultimate bond release for a mine site. These solutions, composed of residual moisture from leaching or processing operations, meteoric water from permeable process components, and dissolved or suspended materials derived from the interaction of moisture with the mine process components provide a mechanism for movement of parameters of concern (PoCs) away from these process components and into the environment. Movement of PoCs through the vadose zone to groundwater provides a mechanism for degradation of groundwater resources. In the state of Nevada, regulations specifically require that operating and closure plans ensure that a site does not “degrade waters of the state of Nevada” (Nev. Admin. Code § 445.350-447, 2016), which include groundwater.

The most conservative (i.e., low-risk) solution management strategies are typically “zero-discharge” or full containment requirement, preventing any release of process solutions to the environment. Such approaches often result in extensive, or technologically/financially infeasible post-closure management and monitoring requirements, possibly extending to hundreds of years. The financial and natural resources spent on zero discharge closures could potentially impact the environment to greater positive effect if spent in locations with greater risk profiles (e.g. legacy mining impacts). Furthermore, groundwater concentrations of many solutes in ore zones are naturally elevated above standards for domestic or agricultural usage (Davis et al., 2010; Runnells et al., 1992). Expenditure of resources to prevent degradation of such waters, or prevention of minimal impacts to better quality waters may or may not be most protective of the environment, when considered against alternative closure and remediation procedures as part of a full life cycle.
analysis. Approaches such as these have been recognized in the management of solid waste per the Resource Conservation and Recovery Act (RCRA) subtitle D, which acknowledges that systems that minimize, but may not completely eliminate leakage can still be considered environmentally protective. Impacts of construction and maintenance of containment and monitoring systems should be weighed against potential impacts to groundwater resources.

One example of such a location where a zero discharge approach would likely not be feasible is the Caselton Tailings impoundment, presented in Chapter 2. At the Caselton Tailings impoundment, excavation and relocation of tailings, or construction of a lined tailings facility would be cost prohibitive, and would likely result in more release of contamination to the environment than implementing a cover system that alters the water balance of the tailings impoundment. One way to assess the potential impact of mining solutions to groundwater resources is through the use of hydrologic flow and transport models. However, model results can be strongly influenced by several factors, including code selection, model conceptualization, temporal data resolution, material property descriptions, choice of boundary conditions, and grid sizing for numerical models. Accordingly, it is important to examine the effect of all modeling variables, and consider modeling outcomes as a range of possibilities which can be used to guide the design of containment, monitoring, or remediation systems.

**Mine Process Components**

Modern mining practice usually consists of the removal of massive amounts of low grade ore for various types of processing to extract valuable components. One side effect of these modern mining methods is the creation of landscape scale emplacements of waste rock, low grade ore, or tailings. Although much of the water that falls on the emplacements is lost to evaporation or evapotranspiration, some portion can percolate through to underlying sediments
or containment systems. Kampf et al., (2002) observed that 2 to 23% of annual precipitation percolates through heap leach facilities to leachate collection systems in Nevada. Although leachate from mining facilities is commonly managed using evaporation cells, this requires long term maintenance, with the associated operational costs. In addition, precipitated solutes from the evaporation cells would ultimately be disposed of in permitted landfills under current operating practice, unless classified as non-hazardous waste (OSWER US EPA, 2016a, 2016b; Younger et al., 2002). Disposal of solutes in a municipal landfill presents many of the same challenges as on-site closure methods. Closure options that require minimal long term maintenance usually involve (1) an alternative cover system that limits infiltration of meteoric water to the mine process component and the associated percolation of solutes into the underlying soil (2) some amount of allowable discharge from the inactive mining facilities. Under such a closure option, one strategy involves utilizing the fluid storage and reactive capacity of the vadose zone to mitigate the percolation of solutes and fluid. The relatively deep vadose zones in many Nevada mining districts could provide an ideal location for this type of closure strategy. However, an understanding of fluid and solute behavior in partially saturated soil, constrained with site specific data, is critical to accurate prediction of the performance of such closure systems. In some locations, this type of closure system would not be protective of the environment. One way to evaluate the effectiveness of such closure systems is with hydrologic and geochemical models.

Proposed Allowable Discharge Procedure

Figure 1 is a flowchart of a possible framework for the allowable discharge approach. In this flow chart, there are several “points of evaluation” for the system performance that would guide decision making by regulatory agencies. The basic premise of the framework is to evaluate the
solutions associated with process components, how far those solutions move through the vadose zone (i.e., assess potential for PoCs from process solution to reach groundwater), and if the solutions reach groundwater, what quantities of PoCs reach groundwater after chemical interaction and attenuation in the vadose zone. The framework is reliant on modeling of solution and PoC migration through the vadose zone and in groundwater. Therefore, identifying the proper models, procedures, data requirements, and quantifying the uncertainties of said models and procedures will be paramount to assuring that any allowable discharge is protective of waters of the state.

In Figure 1, the orange blocks denote two points where modeling of solution and PoC fate and transport will be critical to acceptance of an allowable discharge by the Nevada Division of Environmental Protection, Bureau of Mining Regulation and Reclamation (NDEP-BMRR), while the orange block surrounded by the red box specifically indicates the portion of work that will be conducted to fulfill the requirements of a M.S. in Hydrogeology in the Graduate Program for Hydrologic Sciences at the University of Nevada Reno. In the interest of modeling properly and effectively, the following sections detail a body of work that describes the workings of vadose zone hydrologic models, as well as the impact of modeling decisions on the outcome of hydrologic models.

Chapter 1 comprises work conducted in cooperation with the Nevada Mining Association and the Nevada Department of Environmental Protection with the goal of identifying codes which would be suitable for use as part of an allowable discharge evaluation. In chapter 1, a set of simple hypothetical column models shows the similarity of model results utilizing distinct modeling codes on an identical model set up. In Chapter 2, a realistic hydrologic model of the Caselton tailings impoundment is constructed and analyzed, and several key model inputs are
varied in order to analyze the effect of various model parameterization decisions on modeling outcomes.

Background
A literature review, consisting of background information on cyanide heap leach operations, hydraulic characterization of heap leach piles, and vadose zone model comparison studies has been conducted. Information from the literature review was used to guide the experimental design of model comparison and field studies, and is intended to provide the reader a body of literature from which to gain further insight on the similarities and differences between various modeling codes and procedures.
Characterization and Simulation of Process Components

Decker, (1996) conducted studies on heap materials to determine the hydraulic flow and solute transport parameters within the heap. Decker used data from his own experiments, as well as United States Bureau of Mines (USBM), Reno Research Center column experiments. The USBM conducted column cyanide rinse and tracer experiments on heap materials. The columns were Plexiglas tubes 122 cm long and 15 cm in diameter. Gravel-filled Buchner funnels were placed at the bottom of the column as a filter pack. Fluid collected by gravity drainage was analyzed for Weak Acid Dissociable (WAD) cyanide. WAD cyanide measurements were used in conjunction with continuous EC measurements from NaCl tracer experiments to construct breakthrough curves.

Decker also conducted column experiments on heap materials from the Barrick Goldstrike Mine to determine unsaturated flow parameters. Approximately 420 liters of heap leach ore material was collected from the top of the heap by trenching with a backhoe. Unsaturated hydraulic parameters were determined using a multi-step flow experiment from Eching and Hopmans, (1993). A saturated aliquot of the heap leach material was placed inside a pressurized vessel (Tempe cell) which forced pore liquid through a porous ceramic plate and into a collection system. Continuous mass measurements of the effluent water were taken as the vessel was pressurized at different pressures and allow to equilibrate.

In order to determine solute transport parameters, 6 m column experiments were conducted. The columns were filled with heap leach material and instrumented with eight Time Domain Reflectometry (TDR) probes and eight tensiometers along its length. De-ionized water was pumped into the top of the column by a positive displacement pump, while solutes were pumped to the top with a peristaltic pump. Liquids infiltrated through the column to a
collection system at the bottom. The effluent was continuously monitored with a specific ion probe at the bottom, and collected at specified time intervals with a Manning continuous 24 position sampler.

The data from the column experiments was used to inverse model of the Advection Dispersion Equation (ADE) and a dual porosity formulation of Richards equation. The inverse model fits parameters of the ADE and dual porosity models to the curves generated from the column experiments. The parameters from the inverse models were used to run predictive models.

Kampf et al., (2002) used drainage rates from lined heap leach piles to estimate long term recharge rates at heap leach facilities in Nevada, USA. Drainage rates followed an exponential decline, with steady state precipitation derived drainage achieved in 3 of 8 sites. The remaining 5 sites continued to exhibit a decline in drainage rates during the study period. The steady state drainage rates were used to empirically estimate precipitation derived recharge, under the assumption of steady state conditions, and were compared to other models (Eakin, 1951; Maxey and Eakin, 1949). Empirically estimated precipitation derived drainage ranged from 6 to 160 mm/yr. The drainage rates translated to recharge estimates ranging from 2 to 23% of annual precipitation.

At sites with low precipitation, estimated recharge through the heaps was higher than that predicted by the models. The models with more coarse ore consistency had the highest estimated recharge. Conversely, estimated recharge for high precipitation sites was lower than model predictions. Sites with higher precipitation tended to have well established vegetation covers that helped to limit the infiltration of meteoric waters. Heaps with higher proportions of sloped surface areas to flat surface areas may have higher infiltration and drainage rates. The
permeability of the flat portions of some heaps are thought to have been reduced by the heavy equipment traffic that was necessary to build the heaps. The study concluded that in areas where annual precipitation is <200 mm, heaps with a good vegetation cover will drain at a rate of 6 to 9 mm/yr., or 4 to 7% of annual precipitation.
Model Comparison Studies

Although literature specifically concerned with the water balance of tailings is limited, a wide body of literature for water balance landfill covers provides an in depth analysis of the major issues associated with tailings water balance problems. Several studies pertaining to the numerical simulation of water balance of various infiltration barriers is presented, each of which has a model comparison component.

Fayer et al., (1992) compared field measurements from 8 non-vegetated lysimeters containing a sequence of soils intended to act as a protective hydraulic barrier. The primary objective of the study was to assess the ability of UNSAT-H version 2.0 to simulate the water balance of the protective barrier for durations longer than a year without calibration of model parameters, and to collect information to better inform the model for future predictions. Although the model reproduced much of the water balance behavior of the barrier without calibration, the model over predicted evaporation in the winter and under predicted it in the summer. Testing revealed that the model was sensitive to the hydraulic conductivity function, snow cover, and potential evaporation, and that calibration of the sensitive parameters greatly improved the performance of the model.

Khire et al., (1997) compared simulations from two earthen covers at landfill sites using two water balance models (HELP and UNSAT-H). Hydrologic and meteorological data including precipitation, air temperature, solar radiation, relative humidity, wind speed, wind direction, percolation, overland flow, and soil water content were collected at each test section for three years. Predictions of the water balance were made using the water balance models HELP and UNSAT-H. In general, HELP over predicted percolation, sometimes significantly, and UNSAT-H slightly under predicted percolation. However, both models captured the seasonal variations in
overland flow, evapotranspiration, soil water storage, and percolation. UNSATH captured these variations more accurately than HELP. They also found that both models were unable to accurately reproduce conditions where a significant amount of snow was on the ground.

Khire et al., (1999) compared simulations of a capillary barrier in a semiarid environment. Model input consisted of meteorological data, soil properties, and vegetative information. Estimates of evapotranspiration and soil-water storage agreed reasonably well with the field data. Peak soil-water storage was underestimated during the winter and evapotranspiration was overestimated in late winter. Water contents were simulated fairly well, although the changes in water content of the sand obtained from UNSAT-H were not as large as, and occurred less quickly than, that in the field. Percolation was generally overestimated, which appears to be closely related to underestimates in runoff and storage in the geocomposite drain. Snowmelt, soil freezing, and hysteresis also appear to affect the quality of the simulations.

Albright et al., (2002) conducted a large study on several monitoring stations for the Alternative Cover Assessment Project (ACAP). The ACAP assessed the viability of alternative covers for municipal landfills. The study was broken into several phases. Phase I included a review of existing research sites, selection of additional research sites, detailed code descriptions for HELP, HYDRUS-2D, EPIC, UNSAT-H, and SHAW, sensitivity analysis, code validation, and conclusions and summaries regarding the findings. Ten codes were initially evaluated, but only HELP, HYDRUS-2D, EPIC and UNSAT-H were subjected to detailed evaluation and comparison with field measured data. Water balance type codes (HELP, EPIC) demonstrated several limitations when compared to Richards equation based codes such as HYDRUS-2D and UNSAT-H. However, due to its 1D nature, UNSAT-H cannot simulate processes
that depend on 2D or 3D geometry, such as lateral or surface runoff. Detailed conclusions for each code can be found in the text, but the authors emphasized in general the need for careful consideration regarding meteorological input data, site-specific soil hydraulic parameters, site specific vegetation parameters, and model selection. Because the driving water balance processes vary widely from site to site, model selection should be based matching of the strengths and weaknesses of a particular model to the dominant processes occurring at a particular site.

Scanlon et al., (2002) compared water balance simulation results from seven different codes, HELP, HYDRUS-1D, SHAW, SoilCover, SWIM, UNSAT-H, and VS2DTI, using 1–3 year water balance monitoring data from non-vegetated engineered covers (3 m deep) in warm (Texas) and cold (Idaho) desert regions. A unique aspect of the code comparison study was the ability to compare codes by substituting various simulation approaches such as boundary conditions or hydraulic parameters into a single code and comparing results of the modified and unmodified code. The study found that simulation of infiltration excess runoff was a problem for all codes. Much of the difficulty in accurately simulating surface runoff was related to the implementation of the timing and intensity of precipitation events and evapotranspiration in each code during days with precipitation. UNSAT-H reproduced field measurements most successfully by disaggregating precipitation and applying it at a specified rate, and allowing evaporation to occur throughout the rest of the day. Drainage was simulated to within ± 64 % by most codes. Outliers in simulations results in this study were traced to one of the following: (1) modeling approach (mass balance vs Richards equation) (2) choice of upper boundary condition during precipitation and time discretization of precipitation (3) choice of water retention function, and (4) choice of lower boundary condition. This study also found that water routing codes (e.g.
HELP) perform poorly as they ignore matric gradients, which are often upward in semi-arid environments. Decreased hydraulic conductivity based on the Brooks and Corey water retention function relative to the van Genuchten functions resulted in overestimation in evaporation and underestimation in drainage, while differences in residual water content (> 0 for Brooks and Corey vs 0 for Campbell) did not have a large impact on simulation results.

Seepage face lower boundary condition were the most appropriate for simulating wickless lysimeters, although unit gradient lower boundary conditions should work well for natural systems with monolithic soil profiles near the lower boundary (Scanlon et al., 2002). The seepage face boundary condition was emulated in this study for some models by including a thin gravel layer at the bottom of the soil profile.

Benson et al., (2004, 2005) compared simulations using Vadoze/W and UNSAT-H to field observations from an alternative cover test. While both models had trouble predicting percolation accurately, Vadoze/W (previously SoilCover) simulated runoff, ET, and temporal changes in soil water storage accurately. UNSAT-H had trouble predicting these processes due to the time discretization of precipitation, which affected all subsurface processes. Vadoze/W applied the precipitation at a lower rate that more closely resembled field conditions for this site. Both models had trouble capturing a change in the transpiration pattern during the last winter-summer period of the study.

Ogorzalek et al., (2008) used LEACHM, HYDRUS, and UNSAT-H to predict surface runoff, ET, soil-water storage and percolation for an alternative cover with a capillary barrier. All of the codes were able to capture seasonal variations in the water-balance quantities observed in the field. LEACHM and HYDRUS predicted surface runoff within 18 mm, while UNSAT-H over predicted by at least 239 mm. ET was predicted within 60 mm by all codes when the first year
of data was eliminated, although all ET was over predicted during snowmelt conditions. Consequently, soil-water storage was under estimated for all codes. Observed and simulated percolation matched within 1 mm. The authors emphasize the need to scrutinize surface runoff predictions, and to carefully account for ET and snow melt and accumulation during periods of snow cover.
Research Hypothesis

While model results from mechanistic models for simple well-defined problems should produce similar results, complex realistic models will show significant sensitivity to common modeling decisions made by hydrologic practitioners. Mechanistic modeling of the unsaturated hydrology of the Caselton Tailings impoundment will predict less drainage than previous non-mechanistic HELP models, due to the inclusion of upward ward matric gradients in the mechanistic models.

Research Objectives

1) To assess the sensitivity of unsaturated hydrologic model results to code selection for simple and well defined problems.

2) To assess the potential for percolation of meteoric water through the tailings material at the Caselton Tailings impoundment.

3) To assess the sensitivity of model results at the Caselton Tailings impoundment to various model construction decisions commonly made by hydrologic modelers, including material hydraulic properties, hydraulic property models, boundary conditions, model dimensionality and geometry, spatial discretization, and temporal resolution of input data.
Governing Equations and Solution Techniques for Unsaturated Flow

Governing Equations

Numerical and Analytical codes are used to simulate processes that occur in natural or engineered soils between the atmosphere and the water table. The processes simulated by the water balance code include various components of the water balance equation:

\[ P + Irr - ET - R - D = \Delta S \]

Where \( P = \) Precipitation, \( Irr = \) Irrigation, \( ET = \) Evapotranspiration, \( R = \) Runoff, \( D = \) Drainage, and \( \Delta S = \) change in soil water storage.

Practical applications of water balance codes include land-atmosphere interactions, groundwater recharge estimates, contaminant transport in variably saturated sediments, and performance of engineered cover systems for municipal or mining wastes.

Mechanistic unsaturated hydrologic models deal with the redistribution of water within variably saturated porous media, and are governed by Richards Equation. Typically, the precipitation, irrigation, and evapotranspiration components of the water balance equation are boundary conditions to an unsaturated hydrologic model, while runoff, drainage, and changes in storage are predicted by the model. The 1D, 2D, and 3D formats of Richards Equation are shown below:
\[ \frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[ K_{\psi} \left( \frac{\partial \psi}{\partial z} + 1 \right) \right] - S \]

1D

\[ \frac{\partial \theta}{\partial t} = -\frac{\partial}{\partial y} \left[ K_{\psi} \left( \frac{\partial \psi}{\partial y} \right) \right] - \frac{\partial}{\partial z} \left[ K_{\psi} \left( \frac{\partial \psi}{\partial z} + 1 \right) \right] - S \]

2D

\[ \frac{\partial \theta}{\partial t} = -\frac{\partial}{\partial x} \left[ K_{\psi} \left( \frac{\partial \psi}{\partial x} \right) \right] - \frac{\partial}{\partial y} \left[ K_{\psi} \left( \frac{\partial \psi}{\partial y} \right) \right] - \frac{\partial}{\partial z} \left[ K_{\psi} \left( \frac{\partial \psi}{\partial z} + 1 \right) \right] - S \]

3D

Where \( \frac{\partial \theta}{\partial t} \) represents the change in water content in the model domain over a time period \( \partial t \), \( K_{\psi} \) is the unsaturated hydraulic conductivity for matric suction \( \psi \) and \( S = \) a source/sink/storage term.

The most common form of the 1D and 2D Richards equation are shown above in that one direction is vertical (i.e., ‘z’ axis). This is because the most common problem of interest in unsaturated flow is downward infiltration and percolation. Richards equation is highly non-linear and often requires iterative numerical solutions.

The Water Retention Curve (WRC) describes the relations hip between volumetric moisture content (\( \Theta \)) and \( \psi \), while \( K_{\psi} \) (or, alternatively \( K_{\Theta} \)) describe changes in hydraulic conductivity changes with \( \psi \) (or \( \Theta \)). Multiple formulations for the \( K_{\psi} \) and WRC functions are available in the literature (Brooks and Corey, 1964; Van Genuchten, 1980). The \( K_{\psi} \) function is developed around the WRC function. For example, the van Genuchten-Mualem \( K_{\psi} \) function utilizes parameters and conceptual underpinnings from the van Genuchten WRC and the statistical pore-size distribution model of Mualem, (1976). Studies characterizing the unsaturated hydraulic properties of municipal solid waste (Breitmeyer and Benson, 2014) demonstrated that the selection of the constitutive model does not substantially alter model
predictions, while other studies have found finer grained materials may be more sensitive to constitutive model, especially near saturation (Vogel et al., 2000). Models in Chapters 1 and 2 utilize the van Genuchten WRC, and the van Genuchten-Mualem $K_\theta$ function, as well as the Brooks and Corey WRC and $K_\theta$ function. A schematic illustration of a van Genuchten WRC, showing the effect of changing various van Genuchten parameters is shown in (Figure 2), while a similar figure is shown for a Brooks and Corey WRC in (Figure 3). Figure 4 shows the effects of parameter variation on the van Genuchten – Mualem relative hydraulic conductivity model, while Figure 5 shows the same for the Brooks and Corey relative hydraulic conductivity model. Equations for the van Genuchten – Mualem and Brooks and Corey – Mualem hydraulic property models are presented below:
Van Genuchten-Mualem Model:

\[ \theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[ \frac{1}{1 + (\alpha \psi)^n} \right]^m, \psi < 0 \]

\[ \theta = \theta_s, \psi \geq 0 \]

\[ K_\theta = K_s\theta^l \left[ 1 - \left( 1 - \theta^{1/m} \right)^m \right]^2, \psi < 0 \]

\[ K_\theta = K_s, \psi \geq 0 \]

\[ m = 1 - \frac{1}{n} \]

Where:

- \( \Theta \) = head dependent volumetric moisture content
- \( \Theta_r \) = residual moisture content
- \( \Theta_s \) = saturated moisture content = porosity = \( \phi \)
- \( \alpha \) (1/L) = term related to air entry pressure
- \( n \) = pore size distribution index
- \( \Psi \) = suction of water within the porous medium
- \( l \) = pore interaction term, often assume to be 0.5

Brooks and Corey-Mualem Model:

\[ \theta = \left( \frac{h}{h_b} \right)^{-\lambda}, \text{for } h \geq h_b \]

\[ \theta = \theta_s, \psi < h_b \]

\[ K_\theta = K_s(\theta)^{l+2+\frac{2}{\lambda}}, \text{for } h \geq h_b \]

\[ K_\theta = K_s, \psi < h_b \]

Where:

- \( h \) = suction of water within the porous medium
- \( h_b \) = bubbling pressure (or air entry pressure)
- \( \lambda \) = pore size distribution index
Simplified Models

Models that simplify the Richards equation to obtain approximations of system behavior (e.g. HELP, Heap Leach Draindown Estimator (HLDE)) are widely used in mine permitting and closure, and generally accepted by regulatory agencies. These models are typically formulated by making simplifying assumptions about the governing processes of the system. Simplifying assumptions are typically made on the side of engineering conservatism in order to produce a solution that is conservative, or requiring more mitigation than what is likely to occur in physical reality. While these solutions can be easily implemented, are often free, and provide quick solutions that are easily explained and transparent in their functions, these solutions also tend to simplify governing processes to the point that solutions may not be accurate over wide ranges of system behavior. Most simplified models are developed for the 1D condition in order to reduce the number variables requiring simplification.

Analytical Solutions and Associated Limitations

Analytical models are closed-form or analytical expressions that are solutions to the differential equations that govern a process (e.g. Richards equation for unsaturated fluid movement in porous media). Analytical solutions are typically involve a highly constrained and simplified versions of complex problems that allow for a closed form or analytical solution to the differential equation. Analytical solutions yield equations comprised of constants, variables, and well known operations which can give insight into the behavior of a system. Analytical solutions can be very useful for simulation of problems with simple geometries, and well-defined initial and boundary conditions (e.g. Heber Green and Ampt, (1911)), for validation of numerical simulations of such problems, or to test the reasonability of numerical simulation results with system bounding assumptions. However, analytical solutions are not as useful for problems with complex geometries, or complicated time-varying boundary conditions. An example of a
comparison between analytical and numerical solutions of the Green-Ampt infiltration problem can be seen in Tracy, (2011). Error in analytical models arises from simplification of complex geometry and boundary conditions required to arrive at a solution to the governing differential equation. Although analytical solutions are typically transparent and easily utilized, the solution is often inadequate to predict system behavior over a wide range of time varying system behaviors. Figure 6 illustrates, conceptually, the difference in domain assumptions and definition between an analytical and numerical solution.

**Numerical Simulations and Associated Limitations**

Numerical solutions are approximations to differential equations for which exact solutions are not possible or feasible. Accordingly, all numerical solutions contain error associated with the discrete approximation of the non-linear partial differential equation (Richards equation). Therefore, a disadvantage to a numerical solution is the inherent error introduced by the numerical solution method. However, these errors can be minimized by properly discretizing model domains and time-steps (for transient simulations). The limits/criteria for discretization of time and space model domains is better understood for saturated flow models and is presented in detail by Anderson and Woessner (1992), while some guidance for unsaturated models is presented in Šimunek and Miroslav, (2009). For unsaturated models, it is common practice to vary model discretization to identify the maximum spatial and temporal discretization that accurately captures the length and time scales of the system. Most numerical solution packages automatically change temporal discretization within user defined limits during solution to optimize computational efficiency and stability in the solution. Spatial discretization is still largely static and up to the modeler, although some adaptive spatial discretization routines exist (e.g. SVFlux). In addition to the constraints of numerical solutions in general, the highly non-linear nature of Richards equation results in a highly iterative numerical
solution. The iterative nature of the solution can result in simulations that are numerically unstable and computationally demanding.

**Dimensionality**

Unsaturated hydrologic models also vary by dimensionality. Unsaturated flow can be modeled in 1, 2 or 3 spatial dimensions. As shown in Figure 7, a 1D model assumes a unit-length in the ‘x’ and ‘y’ coordinate directions (a 1D model could also assume unit-lengths in x and z or in y and z but these are less common). The 1D formulation assumes that a condition modeled for any location along the z-axis is identical at all points in the xy plane which has a unit area. In the 2D formulation, conditions at any location in the yz or xz planes are assumed to apply everywhere along the x-axis or y-axis (whichever is inactive in the formulation). Thus, a 1D or 2D model does not preclude interpreting a 3D result, but rather requires assumptions about what happens in the 2nd or 3rd dimension. Implicit in the 1D and 2D solutions is a uniform distribution of the modeled fluid or contaminant across the inactive dimensions of the system.
Chapter 1: Predictive Simulations of Hypothetical Columns

Predictive simulations for this study were conducted on a hypothetical domain representative of a 6-inch nominal diameter infiltrations column with a length of 150 cm and filled with a homogeneous soil profile. Upper boundary conditions were varied to provide two different modeling scenarios (1) A constant flux of 1 cm/day (2) a time-specified flux in the form of hourly step function data generated from a sinusoidal function (Figure 8). Forward simulation results for each modeling code and scenario, consisting of boundary fluxes, changes in soil water storage, and predictions of runoff were compared.

Code Selection

The final list of codes were chosen for evaluation by stakeholders of the project based on their widespread use, documentation, and public domain status for some codes. Most of the codes are mechanistic and use the Richards equation to simulate near surface water balance, although (HELP) is an approximate model and uses a water routing approach (Table 1). The unsaturated flow codes included in this study include:

- **HYDRUS 1D** (version 4.1.6.0110 (Šimůnek et al., 2013); [http://www.pc-progress.com](http://www.pc-progress.com))
- **HYDRUS 2D/3D** (version 2.04.0460 (Šimůnek et al., 2012); [http://www.pc-progress.com](http://www.pc-progress.com))
- **Hydrologic Evaluation of Landfill Performance (HELP)** (Visual HELP, version 2.2.0.3 (Schroeder et al., 1994); [http://el.erdc.usace.army.mil/products.cfm?Topic=model&Type=landfill](http://el.erdc.usace.army.mil/products.cfm?Topic=model&Type=landfill))
- **SVFlux** (Version 2.4.26 (Fredlund and Thode, 2007); [http://soilvision.com/subdomains/svflux.com/](http://soilvision.com/subdomains/svflux.com/); **UNSAT-H** (WinUnsatH version 1.00 (Fayer, 2000); [http://hydrology.pnnl.gov/resources/unsath/software.asp](http://hydrology.pnnl.gov/resources/unsath/software.asp)); and

Detailed Model Parameterization

Simulation 1: Constant Upper Boundary Flux

Soil Characteristics

The soil characteristics were identical for each numerical model for simulation 1, and were represented with the van Genuchten–Mualem water retention and hydraulic conductivity
functions for the Richards equation based codes (van Genuchten, 1980). Parameters for the van Genuchten function can be found in Table 2, and were generated with pedotransfer functions from Rosetta Lite v. 1.1. (Schaap, 2003). Inputs were purely textural, and consisted of a 97.5 percent sand fraction and 2.5 percent clay fraction. The soil texture was chosen for ease of experimental validation at a later date. The HELP model requires porosity, volumetric moisture content at the wilting point (-15 bar) and field capacity (-.33 bar) for a soil, and uses linear regressions developed by W. J. Rawls et al., (1982) to develop a WRC consistent with the equations in Brooks and Corey, (1964) (Schroeder et al., 1994). Volumetric moisture content for wilting point and field capacity were solved for using expressions from van Genuchten, (1980), and yield a moisture content of .0530 at the wilting point and .0532 at field capacity.

Initial Conditions
Initial conditions for all models except for HELP were set in terms of suction, with a uniform 100 cm of suction throughout the soil profile. Initial conditions for HELP must be in terms of moisture content, with a uniform volumetric water content of .0612 corresponding to 100 cm of suction for the van Genuchten WRC described above (Table 2).

Boundary Conditions
The upper boundary condition was set to a 1 cm/day constant flux into the domain for all simulations. For 2D and 3D simulations (HYDRUS, SVFlux, and VS2D), edges of the column were set to a zero specified flux condition. Although a seepage face lower boundary condition may more accurately represent the conceptual model of the infiltration columns, the version of UNSAT-H used in this study does not have the ability to implement this type of boundary condition. Scanlon et al., (2002) described a procedure of inserting an artificial gravel layer below the bottom most layer of the model to approximate a seepage face boundary. Although this procedure would be a feasible alternative to using unit gradient lower boundary conditions,
use of unit gradient boundary conditions for all models ensures that the lower boundary is implemented identically across models, while reducing the numerical complexity of the simulations.

**Temporal and Spatial Discretization**

Spatial discretization for each model was initially run at default spacing or 5 cm if there was not a default value, while time step parameters were left at default values. If numerical simulations did not converge, time step parameters were adjusted or grid spacing was reduced until convergence was achieved. Temporal and spatial discretization is listed for each model in Table 3.

**Simulation 2: Time Varying Upper Boundary Flux**

**Soil Characteristics**

The soil characteristics were identical for each model for simulation 2, and were represented with the van Genuchten – Mualem water retention and hydraulic conductivity functions for the Richards equation based codes (van Genuchten, 1980). Parameters for the van Genuchten - Mualem functions can be found in Table 3, and correspond to a silt loam from Carsel and Parrish, (1988) (Figure 9). The soil parameters chosen for simulation 2 are closer to those likely to be encountered in many field locations. Constitutive properties for the HELP model were developed as described for simulation 1, with moisture contents of .135 at the wilting point and .284 at field capacity calculated from the van Genuchten WRC used in the calculations.
Initial Conditions

Initial conditions for all models except for HELP were set in terms of suction, with a uniform 100 cm of suction throughout the soil profile. Initial conditions for HELP must be set in terms of moisture content, with a uniform volumetric water content of .33 corresponding to 100 cm of suction for the van Genuchten WRC described above (Table 3).

Boundary Conditions

The upper boundary condition was set to either a time-varying specified flux, or an atmospheric boundary condition, with precipitation rate or specified flux rate corresponding to the following hourly function:

\[ P = 5.4 \left( \frac{cm}{day} \right) \sin(X) + 5.4 \left( \frac{cm}{day} \right) \]

Where \( P \) = precipitation rate/specified flux (cm/day), and \( X \) = an array of hours from 0 to 600. Note that the output of the precipitation function is irregular because the input array (0 - 600, increasing by 1) is misaligned with the period of the sin function (0 - 2\( \pi \)).
Precipitation was represented as an hourly step function of precipitation rates (Figure 8) with minimum value equal to 0 cm/day and maximum value equal to 10.8 cm/day, which is equal to the saturated hydraulic conductivity for the silt loam. The precipitation function was chosen such that precipitation values would be very close to the infiltration capacity for the soil, allowing for the possibility that the models with atmospheric boundary conditions would partition a portion of the flow to runoff. VS2D and SVFlux (Standard Edition) could not implement an atmospheric boundary condition due to inherent lack of capability, and licensing availability during the time of the study, respectively. The choice of upper limit for precipitation rate equal to saturated hydraulic conductivity allows for a small enough runoff component that comparison of the remaining water balance components is still valid. For 2D and 3D simulations (HYDRUS, SVFlux, and VS2D), edges of the column were set to a zero specified flux condition. As with simulation 1, lower boundary conditions were set to free drainage for all models.

**Temporal and Spatial Discretization**

Temporal and Spatial discretization was retained from simulation 1, unless convergence issues were encountered. If numerical simulations did not converge, discretization was adjusted until convergence was achieved. Temporal and spatial discretization is listed for each model in Table 3.
Results/Discussion for Column Models

Constant Flux Columns:
Cumulative daily drainage and daily water storage change were compared for each model. For Richards equation based models, all water from the constant flux upper boundary was allocated to an increase in soil water storage for the first 4-6 days (Figure 10). Subsequently, changes in storage decreased to 0 cm/day, and drainage increased from 0 cm/day during the first 4-6 days, to a constant rate of 1 cm/day. Equivalency between the drainage rate and upper boundary flux after 6 days indicates that the models have achieved steady state conditions (Figure 11). The HELP model predicted immediate drainage of soil moisture until the wilting point (~15,000 cm) was reached, which was very near to the residual moisture content for the hydraulic properties used in this simulation. The initial drainage in the HELP model occurs because the HELP model does not consider matric suction. Following the initial drainage, the HELP model predicted that soil moisture would drain at a rate matching the upper boundary condition of 1 cm/day.

Although there is some variance (~1.5 days) between the Richard’s equation based models in terms of the onset of drainage and cumulative drainage (~2.5 cm) the steady state drainage rate of 1 cm/day was achieved in all models. The difference between the model results is 12.4 percent of the mean cumulative drainage total (21 cm) at 25 days. Under longer simulation periods with greater cumulative drainages, the relative difference would become a much smaller and insignificant portion of the cumulative drainage total.

Sin Flux Columns:
Due to the increased complexity of simulation 2, results are split into several sections, each corresponding to a water balance component.
Drainage:

Drainage from the Simulation 2 models commences between 2-4 days, with HELP predicting the earliest drainage near 2 days, and SVFlux predicting the latest drainage near 4.5 days. The remaining models predicted the onset of drainage near 3.5 days (Figure 12, Figure 13). The differences in drainage can be analyzed by comparing cumulative and instantaneous drainage rates for each model.

The slope of the steady state cumulative drainage is the steady state drainage rate. All cumulative drainage rates are near to 5.4 cm/day (Figure 12), which is equal to the average rate of precipitation (or flux for specified flux models) applied at the upper boundary (Figure 8). There are some slight differences in the average rate before ~16 days (Figure 12) due to differences in instantaneous drainage rate over time, which can be seen in Figure 13. However, all models produced mass balances within reasonable limits (Figure 14).

Hydrus 1D and Hydrus 2D/3D solve the mixed form of Richards equation (Celia et al., 1990), which solves for suction and moisture content and is generally more mass conservative than the purely suction based Richards equation. Codes based on the mixed form of Richards equation show more variation in the upper limit of drainage rate (Figure 13). Although the variation in the upper limit of drainage rate is reflective of the model forcing from the upper boundary condition (Figure 8), drainage rate did show sensitivity to implementation of the Richards equation. As an example, the SVFlux model shown in Figure 13, executed using the suction based Richards equation shows much less variation in the upper limit of drainage rate. Execution of SVFlux with increased error tolerance produced variation in the upper limit of drainage rate similar to the mixed equation based codes (Figure 15). However, this option produced erratic variation in input fluxes. Execution of SVFlux with the mixed form of Richards equation resulted in outputs similar to HYDRUS models, although convergence issues were
encountered when the specified upper boundary flux was equal to saturated hydraulic conductivity. HYDRUS encountered similar issues when Simulation 2 was executed as a specified flux model. Finally, variation in the upper limit of drainage rate was successfully reduced by decreasing the water content tolerances for the solution in the VS2D model (Figure 16). The results described above point to the challenging nature of calculating fluxes in an unsaturated model near saturation with the standard van Genuchten–Mualem formulation.

While the central tendency for instantaneous drainage rates is near 5.4 cm/day for all codes, there are differences in the magnitude of variation around the central tendency. SVFlux, HYDRUS 2D/3D and HYDRUS 1D show variation in instantaneous drainage rate on the order of +/- 1 cm, while VS2D varies closer to +/- .6 cm. For all codes, the instantaneous drainage rate increases quickly while the upper boundary flux is near Ks, and then exhibits an exponential shaped drain down curve as the upper boundary flux reduces to zero.

Although there is some variance (~1.5 days) between the Richard’s equation based models in terms of the onset of drainage and cumulative drainage (~5.8 cm) the steady state drainage rate of ~5.4 cm/day was achieved in all models. The difference between the model results is 5.1 percent of the mean cumulative drainage total (113.8 cm) at 25 days. Under longer simulation periods with greater cumulative drainages, the relative difference would become a much smaller and insignificant portion of the cumulative drainage total.

The HELP and UNSAT-H models produce model outputs at minimum temporal resolution of daily intervals. The finest temporal resolution for input data in the HELP model is daily, while the UNSAT-H model accepts hourly input data, but produces output data in daily averaged values at the finest resolution. Accordingly, the drainage rate for HELP is equal to the constant daily specified flux at the upper boundary of 5.4 cm/day, while the average daily
drainage rate for UNSAT-H is near to 5.4 cm/day, showing some deviation due to time averaging of hourly data (Figure 13).

**Changes in Water Storage:**
For the HYDRUS 1D, HYDRUS 2D/3D, SVFlux and VS2D models, changes in storage are tied directly to the upper boundary sinusoidal flux, varying from 0 to 10.8 cm/day for the first \(\sim 3.3 - 4.1\) days. Thereafter changes in storage vary from – 5.4 to 5.4 cm/day, with the average change in storage being 0 (Figure 17). Increases in storage are near to the average rate of 5.4 cm/day for the UNSAT-H and HELP models, with increases in storage returning to zero \(\sim 3.3\) days for the UNSAT-H model, and \(\sim 3\) days for the HELP model. A simple calculation using the initial moisture content (.33), saturated moisture content (.45), and height of the model give 18 cm of storage available at the onset of the Simulation 2. Using the average rate of infiltration of 5.4 cm/day and assuming no drainage, storage space should reach full saturation around 3.3 days from the beginning of Simulation 2. This calculation agrees well with the observations for the HYDRUS, VS2D, and UNSAT-H models. The difference between all models in terms of time to onset of drainage/return to zero water storage changes is \(\sim 1.2\) days, or 4.8 percent of the total simulation time.

**Infiltration Rate:**
Instantaneous infiltration rate varies from 0 cm/day to the maximum upper boundary flux of 10.8 cm/day for HYDRUS 1D, HYDRUS 2D/3D, VS2D and SVFlux (Figure 18). The infiltration rate for HELP is equal to the constant daily specified flux at the upper boundary of 5.4 cm/day, while the average daily drainage rate for UNSAT-H is near to 5.4 cm/day, showing some deviation due to time daily averaging of hourly data, as described previously.
Runoff:

VS2D and the version of SVFlux available for this study do not support an atmospheric upper boundary condition, and the upper boundary condition was implemented in those models as a time varying specified flux. Accordingly, the total amount of flux specified per time step by the sin function is forced across the upper boundaries in these models, and runoff is not generated. Because the finest temporal resolution for the HELP model is daily, the precipitation rate for HELP is set at a constant rate of 5.4 cm/day. Accordingly, the precipitation rate never exceeds the infiltration capacity, and no runoff is generated for this model. Plots of cumulative runoff and runoff rate for HYDRUS 1D, HYDRUS 2D/3D, HELP, and UNSAT-H are provided in Figure 19. The models predicted .33, .71, 0.00 and 6.45 cm of cumulative runoff, respectively. Stated in the context of the 135 cm of applied surface flux over the 25 day simulation, the models predict 0.2, 0.5, 0.0, and 4.8 percent runoff, respectively.

Notable Differences/Issues Encountered During Simulations

All codes encountered convergence issues near saturation for simulation 2, in the air entry region of the WRC. In this region, small changes in \( \psi \) (which effect changes in \( \theta \)) produce large changes in \( K_\theta \), and the \( K_\theta \) function is highly non-linear. Consequently, much iteration on the \( K_\theta \) function is required to achieve convergence of the solution. Convergence issues near saturation are well-documented, and explained in detail in Vogel et al., (2000). One solution to this problem is the use of a modified constant air entry value in the 0-4 cm suction range as detailed in Schaap and van Genuchten, (2006). Use of the 2cm air entry van Genuchten model for Simulation 2 provided consistent results in terms of cumulative drainage, while drainage rate exhibited much less variability with the 2cm air entry model (Figure 20). UNSAT-H has the option of specifying the range of suctions which soils can wet up to. Limiting the pressure to be further from 0 (full saturation) is another method to prevent the convergence issues, although
accuracy issues can arise from this option. The issues near saturation were amplified for models that were executed as specified flux models (SVFlux, VS2D), because the entire precipitation function was forced across the upper boundary, which increased the saturation state to very near full saturation.

Several times during the course of the model comparisons, what appeared to be a substantive difference between modeling codes was attributed to differences in model setups, most commonly variations in parameter descriptions between codes, or incorrect unit conversions. Once the differences were addressed, model results were nearly identical between models. In a sense, executing a model in more than one code could serve as a sort quality control measure, where differences between codes may draw attention to incorrect model setup.

Finally, in use of the varying codes for the comparisons it became apparent that some codes were intended for the type of simulations conducted, while others were not. As an example, the HELP model is intended to be used with daily or monthly average climate data, while input to the UNSAT-H model used in this study is cumbersome at hourly intervals. Newer versions of the UNSAT-H model are available, although there are no readily available GUIs, which makes the learning curve for operation of this model steep. In order to execute the UNSAT-H model on hourly data, input files were created with the aid of a scripting language, while the HELP model was ultimately being incapable of execution on hourly data.

Conclusions

Chapter 1 demonstrates that Richards equation based codes should produce similar cumulative and transient outputs for simple problems because the same governing equation is solved by each code. The simulations presented in this chapter are identical in terms of
geometry, initial conditions and boundary conditions. It follows that the slight differences between solutions for each code are due to differences in how the Richards equation is implemented in each code. For more complicated problems, specific implementation of boundary conditions will play a larger factor in solution differences. As an example, Scanlon et al., (2002) found that UNSAT-H simulated precipitation excess runoff better than other compared codes by disaggregating precipitation and applying it at a specified rate, and allowing evaporation to occur throughout the rest of the day.

The HELP model does not solve Richards equation, and so the results for that model differ more than the Richards equation based codes do from each other. The main difference between HELP and the other codes for the simulations presented in Chapter 1 is that the HELP model does not simulate matric gradients, which allows drainage to occur sooner than the other models, which initially partition more water to storage. For the Chapter 1 simulations, matric gradients do not play a large role because there is no atmospheric potential at the upper boundary in Simulations 1 and 2. However, steep upward matric gradients near the soil surface are present in many arid and semiarid climates. Upward matric gradients can have a large impact on water balance, and ignoring them is inappropriate for most semiarid to arid climates.

Another significant difference is the ability to simulate time periods smaller than 1 day. The HELP and UNSAT-H models used in this study were not capable of hourly outputs, and thus could not be compared to the other models on this time scale. The inability to simulate smaller time periods may produce inaccurate results for climates with convective storms that produce precipitation events that last < 1 hour.

In Chapter 2, the differences highlighted in Chapter 1 simulations and the literature review are examined by implementing realistic boundary conditions and several variations on
key model parameters in a semiarid climate, using HYDRUS 1D and HYDRUS 2D. The results are compared to a HELP simulation that utilized monthly climate data from a climate generation routine.
<table>
<thead>
<tr>
<th>Model</th>
<th>Public/Private</th>
<th>Process Summary for Near Surface Hydrologic Modeling</th>
<th>Numerical Solution Method</th>
<th>Geochemical Summary</th>
</tr>
</thead>
</table>
| HYDRUS 1D | Public | Numerically solves the Richards equation for simulating variably-saturated water flow. | The governing flow and transport equations are solved numerically using Galerkin type linear finite element schemes. Integration in time is achieved using an implicit (backwards) finite difference scheme for both saturated and unsaturated conditions. Additional measures are taken to improve solution efficiency for transient problems. Including automatic time step adjustment and adherence to preset ranges of the Courant and Peclet numbers. The water content term is evaluated using the mass conservative method proposed by Celia et al. (1990). Possible options for minimizing numerical oscillations in the transport solutions include upstream weighing, artificial dispersion, and/or performance indexing. HYDRUS implements a Marquardt-Levenberg type parameter estimation technique for inverse estimation of selected soil hydraulic and/or solute transport and reaction parameters from measured transient or steady-state flow and/or transport data (Šimůnek et al., 2013). | Standard Solute Transport (ADRE) | Major ion chemistry (UNSATCHEM Model):  
- Major ion equilibrium/kinetic reactions  
- Major ion sorption  
- Chemical effects on hydraulic conductivity  
- Transport of multiple components  
- Broad range of mixed equilibrium/kinetic biogeochemical reactions  
- Interactions with minerals, gases, exchangers, and sorption surfaces based on thermodynamic equilibrium, kinetic, or mixed kinetic/equilibrium reactions |
| HYDRUS 2D/3D | Private | Numerically solves the Richards equation for saturated-unsaturated water flow. | The governing equations are solved numerically using a Galerkin type linear finite element method applied to a network of triangular elements. Integration in time is achieved using an implicit (backwards) finite difference scheme for both saturated and unsaturated conditions. The resulting equations are solved in an iterative fashion, by linearization and subsequent Gaussian elimination for banded matrices, a conjugate gradient method for symmetric matrices, or the ORTHOMIN method for asymmetric matrices. Additional measures are taken to improve solution efficiency in transient problems, including automatic time step adjustment and ensuring that the Courant and Peclet numbers do not exceed preset levels. The water content term is evaluated using the mass-conservative method proposed by Celia et al. (1990). To minimize numerical oscillations upstream weighing is included as an option for solving the transport equation (Šimůnek et al., 2012). | Standard Solute Transport (ADRE) | Major ion chemistry (UNSATCHEM Model):  
- Major ion equilibrium/kinetic reactions  
- Major ion sorption  
- Chemical effects on hydraulic conductivity  
HP2 (Loosely coupled HYDRUS 2D and PHREEQC):  
- Transport of multiple components  
- Broad range of mixed equilibrium/kinetic biogeochemical reactions  
- Interactions with minerals, gases, exchangers, and sorption surfaces based on thermodynamic equilibrium, kinetic, or mixed kinetic/equilibrium reactions |
<p>| HELP | Public/Private | Runoff is computed using the SCS method based on daily amounts of rainfall and snowmelt. Potential evapotranspiration is modeled by an energy-based Penman method. The evaporative zone depth is assumed to be constant throughout the simulation period. The HELP program assumes Darcian flow for vertical drainage through homogeneous, temporarily uniform soil and waste layers. Vertical drainage is assumed to be driven by gravity alone and is limited only by the saturated hydraulic conductivity and available storage of lower segments. The vertical drainage routine does not permit capillary rise of water from below the evaporative zone depth. The lateral drainage model is based on the assumption that the lateral drainage rate and average saturated depth relationship that exists for steady-state drainage also holds for unsteady drainage. | Does not solve a differential equation numerically. | Drainage rates can be used as input to external geochemical model or analytical solution to ADRE |
| SV FLUX | Private | SVFlux™ is designed to model seepage and groundwater in soils. It is a 1D, 2D, axisymmetric and 3D finite element program for calculating saturated and unsaturated groundwater flow. Numerically solves the Richards equation. | Finite element analysis by the Galerkin method - the solver uses advanced features such as preconditioning of the convergence matrix as well as staging and automatic mesh refinement to achieve solutions with greater stability than any other software currently available. | Drainage rates can be used as input to external geochemical model or analytical solution to ADRE |
| | | | | CHEMFlux package can model fully coupled ADRE, with adsorption and decay options |</p>
<table>
<thead>
<tr>
<th>Model</th>
<th>Public/Private</th>
<th>Process Summary for Near Surface Hydrologic Modeling</th>
<th>Numerical Solution Method</th>
<th>Geochemical Summary</th>
</tr>
</thead>
<tbody>
<tr>
<td>UNSAT-H</td>
<td>Public</td>
<td>UNSAT-H is a FORTRAN computer code used to simulate the one-dimensional flow of water, vapor, and heat in soils. The code addresses the processes of precipitation, evaporation, plant transpiration, storage, and deep drainage. The UNSAT-H computer code is used to understand the movement of water, heat, and vapor in soils. The UNSAT-H model simulates liquid water flow using Richards equation (Richards 1931), water vapor diffusion using Fick’s law, and sensible heat flow using the Fourier equation. The mathematical equations that describe the state and dynamics of the modeled system are written in an implicit finite-difference form. The user must specify an averaging scheme for internodal hydraulic and vapor conductivities; choices include arithmetic (and arithmetic-weighted), geometric, and harmonic. Heat internodal conductances are calculated as arithmetic means. The resulting equations are solved using an iteration technique (either standard or modified Picard) with the Thomas algorithm. The solution strategy for each iteration is to solve the water flow equations, then solve the heat flow equations. After the second and subsequent iterations, the convergence criteria are checked. Drainage rates can be used as input to external geochemical model or analytical solution to ADRE.</td>
<td>For the flow equation, spatial derivatives are approximated by central differences written about grid block boundaries. Time derivatives are approximated by a fully implicit backward scheme. Nonlinear conductance terms, boundary conditions, and sink terms are linearized implicitly. Relative hydraulic conductivity is evaluated at cell boundaries by using full upstream weighting, the arithmetic mean, or the geometric mean of values from adjacent cells. Saturated hydraulic conductivities are evaluated at cell boundaries by using distance-weighted harmonic means. Nonlinear conductance and storage terms can be represented by algebraic equations or by tabular data.</td>
<td>Drainage rates can be used as input to external geochemical model or analytical solution to fully coupled ADRE (Transport equation) with linear, freundlich, and langmuir sorption isotherms, and ion-exchange capabilities.</td>
</tr>
<tr>
<td>VS2D</td>
<td>Public</td>
<td>Computer program VS2DT solves problems of water and solute movement in variably saturated porous media. The finite difference method is used to approximate the flow equation, which is developed by combining the law of conservation of fluid mass with a nonlinear form of Darcy’s equation (Richards eq.), and the advection-dispersion equation. The model can analyze problems in one and two dimensions with planar or cylindrical geometries. There are several options for using boundary conditions that are specific to flow under unsaturated conditions: infiltration with ponding, evaporation, plant transpiration, and seepage faces. For the flow equation, spatial derivatives are approximated by central differences written about grid block boundaries. Time derivatives are approximated by a fully implicit backward scheme. Nonlinear conductance terms, boundary conditions, and sink terms are linearized implicitly. Relative hydraulic conductivity is evaluated at cell boundaries by using full upstream weighting, the arithmetic mean, or the geometric mean of values from adjacent cells. Saturated hydraulic conductivities are evaluated at cell boundaries by using distance-weighted harmonic means. Nonlinear conductance and storage terms can be represented by algebraic equations or by tabular data.</td>
<td>Drainage rates can be used as input to external geochemical model or analytical solution to fully coupled ADRE (Transport equation) with linear, freundlich, and langmuir sorption isotherms, and ion-exchange capabilities.</td>
<td></td>
</tr>
</tbody>
</table>
Table 2. Model parameters for Simulation 1

<table>
<thead>
<tr>
<th>Model</th>
<th>Model Scenario</th>
<th>Lower B.C. Used</th>
<th>Upper B.C. Used</th>
<th>Water Retention Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>HYDRUS 1D</td>
<td>Simulation 1</td>
<td>Unit gradient</td>
<td>Constant flux (1 cm/day)</td>
<td>V.G.¹</td>
</tr>
<tr>
<td>HYDRUS 2D/3D</td>
<td>Simulation 1</td>
<td>Unit gradient</td>
<td>Constant flux (1 cm/day)</td>
<td>V.G.¹</td>
</tr>
<tr>
<td>SV Flux</td>
<td>Simulation 1</td>
<td>Unit gradient</td>
<td>Constant flux (1 cm/day)</td>
<td>V.G.¹</td>
</tr>
<tr>
<td>UNSAT-H</td>
<td>Simulation 1</td>
<td>Unit gradient</td>
<td>Constant flux (1 cm/day)</td>
<td>V.G.¹</td>
</tr>
<tr>
<td>VS2D</td>
<td>Simulation 1</td>
<td>Unit gradient</td>
<td>Constant flux (1 cm/day)</td>
<td>V.G.¹</td>
</tr>
<tr>
<td>HELP</td>
<td>Simulation 1</td>
<td>Unit gradient</td>
<td>Constant flux (1 cm/day)</td>
<td>Other²</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Model</th>
<th>K(Θ,h) Function</th>
<th>Spatial Discretization</th>
<th>Minimum Time Step</th>
<th>Initial Time Step</th>
</tr>
</thead>
<tbody>
<tr>
<td>HYDRUS 1D</td>
<td>V.G. / Mualem</td>
<td>400 nodes uniform spacing</td>
<td>1x10⁻⁶ day</td>
<td>1x10⁻⁵ day</td>
</tr>
<tr>
<td>HYDRUS 2D/3D</td>
<td>V.G. / Mualem</td>
<td>117 nodes, 64 1D elements, 168 2D Elements, 5 cm elements</td>
<td>1x10⁻⁵ day</td>
<td>1x10⁻⁴ day</td>
</tr>
<tr>
<td>SV Flux</td>
<td>V.G. / Mualem</td>
<td>5 cm mesh spacing, automatic refinement</td>
<td>1x10⁻¹⁸ day</td>
<td>1x10⁻⁴ day</td>
</tr>
<tr>
<td>UNSAT-H</td>
<td>V.G. / Mualem</td>
<td>50 nodes uniform spacing</td>
<td>1x10⁻⁷ day</td>
<td>Automated</td>
</tr>
<tr>
<td>VS2D</td>
<td>V.G. / Mualem</td>
<td>1200 .95 x 1 cm grid cells</td>
<td>1x10⁻⁴ day</td>
<td>1x10⁻⁴ day</td>
</tr>
<tr>
<td>HELP</td>
<td>Campbell, 1974</td>
<td>N/A</td>
<td>1 day</td>
<td>1 day</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Model</th>
<th>Initial Condition</th>
<th>Model Run Time</th>
<th>Soil Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>HYDRUS 1D</td>
<td>h = -100 cm</td>
<td>.79 s</td>
<td>Θr = .053</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Θs = .375</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>α (1/cm) = .033</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>n = 4.087</td>
</tr>
<tr>
<td>HYDRUS 2D/3D</td>
<td>h = -100 cm</td>
<td>.32 s</td>
<td>Ks = 1213.96 cm/day</td>
</tr>
<tr>
<td>SV Flux</td>
<td>h = -100 cm</td>
<td>23 s</td>
<td>l = .5</td>
</tr>
<tr>
<td>UNSAT-H</td>
<td>h = -100 cm</td>
<td>25 s</td>
<td></td>
</tr>
<tr>
<td>VS2D</td>
<td>h = -100 cm</td>
<td>48 s</td>
<td></td>
</tr>
<tr>
<td>HELP</td>
<td>vwc = .0612</td>
<td>&lt; 1 s</td>
<td></td>
</tr>
</tbody>
</table>

1. V.G. - van Genuchten
2. See (Schroeder et al. 1994) for a detailed explanation of water retention in HELP.
Table 3. Model parameters for Simulation 2.

<table>
<thead>
<tr>
<th>Model</th>
<th>Model Scenario</th>
<th>Lower B.C. Used</th>
<th>Upper B.C. Used</th>
<th>Water Retention Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>HYDRUS 1D</td>
<td>Simulation 2</td>
<td>Unit gradient</td>
<td>$P = 5.4 \sin(x) + 5.4 \text{ (cm/hr)}$</td>
<td>V.G.¹</td>
</tr>
<tr>
<td>HYDRUS 2D/3D</td>
<td>Simulation 2</td>
<td>Unit gradient</td>
<td>$P = 5.4 \sin(x) + 5.4 \text{ (cm/hr)}$</td>
<td>V.G.¹</td>
</tr>
<tr>
<td>SV Flux</td>
<td>Simulation 2</td>
<td>Unit gradient</td>
<td>$P = 5.4 \sin(x) + 5.4 \text{ (cm/hr)}$</td>
<td>V.G.¹</td>
</tr>
<tr>
<td>UNSAT-H</td>
<td>Simulation 2</td>
<td>Unit gradient</td>
<td>$P = 5.4 \sin(x) + 5.4 \text{ (cm/hr)}$</td>
<td>V.G.¹</td>
</tr>
<tr>
<td>VS2D</td>
<td>Simulation 2</td>
<td>Unit gradient</td>
<td>$P = 5.4 \sin(x) + 5.4 \text{ (cm/hr)}$</td>
<td>V.G.¹</td>
</tr>
<tr>
<td>HELP</td>
<td>Simulation 2</td>
<td>Unit gradient</td>
<td>$P = 5.4 \sin(x) + 5.4 \text{ (cm/hr)}$</td>
<td>Other²</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Model</th>
<th>K(Θ,h) Function</th>
<th>Spatial Discretization</th>
<th>Minimum Time Step</th>
<th>Initial Time Step</th>
</tr>
</thead>
<tbody>
<tr>
<td>HYDRUS 1D</td>
<td>V.G. / Mualem</td>
<td>400 nodes .375 cm uniform spacing</td>
<td>$1x10^{-6}$ day</td>
<td>$1x10^{-5}$ day</td>
</tr>
<tr>
<td>HYDRUS 2D/3D</td>
<td>V.G. / Mualem</td>
<td>1015 nodes, 212 1D elements, 1816 2D elements, 1.5 cm elements</td>
<td>$1x10^{-4}$ day</td>
<td>$1e^{-8}$ day</td>
</tr>
<tr>
<td>SV Flux</td>
<td>V.G. / Mualem</td>
<td>5 cm mesh spacing, automatic refinement</td>
<td>$1x10^{-18}$ day</td>
<td>$1x10^{-4}$ day</td>
</tr>
<tr>
<td>UNSAT-H</td>
<td>V.G. / Mualem</td>
<td>50 nodes uniform spacing</td>
<td>$1x10^{-20}$ day</td>
<td>Automated</td>
</tr>
<tr>
<td>VS2D</td>
<td>V.G. / Mualem</td>
<td>400 .375 cm grid cells</td>
<td>$1x10^{-9}$ day</td>
<td>$1x10^{-4}$ day</td>
</tr>
<tr>
<td>HELP</td>
<td>Campbell, 1974</td>
<td>N/A</td>
<td>1 day</td>
<td>1 day</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Model</th>
<th>Initial Condition</th>
<th>Model Run Time</th>
<th>Soil Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>HYDRUS 1D</td>
<td>$h = -100 \text{ cm}$</td>
<td>19.25 s</td>
<td>$\Theta_r = .067$</td>
</tr>
<tr>
<td>HYDRUS 2D/3D</td>
<td>$h = -100 \text{ cm}$</td>
<td>46.6 s</td>
<td>$\Theta_s = .45$</td>
</tr>
<tr>
<td>SV Flux</td>
<td>$h = -100 \text{ cm}$</td>
<td>1 m21 s</td>
<td>$\alpha (1/cm) = .02$</td>
</tr>
<tr>
<td>UNSAT-H</td>
<td>$h = -100 \text{ cm}$</td>
<td>11 s</td>
<td>$n = 1.41$</td>
</tr>
<tr>
<td>VS2D</td>
<td>$h = -100 \text{ cm}$</td>
<td>12 m4 s</td>
<td>$K_s = 10.8 \text{ cm/day}$</td>
</tr>
<tr>
<td>HELP</td>
<td>vwc = .33</td>
<td>&lt;1 s</td>
<td>$l = .5$</td>
</tr>
</tbody>
</table>

1. V.G. - Van Genuchten
2. See (Schroeder et al. 1994) for a detailed explanation of water retention in HELP.
Chapter 1 Figures

Figure 1. Flow chart for proposed closure procedure. Orange blocks denote steps dependent on numerical modeling, while the red box surrounds the work detailed in this thesis.
Figure 2. Illustration of a van Genuchten WRC, showing the effect of changes in various parameters.
Figure 3. Illustration of a Brooks and Corey WRC, showing the effect of changes in various parameters.
Figure 4. Illustration of a van Genuchten - Mualem relative hydraulic conductivity model, showing the effect of changes in various parameters.
Figure 5. Illustration of a Brooks and Corey - Mualem relative hydraulic conductivity model, showing the effect of changes in various parameters.
Q is the flow term and in analytical solutions is based on an assumed and simplified hydrologic flow condition.

\[ \theta = \frac{V_w}{AH} \]

\[ \Delta V_w = [P - ET - Q + S] \]

This is the flow term and is solved iteratively at each node or element using a numerical solution to the partial differential equation.

\[ \frac{\partial \theta}{\partial t} = P - ET - \frac{\partial K_{\psi}}{\partial z} - \frac{\partial}{\partial z} \left( K_{\psi} \frac{\partial \psi}{\partial z} \right) - S \]

Figure 6. Illustration of analytical (top) and numerical conceptual flow models (1D condition shown).
Figure 7. Illustration of model dimensionality and discretization.

Figure 8. Step Function of Sinusoidal Precipitation data used as the time varying specified flux for the upper boundary condition in Simulation 2.
Figure 9. Hydraulic properties for soils in Simulations 1 and 2.

Figure 10. Daily change in water storage for Simulation 1.
Figure 11. Cumulative drainage for Simulation 1.

Figure 12. Cumulative drainage for Simulation 2.
Figure 13. Instantaneous drainage rates for Simulation 2.
Figure 14. Cumulative mass balance errors for Simulation 2.
Figure 15. Results for SVFlux simulation with increased error tolerance.

Figure 16. Results for VS2D with decreased error tolerance.
Figure 17. Changes in soil water storage for Simulation 2.
Figure 18. Instantaneous infiltration rates for Simulation 2.
Figure 19. Cumulative runoff for Simulation 2 models with atmospheric type boundary conditions.

Figure 20. Results for Simulation 2 with varying soil water property model. The van Genuchten-Mualem model is shown in red, while the modified (with 2cm air entry pressure) van Genuchten-Mualem model is shown in black.
Chapter 2: Assessment of Percolation at Caselton Tailings Impoundment

Introduction

Field and laboratory investigations, as well as predictive hydrologic simulations of the Caselton tailings impoundment were conducted to assess the likelihood of percolation of meteoric water through the tailings to the underlying alluvium. Simulations were conducted with mechanistic models to accurately capture the dynamics of unsaturated flow at appropriate spatial and temporal scales, and to assess the effects of various modeling decisions on the outcome of a predictive simulation (e.g. element size, code selection, conceptual model).

Location, Geography, and Climate

The Caselton Tailings impoundment is located in Lincoln County, in eastern Nevada, approximately 110 miles south of Ely, Nevada and 170 miles north of Las Vegas, Nevada (Figure 21). Populated areas in proximity to the tailings impoundment include the unincorporated communities of Pioche, NV (three miles northeast) and Caselton Heights (one mile northeast).

Regional geography near the site is typical of the Basin and Range Province: North to northwest trending mountain ranges separated by arid sedimentary basins bounded by range-front normal faulting. Regionally, elevations range from as low as 5,000 feet near Panaca, NV, up to 9,305 feet at Highland Peak. Sage brush, mountain mahogany, juniper and piñon pine dominate valleys and lower elevation slopes, while sparse ponderosa pine and aspen have been observed at higher elevations (Hayes, L.D., 1971).

Climate data from 1945 to 2005 in Pioche, NV (Western Regional Climate Center, 2016) details that climate in the area is typical of the great basin, with low annual precipitation (.3 m), hot summers, and cool winters. Minimum winter temperatures as low as -18 - 23°C (0 - 10° F)
are observed, although average minimum winter temperatures range from -6 to 6 °C (21 - 43°F) in January. Summer temperatures may reach 38 °C (100°F), although average summer temperatures range from 15 to 31 °C in July (58 - 88 °F) (Figure 22). Winter precipitation is dominant, with an average snow depth of 3 – 8 cm of from December to March (Western Regional Climate Center, 2016). Snowfalls one foot deep are not uncommon, but usually disappear from the ground within a week (Hayes, L.D., 1971). Precipitation is usually mixed snow and rain from December to March, while sparse rainfall comprises precipitation from April through November (Figure 23).

**Caselton Mine Site History**

The Caselton site is located within the Pioche Mining District. Throughout active production years (1869-1957), the Pioche Mining District produced over 6 million tons of ore valued at approximately $100 million. These production numbers include historic mining operations in the Bristol, Pioche, and Highland mountain ranges. Most production from the Pioche Mining District was from elongate lead-zinc-silver ore zones in the Lower Cambrian Combined Metals limestone member of the Pioche Shale. Additional production came from precious metal veins in the lowermost Cambrian Prospect Mountain quartzite (Hayes, L.D., 1971).

Ore was discovered in 1869 in the Pioche Hills south of present day Pioche. During the height of production in the 1870s, the district produced over $21 million in bullion, mostly from ore-bearing quartz veins in the Prospect Mountain quartzite. By the turn of the century, these rich ores had been depleted, and the direct smelting of oxidized Pb-Zn-Cu ore gave the district new life. The completion of Combined Metals Reduction Company’s flotation mill in Bauer, Utah in 1923 initiated the mining of mixed sulfide replacement orebodies in the Combined
Metals limestone bed. The Bauer mill, and the later one built at Caselton, were fed by ore from the Caselton, Prince, and Ely Valley mines until 1957, by which time the minable reserves of all three mines had been depleted. In 1964, the Caselton mill was reopened to process ore from the Pan American Mine in the Highland Range, 16 miles to the west. Commercial production of ore from the Pioche mining district ceased in 1968, when the Pan American Mine was closed as a result of litigation (Hayes, L.D., 1971).

After 1976, the ownership of the tailings changed hands numerous times, and various levels of tailings reprocessing occurred. The Caselton site was acquired by the Kerr McGee Corporation (KMC). In 2005, KMC sold off its’ chemical processing division by IPO as Tronox. On January 12, 2009, Tronox filed for bankruptcy by filing voluntary petitions for relief under Chapter 11 of the U.S. Code in the U.S. Bankruptcy Court for the Southern District of New York. On August 11, 2009, the U.S. Department of Justice filed proofs of claim on behalf of EPA to recover past and future environmental response costs relating to 18 named sites in seven EPA Regions. On February 14, 2011, a bankruptcy settlement and several trusts established thereby went into effect. The funds from the Tronox settlement related to the Caselton Tailings are managed by the Multistate Environmental Response Trust (OECA US EPA, 2016). The lead agency responsible for remedial action related to the Caselton Tailings is the Nevada Division of Environmental Protection (NDEP), and the Caselton Tailings are located on U.S. Bureau of Land Management (BLM) land.
Mine, Mill, and Related Structures and Features

Topographically up gradient of Caselton Wash are several features that are related to the industrial history of the site, including the Caselton Mine, Caselton Mill and Caselton Mill tailings to the north, and Caselton Heights to the east. The mine, mill, and tailings represent potential sources for contaminant migration, and Caselton Heights represents one potential receptor for said contaminants (Dynamac Corporation, 2010).

Caselton Wash

There are ten earthen dams associated with nine separate tailings impoundments in Caselton Wash, with the most up-gradient pond being Pond 1 and the farthest down-gradient pond being Pond 9. The tenth dam (for 9 impoundments) is located within Pond 6 as a partial dam (Figure 21). The dams are hypothesized to be constructed of soils sourced near Caselton Wash (Dynamac Corporation, 2010).

Caselton Wash is a major drainage feature, and is incised approximately 70 feet into the Quaternary-aged alluvium and Tertiary Panaca Formation, a hydraulically deposited volcanic tuff (Westgate and Knopf, 1932). The condition of the tailings dams is discussed at length in Attachment A of the EECA for the Caselton Wash tailings impoundments (Dynamac Corporation, 2010). The surfaces of Ponds 1 through 4 are irregular and characterized by mounds and pits that are a result of ongoing mineral claims and unsuccessful small-scale reprocessing operations. During site investigations and visits in 2000, November, 2015, and August 2016, two pits, one in Pond 3 and one in Pond 4 contained water (Figure 24). Ponds 5 through 9, are topographically flat with well-defined dams.
Geology/Hydrology

Geology

Caselton is located within the Ely Range, a minor, geomorphically discordant mountain uplift about 14 miles long. The Ely Range strikes northwest toward a junction with the elongate Highland-Bristol chain, which has the northerly orographic trend more characteristic of the Great Basin. Within the Ely Range, Cambrian limestones, dolomites, shales and quartzite are hosts for lead, zinc, and silver ore deposits resulting from sulfide ore replacement of limestone layers within specific lithologic units (Merriam and Palmer, 1964).

Hydrothermal fluids associated with Tertiary-aged intrusions within the Pioche Shale brought resulted in sulfide ore replacement of limestone layers, producing highly mineralized bedded ore deposits (Vikre and Browne, 1999). The sulfide ore is the source of acid generating tailings in Ponds 1 through 4. Partial oxidation through natural weathering of manganosiderite produced manganese oxide ore in many locations. The manganese oxide dominated ore is the source of the carbonate/oxide tailings in Ponds 5 through 9 (Dynamac Corporation, 2010). The Caselton Wash tailings are located in a segment of Caselton Wash that crosses a moderately flat pediment of Quaternary alluvium along the southwestern flank of the Pioche Hills.

Surface Water Hydrology

The Caselton Wash tailings are emplaced within the Caselton Wash, a major drainage feature which is incised about 70 feet into a pediment of Quaternary alluvium. Down gradient of the tailings ponds, Caselton Wash widens as smaller drainages join Caselton Wash, increasing the size of the drainage basin. Caselton Wash is ephemeral for its entire length, and joins Meadow Valley Wash near the town of Panaca, NV. Meadow Valley Wash is intermittent to perennial where it flows through Meadow Valley, and is extensively diverted for irrigation (Dynamac Corporation, 2010)(Figure 25).
Most runoff into the Caselton tailings ponds originates west and northwest of the ponds from snowmelt or rainfall on the northeast side of the Highland Range. Approximately 12 square miles (31 square kilometers) of mountain watershed drains towards the tailings ponds in Caselton Wash and its tributaries at the northern end of the tailings ponds. Additional drainage can enter the tailings ponds from the northeast through three small channels draining the Caselton Heights community as well as a fourth drainage originating from the Price Mine/Camp area. The drainages originating from Caselton Heights and the Prince Mine/Camp area are each less than one square mile (2.6 square kilometers) in area.

**Hydrogeology**

The Caselton Tailings impoundment lies within the boundaries of the Great Basin Regional Aquifer (Harrill et al., 1988). The Great Basin Regional Aquifer System contains three principal hydrogeologic units: basin-fill deposits, carbonate rocks, and non-carbonate rocks. The basin-fill deposits are composed of unconsolidated silt, clay, gravel, and sand. The carbonate rocks are massive consolidated Paleozoic strata, while the non-carbonate rocks are largely volcanics. The volcanics consist mostly of tuffs and basalts of Tertiary age. Generally, the basin-fill aquifers overlie the volcanics, which overlie the Paleozoic carbonate aquifers. In some instances the volcanics are topographically higher, while the basin-fill aquifers are always located in the accommodation spaces between mountain ranges created by basin and range faulting.

Groundwater flow in deeper fractured carbonate-rock aquifers moves in response to regional topography and large scale recharge and discharge features. Groundwater within the basin-fill zones generally flows from mountain front recharge along the margin of valleys to the basin centers, where groundwater is internally drained by evaporative discharge, or drained by
underlying carbonate-rock aquifer systems. The basin-fill aquifer often reaches thicknesses of several thousand feet. Many basin-fill aquifers, especially when composed of gravel and sand deposits, are highly productive. Wells constructed in these aquifers are commonly used for agricultural, domestic, or municipal use. The carbonate-rock aquifer is highly fractured in many areas, and receives recharge in exposed high altitude areas with higher precipitation rates and lower evapotranspiration rates. Water from the carbonate aquifer feeds many of the large, perennial low-elevation springs present in the Great Basin, and in some cases can provide recharge to the overlying basin-fill aquifer (Dynamac Corporation, 2010). Volcanic rocks act as aquifers at a few key areas, including the Fallon, NV area, western Nevada, and the Nevada Test site. Basalt flows, lava flows, and welded tuffs generally act as aquifers, while ash-flow and air-fall tuffs generally have lower permeability (Harrill et al., 1988; Harrill and Prudic, 1998).

Although no recent water level data are available in the immediate vicinity of the Caselton Tailings, Westgate and Knopf, (1932) documented that the pre-mining water level was encountered in 1926 on the 1,200 foot level (5,146 ft. amsl) of the Combined Metals Mine, but later declined to the 1,400 foot level (4,946 ft. amsl). Subsequent mining and dewatering (through 1957) likely lowered the groundwater level further. With the cessation of mining and dewatering efforts in 1957, groundwater levels have likely recovered to between the 1957 low, and the pre-mining groundwater elevation encountered in 1926. With a ground elevation of approximately 5,800 feet (1770 m) on the Caselton Tailings, depth to groundwater would have a lower bound of 800 feet (244 m), unless perched groundwater zones exist between the Quaternary alluvium and the regional carbonate aquifers.
**Previous Work**

L.D. Hayes, (1971) prepared a report for Humble Oil & Refining Co. detailing the mining history, geology, climate, mineralization history, and mineral exploration in the Pioche Mining District. An Engineering Evaluation/Cost Analysis (EECA) was conducted by Dynamac Corporation and CALIBRE Systems, Inc. for the U.S. Army Corp of Engineers, Albuquerque District in 2010 (Dynamac Corporation, 2010). The EECA contains extensive background details for the Caselton Site such as location, weather, geology, hydrology, hydrogeology, soils, and ecosystem, among other items. The EECA also characterized the source, nature, and extent of contamination associated with the tailings material located within Caselton Wash. Also detailed in the EECA was a streamlined risk evaluation and series of removal alternatives. As part of the EECA, a series of HELP models for remedial alternatives was presented. Brown and Caldwell, (2015) prepared a Conceptual Site Model that outlined the various components of the broader site, including the mill, mine site, additional tailings ponds up gradient of Caselton Wash, and Caselton Wash tailings.

**Field and Laboratory Data Collection**

Field investigations at the Caselton site were conducted during November, 2015, and included in-situ, field saturated hydraulic conductivity testing, determination of tailings in-situ density, and collection of tailings samples for subsequent laboratory analysis. Laboratory investigations consisted of WRC development by several methods, as well as determination of field moisture content, bulk density, and saturated hydraulic conductivity. Field investigations were conducted on Ponds 3 and 7, with Pond 3 representative of the sulfide tailings ponds, and Pond 7 representative of the oxide tailings ponds. Synthetic Precipitation and Leaching Procedure and bio accessibility results in Dynamac Corporation, (2010) indicate that the acid generating sulfide tailings in Ponds 1-5, with a pH of ~3.3, are more likely to mobilize lead,
arsenic, and other metals in the environment than the manganese oxide dominated tailings (pH ~8) in Ponds 6-9. Although a significant amount of lead was mobilized from the oxide tailings under aggressive acid digestion, the conditions of the digestion are not representative of conditions that would be observed in the field. Accordingly, the oxide tailings were not characterized beyond field saturated hydraulic conductivity, while the further characterization of the sulfide tailings is outlined in the subsequent sections.

**Determination of In-situ tailings density**

Field density measurements were collected on Ponds (3 and 7). Density measurements were collected using the sand-cone and drive-cylinder methods for Pond 3 while only the sand-cone method was used for Pond 7 (Table 4). The oxide tailings at Pond 7 were well cemented and too hard for effectively driving cores, making the drive core method impractical.

**Sand-Cone Method**

To obtain in place soil densities using the sand cone method (Table 4), a test hole is hand excavated in the soil to be tested and all the material from the hole is saved in a container. The hole is filled with free flowing sand of a known, calibrated dry density, and the volume is determined. The in-place wet or total density of the soil is determined by dividing the wet mass of the removed material by the volume of the hole. The water content of the material from the hole is determined and the dry mass and the dry density of the in-place material are calculated using the wet mass of the soil, the water content, and the volume of the hole (*ASTM D1556/D1556M, 2015*).
Drive-Cylinder Method
In place tailings densities were obtained using the drive-cylinder method (Table 4). To obtain in place soil densities using the drive-cylinder method, a thin walled metal cylinder is driven into the soil. The metal cylinder containing soil is retrieved, and the ends of the cylinder are trimmed with a straight edge. The mass and water content of the soil is determined on-site or the sample is stored to prevent soil and water loss until such determinations can be made (ASTM D2937-10, 2010).

Measurement of Field Saturated Hydraulic Conductivity Data on Caselton Wash Tailings
Saturated hydraulic conductivity $K_s$ is a key parameter for determination of unsaturated flow, because models for $K_{\phi}$ are dependent on $K_s$. $K_s$ is a fundamental soil hydraulic property that describes how much fluid will a saturated porous medium can convey under a given hydraulic gradient. A variety of methods exist for determination of hydraulic conductivity in the field ($K_{fs}$) and in the laboratory ($K_s$) (Olson and Daniel, 1981). $K_{fs}$ is often the preferred parameter because a larger volume of soil is permeated, taking into account the effects of macrostructure and preserving in place soil structure better than laboratory tests, while laboratory methods often provide economy.

Early methods for determination of $K_{fs}$ involved measurement of ponded infiltration from a single ring infiltrometer, and assumed one-dimensional, vertical flow (Bouwer, 1986; Daniel, 1989). Single ring approaches overestimated $K_{fs}$ due to lateral divergence of flow from capillarity of unsaturated soil surrounding the infiltration area, and excess head gradients from water ponding in the ring. Subsequent attempts to correct for lateral divergence involved the addition of an outer ring to buffer the flow in the inner ring. Such attempts were successful with large dual-ring infiltrometers, while smaller dual-ring infiltrometers still overestimated infiltration rates (Swartzendruber and Olson, 1961a, 1961b). Reynolds and Elrick, (1990)
presented the two-ponding head approach for determining $K_{fs}$, macroscopic capillary length ($\alpha$),
and matric flux potential ($\psi_m$). The two-ponding head approach accounts for soil capillarity,
depth of ponding, ring radius, and depth of ring insertion, but is insensitive to depth of ponding
and soil hydraulic properties. As a consequence, the procedures for calculating $K_{fs}$ are based on
averaged shape factors for the ring and ponding at multiple levels in the ring. This approach
offers significant decreases in the time required to measure low conductivity soils, because large
ponding heads can be applied without adverse effect.

Measurements of $K_{fs}$ were collected on Ponds 3 and 7 using a Decagon Devices
DualHead Infiltrometer (Decagon Devices, Inc., 2016a)(Table 5). The Decagon Devices DualHead
Infiltrometer implements a modified version of the Reynolds and Elrick, (1990) method to
estimate $K_{fs}$ (Decagon Devices, Inc., 2016a).
Laboratory Analysis of Soil Samples
Density and Moisture Content Determination

Soil samples were excavated using a trowel or shovel, and placed in Ziploc® bags to prevent moisture loss. Samples were weighed, then dried for 24 hours at 105°C. Dried samples were re-weighed to determine moisture content on a mass basis in accordance with ASTM D2216, (2010):

\[
w = \frac{M_w}{M_s} \times 100
\]

\(w\) = water content, %
\(M_w\) = mass of water
\(M_s\) = mass of oven dry specimen

To determine dry bulk density and volumetric moisture content, soil samples were then calculated in accordance with ASTM D7263, (2009) (Table 4):

\[
\rho_m = \frac{M_t}{V} ; \rho_d = \frac{\rho_m}{1 + \frac{w}{100}}
\]

\(M_t\) = mass of moist/total soil specimen
\(V\) = volume of moist soil specimen
\(\rho_m\) = density of total (moist) soil specimen
\(\rho_d\) = dry density of soil
\(w\) = water content of soil specimen (in percent), to nearest four significant digits.
Saturated Hydraulic Conductivity Determination

Saturated hydraulic conductivity ($K_s$) was determined at various effective stresses (simulated depths) using a flexible wall permeameter (Figure 26, Table 5) and the falling head, rising tail method (*ASTM D5084*, 2010). Loose samples were re-packed to field dry density in the flexible wall permeameter. After placement in the flexible wall permeameter, samples were saturated, and hydraulic conductivity was determined at varying confining stress. For the falling head, rising tail method, $K_s$ is determined with the following equation:

$$K_s = \frac{a_{in} \cdot a_{out} \cdot L}{(a_{in} + a_{out}) \cdot A \cdot \Delta t \cdot \ln \left( \frac{\Delta h_1}{\Delta h_2} \right)}$$

Where:

- $a_{in}$ = cross-sectional area of the reservoir containing the influent/inflow liquid
- $a_{out}$ = cross-sectional area of the reservoir containing the effluent/outflow liquid
- $L$ = length of specimen
- $A$ = cross-sectional area of specimen
- $\Delta t$ = interval of time over which the flow occurs
- $\Delta h_1$ = head loss across the permeameter/specimen at $t_1$
- $\Delta h_2$ = head loss across the permeameter/specimen at $t_2$

Saturated hydraulic conductivity varied over two orders of magnitude, from $1 \times 10^{-4}$ to $1 \times 10^{-6}$ cm/s (Table 5). Although available literature shows smaller variations in $K_s$ with stress (Aubertin et al., 1996), tailings vary widely in terms of composition, material properties, and consolidation behavior. Further testing is required to constrain tailings properties with variation in burial depth, composition, and location.
Development of Water Retention Curves

The Water Retention Curve (WRC) describes the relationship between volumetric moisture content (Θ) and ψ, while $K_\psi$ (or, alternatively $K_\Theta$) describe changes in hydraulic conductivity changes with ψ (or Θ). Multiple formulations for the $K_\psi$ and WRC functions are available in the literature (Brooks and Corey, 1964; Van Genuchten, 1980). The $K_\psi$ function is developed around the WRC function. For example, the van Genuchten-Mualem $K_\psi$ function utilizes parameters and conceptual underpinnings from the van Genuchten WRC and the statistical pore-size distribution model of Mualem, (1976). Here, a combined set of equations describing the water retention and $K_\psi$ properties of a granular matrix will be referred to as a hydraulic property model. The hydraulic property models used in this thesis are defined as follows:
Van Genuchten-Mualem Model:

\[ \theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[ \frac{1}{1 + (\alpha \psi)^n} \right]^m, \psi < 0 \]

\[ \theta = \theta_s, \psi \geq 0 \]

\[ K_\theta = K_S \theta^l \left[ 1 - \left( 1 - \theta^{1/m} \right) \right]^2, \psi < 0 \]

\[ K_\theta = K_S, \psi \geq 0 \]

\[ m = 1 - \frac{1}{n} \]

Where:

\( \Theta \) = head dependent volumetric moisture content

\( \Theta_r \) = residual moisture content

\( \Theta_s \) = saturated moisture content = porosity = \( \phi \)

\( \alpha \) (1/L) = term related to air entry pressure

\( n \) = pore size distribution index

\( \psi \) = suction of water within the porous medium

\( l \) = pore interaction term, often assume to be 0.5

Brooks and Corey-Mualem Model:

\[ \theta = \left( \frac{h}{h_b} \right)^{-\lambda}, \text{for } h \geq h_b \]

\[ \theta = \theta_s, \psi < h_b \]

\[ K_\theta = K_S \left( \theta \right)^{l+2+\left( \frac{2}{\lambda} \right)}, \text{for } h \geq h_b \]

\[ K_\theta = K_S, \psi < h_b \]

Where:

\( h \) = suction of water within the porous medium

\( h_b \) = bubbling pressure (or air entry pressure)

\( \lambda \) = pore size distribution index
Because WRC parameters govern the $K_\psi$ and water storage properties for a granular matrix, variation in WRC parameters can produce large differences in modeling results. Accordingly, it is important to characterize the WRC as accurately as possible. WRCs for the tailings materials were developed using the hanging column method (0-80 kPa), the pressure plate method (0-1500 kPa) and the chilled mirror hygrometer method (500 kPa to 100 MPa) (Figure 27). Additionally, unsaturated hydraulic properties for tailings from Pond 3 and alluvial materials were generated with particle size distribution data from Dynamac Corporation, (2010) and the Rosetta Lite software package (Schaap, 2003).

**Sample Preparation**

All WRC test specimens were prepared by packing specimen rings with tailings material to field dry density. Since the specimens were sealed, field water content was preserved in the sample tailings. Tailings specimens were prepared for the hanging column and pressure plate methods by placing tailings material in retaining rings with filter paper and a slotted sample retainer on one end. Subsequently, samples were placed on a slotted surface such that the bottom of the specimen was in contact with degassed, deionized water and allowed to wet via capillary action. The water level was risen to just below the top of the retaining ring such that the sample became fully saturated. The hanging column and pressure plate methods involve the use of a porous plate that is in direct hydraulic connection (physically contacting the bottom of the specimen) with the sample during the duration of the test. The porous plate must have an air entry pressure that is greater than the highest matric suction to be applied during testing, in order to maintain hydraulic connection with the sample. Porous plates are prepared for testing by submersion in degassed, ionized water under vacuum until completely saturated with degassed water.
**Hanging Column Method**

The hanging column method induces flow from the sample by lowering pore water pressure while pore gas pressure remains at atmospheric pressure. This is accomplished using a system of hanging columns of water that can be raised or lowered in relation to the sample height to create a pressure differential between the sample and the hanging column. Pore water pressure is lowered in discrete steps, inducing outflow into horizontal volumetric outflow burettes. The outflow from the sample is allowed to continue until the specimen reaches equilibrium (i.e., outflow rate approaches zero) *(ASTM D6836, 2008)* (Figure 28).

**Pressure Plate Method**

The pressure plate method induces flow from the sample via the axis translation principle *(Vanapalli et al., 2008)* by increasing pore gas pressure while pore water pressure is kept at atmospheric pressure. Pore gas pressure is lowered in discrete steps, inducing outflow into a receptacle with known mass. The receptacle is periodically weighed to track the amount of outflow from the sample. The outflow from the sample is allowed to continue until the outflow rate approaches zero. At this point, the sample is considered to be in equilibrium with the applied pressure, and a new, higher pore gas pressure is applied *(ASTM D6836, 2008)* (Figure 29).
**Chilled Mirror Hygrometer Method**

In the chilled mirror hygrometer method, the activity of pore water is measured using a chilled mirror hygrometer, after which the total suction is computed using the Kelvin equation:

\[
\ln \left( \frac{p}{p_0} \right) = \frac{2\gamma V_m}{rRT},
\]

Where:

- \( P \) = actual vapor pressure
- \( P_0 \) = saturated vapor pressure
- \( \gamma \) = surface tension
- \( V_m \) = molar volume of the liquid (water)
- \( R \) = universal gas constant
- \( r \) = radius of the droplet
- \( T \) = temperature

The chilled mirror hygrometer method is typically only used for suctions greater than 1,000 kPa, which correspond to the portions of the WRC with lowest \( \Theta \). In this pressure range, osmotic suction is small compared to matric suction, so the total suction derived from the test is comparable to matric suction. Specimens are dried to the desired water content, and then placed inside a sealed sampling chamber. Water vapor in the pore space eventually comes into equilibrium with the water vapor in the air in the sample chamber. The top of the sample chamber consists of a chilled mirror, on which the water vapor can condense. An optical sensor in the sample chamber detects the amount of condensed water on the chilled mirror (Decagon Devices, Inc., 2016b) (Figure 30).
Grain Size Distribution Method

Unsaturated hydraulic properties were generated from particle size distributions from Pond 3 as well as alluvial sediments that were gathered as part of the EECA (Dynamac Corporation, 2010). Particle size distributions were used as inputs for the Rosetta Lite software package (Schaap, 2003). Rosetta predicts the hydraulic properties of a granular matrix based on grain size distributions, utilizing pedotransfer functions based on neural networks (Schaap and Bouten, 1996). While grain size distributions are much easier to experimentally determine than the hydraulically based methods, parameter estimations for hydraulic property models estimated with pedotransfer functions can vary widely from more rigorous methods. As an example, there are major differences between the $\Theta_s$, $\alpha$, and $n$ parameters for the tailings developed using rigorous laboratory methods, and the properties developed using the Rosetta–grain size distribution method (Figure 31, Table 6). However, the Rosetta–grain size distribution method did predict a $K_s$ close to the experimentally determined value at a simulated depth of 1.1 m (Table 5, Table 6).

Fitting of Data to Hydraulic Property Model

Equilibrium water content data from all tailings characterization methods were aggregated, and regressed to develop parameters for the hydraulic property models used in the simulations (Figure 32). For all models, a saturated water content (equal to porosity) of 0.53 was used. The calculation of saturated water content is based, in part, on an assumption of a specific gravity of 2.65 g/cm$^3$ for the tailings solids. However, recent work has shown that the specific gravity for the tailings solids may be as low as 2.4 g/cm$^3$, due to the high abundance of gypsum and other low density minerals in the tailings. Future determination of the tailings solids specific density will help to constrain the saturated water content of the tailings.
The van Genuchten hydraulic property model parameters show less sensitivity to constraint of saturated water content than the Brooks and Corey model. Unconstrained van Genuchten model fits to the experimental data resulted in saturated water content estimation of 0.52, while unconstrained Brooks and Corey model fits to experimental data resulted in saturated water content estimation of 0.49. Regression of a non-linear function with multiple fitting parameters is a non-unique process, so the choice of whether to fix one or more fitting parameters, with or without physical justification, will impact the estimates for the remaining parameters.
Predictive Simulations of Caselton Tailings

Predictive simulations of the Caselton Tailings impoundment were conducted to assess the likelihood of percolation of meteoric water through the tailings to the underlying alluvium. Simulations were conducted with a mechanistic model to accurately capture the dynamics of unsaturated flow at appropriate spatial and temporal scales. Hydrologic modeling was performed using HYRUS 2D/3D (Šimůnek et al., 2012) and HYDRUS 1D (Šimůnek et al., 2013). Models were parameterized for a base case model in both HYDRUS 2D/3D, which was then altered to evaluate the effects of various, common modeling decisions. The results of these models are presented as a sensitivity analysis. Although a true modeling sensitivity analysis would require a multi-trial approach such as Monte-Carlo simulations, the sensitivity analysis in this study addresses variation that arises from common modeling decisions that must be made by environmental practitioners when evaluating tailings as a hydrologic system.

Base Case Model

The base-case model consists of a simulation conducted in HYDRUS 2D/3D, with realistic channel geometry, small finite element mesh, daily boundary condition data, unit gradient lower boundary condition, and utilizes the van Genuchten-Mualem hydraulic property model (van Genuchten, 1980).

Model Dimensionality and Geometry

A variety of geometries were implemented to test the sensitivity of the model to using realistic vs simplified geometries, and to provide simulations that are consistent with the geometries used in previous simulations at the site. Realistic geometries for predictive simulations of the Caselton tailings impoundment were constructed from depth to the tailings – alluvium interface, compiled from boring logs of the tailings material gathered from Dynamac Corporation, (2010), and used in conjunction with land surface elevation data from the USGS.
National Elevation Dataset Digital Elevation Model (DEM) (“USGS National Elevation Dataset,” 2013) to create upper and lower bounding surfaces for the tailings. Both surfaces were interpolated with a Triangular Irregular Network (TIN) algorithm, after which their elevation was extracted along a 2-Dimensional profile across Pond 2 (Figure 33).

Simplified geometries, which consisted of 1D and 2D uniform depth domains, assumed an average tailings depth of 4.6 m and were consistent with previous site models. However, in order to provide water storage results that were consistent across varying geometry, the 1D and 2D uniform depth results were normalized to an approximated average depth of the 2D realistic channel geometry. In order to approximate the average depth of an irregular polygon, we can first begin by thinking about a rectangular polygon, and then extending that line of thought to an irregular polygon. A rectangular polygon can be thought of as a small buffer (with radius = r) around a line, with some small error arising from non-circular ends of the polygon.
Thus:

\[ 2r = h \]

\[ P = 2L + 2h \]

\[ A \approx h \times L \]

and \( w \) and \( L \) can be recovered as the roots of the quadratic equation:

\[ x^2 - \left( \frac{P}{2} \right) x + A, \]

yielding:

\[ h = \frac{P - \sqrt{P^2 - 16A}}{4} \]

Where:

\( P \) = perimeter length
\( A \) = cross sectional area of the realistic geometry cross section
\( w \) = average polygon width
\( h \) = average polygon height

Utilizing this procedure with perimeter length and cross-sectional area from the 2D realistic channel geometry yields an average depth of 4.9 m. For 2D simulations, the realistic channel geometry and 4.6 m uniform depth geometry were used, and the 2D fluxes were normalized to 1D fluxes by division with the widths of the upper and lower tailings surfaces for atmospheric and lower boundary fluxes, respectively.
Hydraulic Property Model

Sensitivity to hydraulic property model was examined by conducting simulations with variable hydraulic property models, including the van Genuchten, (1980) model, a version of the van Genuchten-Mualem model modified with a 2 cm air entry pressure described in Vogel et al., (2000), and the Brooks and Corey, (1964) model. The Brooks and Corey model predicts higher $K_\psi$ values and a higher air entry pressure, while the van Genuchten model predicts the lowest $K_\psi$ values, and has an air entry value of 0 cm. The van Genuchten model with a 2 cm air entry pressure retains the smooth shape of the retention curve from the van Genuchten model, and predicts $K_\psi$ values between the van Genuchten and Brooks and Corey models (Figure 32). Equations relating to the van Genuchten and Brooks and Corey hydraulic property models are presented in the previous sections, and illustrated in Figure 2 - Figure 5.

The hydraulic property models differ most in the air entry region of the WRC, with the standard van Genuchten model having an air entry pressure of 0 cm, and the Brooks and Corey model having the greatest (~10 cm for the tailings) (Figure 34). The models also differ slightly in the middle to dry portions of the WRC in the shape of exponentially declining water content with suction. Differences in air entry pressures, as well as shape fitting parameters for the hydraulic property models cause significant increases in $K(\Psi)$ throughout the saturation range. Importantly, the rate at which $K_\psi$ changes near saturation is much lower in the 2 cm van Genuchten model and the Brooks and Corey model (Figure 34). The lower rate of change allows for a more accurate and less iterative numerical solution of Richards equation, as well as improved modeling of water retention properties for materials with significant air entry pressures (Vogel et al., 2000).
Hydraulic Properties

To account for the uncertainty in tailings properties, simulations were conducted with a variety of material descriptions that could potentially describe the tailings material (Table 6, Figure 31). Materials in the hydraulic properties sensitivity group are described with a set of closed-form equations resembling those of van Genuchten, (1980) who used the statistical pore-size distribution model of Mualem, (1976) to obtain a predictive equation for the unsaturated hydraulic conductivity function. Materials used in the hydraulic properties sensitivity group include: a loam from Carsel and Parrish, (1988), tailings from Pond 3 and alluvial material developed with grain size distribution and the Rosetta Lite software package (Schaap, 2003), as well as tailings from Pond 3 developed from laboratory derived equilibrium water retention data. The laboratory derived tailings were described with a saturated hydraulic conductivity from the field saturated hydraulic conductivity testing, as well as hydraulic conductivity at a simulated depth of 1.1m (Table 6, Figure 31). These materials were chosen, because they all represent hydraulic properties and hydraulic property parameterization methods that a practitioner could feasibly use to parameterize a model of the Caselton Tailings impoundment. The hydraulic properties for the tailings in the HELP models (Dynamac Corporation, 2010) is also included in Figure 31 to illustrate the differences between the laboratory developed WRCs used in this study, and those used in the HELP simulations.

Finite Element Discretization

Several finite element mesh sizes were used in the various models implemented at the Caselton Tailings impoundment. Mesh sizes in the finite element discretization sensitivity group consisted of a large mesh (3.7 m global), a medium mesh (.6 m global with .2 m refinement at the atmospheric boundary), and a small mesh (.2 m global with 3.3 cm refinement at the atmospheric boundary) (Table 7). For the small and medium meshes, element size refinements were placed at the atmospheric boundary, where more elements are needed to accurately simulate the steep, non-linear hydraulic gradients commonly present (Figure 33, Figure 35). 1D models utilized 1D finite element discretization equal to the small grid for the 2D models. Additional mesh sizes were required for convergence in the hourly simulation, as well as the material boundary simulation (Table 7). For the hourly simulation, refinement was increased to 1.5 cm near the atmospheric boundary, while refinement was increased to 2 cm above and below the material boundary for the material boundary simulation.

Initial Conditions

Initial conditions for steady state models were specified in terms of pressure head. Conceptually, the initial conditions can be thought of as being in equilibrium with a water table located 10 m below the lowest located element in the model. Numerically, the lowest element in the model was set to a value of -10 m, with a linearly decreasing pressure head gradient projected to the atmospheric boundary. Steady state models were executed with repeated intervals of the 15.4 years of on-site climate data (August, 1999 to January, 2015) until steady state drainage rates were achieved (Figure 36, Figure 37). After the models reached steady state conditions, final head distributions from the steady state models were used as initial conditions for transient models. Transient models were executed one time on the 15.4 year record of input data.
Boundary Conditions

Upper Boundary Conditions

Upper boundaries in all simulations were modeled with an atmospheric boundary condition. Inputs for the atmospheric boundary conditions consist of hourly records of precipitation and potential evaporation. Because vegetation is sparse to non-existent on the surface of the tailings material, transpiration is assumed to be negligible. Potential evaporation is calculated using the Penman equation for evaporation from an open water source (Penman, 1948):

\[
E_{\text{PEN}} = \frac{\Delta}{\Delta + \gamma} \times \frac{Rn - G}{\lambda} + \frac{\gamma}{\Delta + \gamma} \times \frac{C(f_u)D}{\lambda}
\]

Where:

- \(E_{\text{PEN}}\) = potential open water evaporation (mm/hr)
- \(\Delta\) = slope of the saturation vapor pressure curve (Pa/°K)
- \(\lambda\) = latent heat of vaporization of water (J/kg)
- \(\gamma\) = psychometric coefficient (Pa/°K)
- \(Rn\) = net radiation at the surface (J/m\(^2\)/hr)
- \(G\) = soil heat flux(J/m\(^2\)/hr)
- \(C\) = constant of proportionality (J/m\(^2\)/hr/Pa)
- \(D = (e_s - e_a)\) is vapor pressure deficit (Pa)
- \(f_u\) = wind function(m/s * Pa),

\[
f_u = a_u + b_u u
\]

Where \(a_u\) and \(b_u\) are wind function coefficients and \(u\) is wind speed at 2 m above ground surface. The original penman equation coefficients of \(a_u = 1\) and \(b_u = .536\) are assumed.

15.4 years of hourly observations of air temperature, relative humidity, and wind speed from August, 1999 to January, 2015 were obtained from a meteorological station located in the nearby town of Pioche, NV, managed by the Community Environmental Monitoring Program (“CEMP,” 2016). Incoming extraterrestrial shortwave radiation was calculated on an hourly
basis for the site using solar geometry and site location information (Allen et al., 1998). Ground level incoming short wave radiation values were obtained from the National Renewable Energy Laboratory (NREL) National Solar Radiation Database (NSRDB) as Global Horizontal Irradiance (GHI) (“NSRDB,” 2016). GHI from the NSRDB is a modeled product, and represents the total amount of shortwave radiation received from above by a surface horizontal to the ground. GHI includes Direct Normal Irradiance (DNI) and Diffuse Horizontal Irradiance (DIF) (“NSRDB,” 2016).

Input data were aggregated and temporally aligned, after which penman open water potential evaporation was calculated utilizing the Meteorology and Evaporation Function Modules for Python (Waterloo, 2012)(Figure 38). The routine was modified with a stefan-boltzman constant for hourly time steps, and an additional loop for calculating evaporation during nighttime hours based on an estimated soil heat flux (G) (Allen et al., 1998):
\[ G_{\text{day}} = .1 \times R_{\text{net}}; \quad G_{\text{night}} = .5 \times R_{\text{net}} \]

Net radiation was estimated as:

\[ R_{\text{net}} = R_{\text{net,shortwave}} - R_{\text{net,longwave}} \]

\[ R_{\text{net,longwave}} = f \varepsilon \sigma (T_{\text{air}^{\circ C}} + 273.15)^4 \]

\[ R_{\text{net,shortwave}} = R_s (1 - \alpha) \]

\[ f = \left(1.35 \times \frac{R_s}{R_{s0}}\right) - .35 \]

\[ R_{s0} = (0.75 + 2 \times 10^{-5} \times Z) \times R_{\text{ext}} \]

Where:

- \( R_{\text{net}} \) = net radiation = incoming radiation – outgoing radiation
- \( f \) = a cloud factor calculated from the ratio of top of ground level shortwave radiation ground level clear sky radiation (Allen et al., 1998)
- \( \varepsilon \) = emissivity of the air
- \( \sigma \) = Stefan-Boltzmann constant
- \( R_s \) = incoming shortwave radiation at ground level (GHI)
- \( \alpha \) = albedo
- \( R_{s0} \) = clear sky radiation
- \( R_{\text{ext}} \) = top of atmosphere extraterrestrial radiation
- \( Z \) = elevation in meters

The atmospheric boundary condition in HYDRUS 1D and 2D allows evaporation to occur at up to the potential rate when the head at the surface node is between 0 and a user-specified maximum suction value designated \( h_A \). If the specified flux from the atmospheric boundary condition causes suction to reach \( h_A \), the boundary condition changes from a specified flux boundary condition to a constant head boundary condition, and evaporation is controlled by the rate at which water can be transmitted to the upper boundary.
Generally, \( h_A \) is selected such that the corresponding water content is at least 0.005 higher than the residual water content. Selection of this parameter is especially important especially for coarse-textured soils (sands), which have a very steep retention curve. Small changes in water contents in the dry range lead to large changes in the pressure heads, which can make the numerical solution unstable (Šimůnek et al., 2012). Additionally, the effect of including suctions at the atmospheric boundary greater than 100 m is usually negligible, as predicted \( K_\psi \) in this pressure range is effectively zero for many soils, which limits fluxes to near zero. Ebrahimi et al., (2004) suggest a lower limit of \( 10^{-12} \) cm/s for \( K_\psi \). Evaporation in the HELP model is governed by an analytical model with early and late stage rates patterned after Ritchie, (1972).

For models presented here, the \( h_A \) was set to 100 m suction. Suctions at the atmospheric boundary can be calculated from relative humidity and temperature:

\[
H_r = e^{\left( \frac{h_A Mg}{RT} \right)}
\]

Where:

\( H_r \) = relative humidity
\( M \) = Molecular weight of water
\( g \) = gravitational constant
\( R \) = universal gas constant
\( T \) = temperature
\( h_A \) = minimum pressure head allowed at the atmospheric boundary

Although calculated suctions commonly exceed 100 m by orders of magnitude, numerical instabilities due to extremely sharp head gradients near the atmospheric boundary can result if those values are implemented in the model.
Lower Boundary Conditions
Lower boundary conditions were simulated with either a unit gradient boundary condition, a seepage face boundary condition, or a material interface intended to simulate the interface of the tailings material with the native alluvium material (Table 7).

Unit Gradient Boundary Condition
A unit gradient boundary condition simulates a scenario where matric gradients are not present, or small enough that their effect on the total head distribution is negligible. In this case, elevation gradients are the only contributor to the total hydraulic gradient. Although no suction measurements near the tailings/alluvium interface exist at this time, observational studies at similar locations suggest that a unit hydraulic gradient may exist as near as 20 cm to the surface (McCord, 1991; McCord et al., 1991; Sisson, 1987). However, the hydraulic gradient is likely to deviate from unit gradient conditions at the tailings/alluvium interface.

Material Interface
The lower boundary condition can be simulated explicitly by including a layer of material bounding the lower surface of the tailings material with material properties corresponding to the native alluvium present at the site. Grain size distribution and bulk density from a surface sample near Pond 4, presented in (Dynamac Corporation, 2010), was used to generate the parameters for the van Genuchten – Mualem hydraulic property model using Rosetta Lite. The sample was 41.6 percent sand, 45.8 percent silt, and 12.6 percent clay by mass, with a bulk density of 1.6 g/cm³ (Table 6). The lower boundary condition for the alluvium was set to be a constant head value of 0 m (saturated) at 245 m below ground surface.
Seepage Face Boundary Condition

Seepage face boundary conditions simulate a scenario where the porous media is exposed to the atmosphere, with fluid seeping from the porous media. Fluid is allowed to flow across the boundary when total head is greater than 0 (or another user-defined value, if appropriate). Pressure buildup continues until some amount of water leaves the domain, which reduces the pressure head. Pressure head must again accumulate due to redistribution of fluid or additional fluid flux into the domain before more fluid can pass through the seepage face boundary. Scanlon et al., (2002) showed that seepage face boundary conditions can be approximated by placing a coarsely textured material next to a fine grained material for codes that do not explicitly simulate this boundary condition. The material interface between the fine grained tailings and the relatively coarse grained alluvium may behave as a seepage face boundary in this fashion.
Results/Discussion of Caselton Models

Results of Caselton models are presented for the “base case” model in terms of transient results over the 15.4 year simulation period, and steady state drainage rates from the steady state base case model. The base-case consists of a HYDRUS 2D flow model, constructed with the small finite element mesh (.2 m with 3.3 cm refinement at the atmospheric boundary), daily atmospheric data, van Genuchten parameters based on laboratory retention data and field-saturated hydraulic conductivity, and free drainage lower boundary condition (Table 7). Remaining simulations are discussed in terms of sensitivity to model parameters (Table 7, Figure 39).

The hydraulic properties and lower boundary condition sensitivity groups were conducted in HYDRUS 1D, while the hydraulic property model, finite element discretization, geometry, and temporal data resolution sensitivity groups were conducted in HYDRUS 2D (Table 7, Figure 35). In order to control for the effect of dimensionality on the sensitivity analysis, a HYDRUS 1D model equivalent to the HYDRUS 2D base case model in all aspects except for dimensionality was also constructed. Relative differences between 2D models (Table 7) are discussed in terms of their relative difference to the 2D base case model, while differences for 1D models are compared to the 1D base case.

Base Case Results

Figure 40 details increases in water storage and cumulative drainage for the base case that are driven by extended winter precipitation events where precipitation rates are greater than evaporation rates (Figure 40). Specifically, where precipitation rates are greater than evaporation rates, infiltration occurs (Figure 41). Conversely, when evaporation rates are greater than precipitation rates, water leaves the tailings via evaporative flux (Figure 40). Net
evaporative conditions are present for the majority of time under the climatic conditions at the Caselton Tailings impoundment at all temporal resolutions (Figure 41). Flux rate across the upper boundary is not always equal to the difference between precipitation and evaporation rates. The controls on the rates of infiltration or evaporation are total head gradients, and head dependent hydraulic conductivity $K(\psi)$. For infiltration, $K(\psi)$ increases in the direction of the total gradient as pore spaces in front of the infiltration front are filled with water. For evaporation, $K(\psi)$ decreases in the direction of total gradient. Consequently, even in the presence of large upward gradients near the atmospheric boundary, $K(\psi)$ is limited to a degree that evaporative flux rates are low over long period of time. This behavior is shown in the model results in Figure 40 and has been demonstrated in the literature (Shah et al., 2007). Evaporation rates increase quickly after an infiltration event, and decay to near zero soon afterward as the tailings surface dries.

Infiltration events occur at or near the rate of applied precipitation in most cases. Two significant infiltration events (~.2 m) occur during the 15.4 year simulation period; one from September 2004 – May 2005, and one from December 2010 – April 2011 (Figure 40). Both of the infiltration events occurred during extended periods of low potential evaporation, and sustained precipitation. Water from infiltration events is partitioned mostly to water storage, after which the infiltrated water is lost to evaporative flux and drainage over a longer time period (Figure 40). For the base case model, and in all models, insignificant amounts of runoff were predicted. The 2D base case model produced .15 m of cumulative drainage over the 15.4 year simulations period, -.15 m of cumulative atmospheric flux, and an average water storage of ~1.35 m (Figure 40). The steady state drainage rate for the 2D base case simulation was 9.5
mm/yr., or about 4% of average annual precipitation over the 15.4 year simulation period (.23 m) (Table 7).

Compared to percolation rates observed in the Alternative Landfill Cover Demonstration (ALCD), the percolation rates at the Caselton Tailings impoundment are significant (US EPA, 2011). The ALCD reported precipitation and percolation rates for 3 evapotranspirative covers and 3 resistive barrier covers constructed on a landfill in Albuquerque, New Mexico. Percolation rates in the ALCD for RCRA Subtitle D covers ranged from 3.56 mm/yr. two years after construction to .74 mm/yr. 7 years after construction, while evapotranspirative covers ranged from 0.54 mm/yr. one year after to 0 mm/yr. 6 years after construction. A significant difference between the Caselton Tailings impoundment and the ACLD, is that the evapotranspirative covers in the ALCD were vegetated. Increased evapotranspiration from the vegetation caused percolation rates to decrease to 0 for all covers but the subtitle D cover within 4 years, while the lack of vegetation on the Caselton Tailings is likely contributing to ongoing percolation through the tailings. The predicted 2D base case percolation rates (9.5 mm/yr.) at the Caselton Tailings impoundment are greater than the RCRA subtitle D percolation rates by a factor of 3 - 13, and greater than the evapotranspirative by at least a factor of 17 (calculated at one year after construction of the ACLD evapotranspirative covers).
Sensitivity Analysis

Sensitivity to Hydraulic Property Model

Sensitivity to hydraulic property model was tested using the van Genuchten–Mualem model (Mualem, 1976; van Genuchten, 1980) in the base case simulation, the van Genuchten–Mualem model with an air entry value of 2 cm, and the Brooks and Corey, (1964) model. Evaporative flux (seen in Figure 42 as positive cumulative atmospheric flux) was greatest with Brooks and Corey model, and lowest with the standard van Genuchten model. Differences in evaporative flux are due primarily to higher predicted $K(\psi)$ at high suction in the Brooks and Corey and 2 cm van Genuchten-Mualem models relative to the van Genuchten model (Figure 32, Figure 34). Infiltration events behaved largely similarly, as infiltration is not a $K(\psi)$ limited process in most cases (Figure 43). Due to decreased evaporative flux relative to the other models, drainage was greatest with the standard van Genuchten model. Conversely, increased evaporative fluxes in the Brooks and Corey and 2 cm van Genuchten models decreased the amount of water available for drainage from the lower boundary. Results for varying hydraulic property model compared to the 2D base case simulation resulted in differences of -.08 m, .11 m and -.2 m in terms of cumulative drainage, cumulative atmospheric flux, and average water storage over the 15.4 year simulation period (Figure 42). Use of varying hydraulic property model affected steady state drainage rates by as much as .006 m/yr. or a 59.7% decrease with respect to the 2D base case simulation (Table 7, Figure 42).

Sensitivity to Hydraulic Properties

Sensitivity to van Genuchten parameters and hydraulic conductivity was tested using a variety of parameterization methods. Parameters were developed from: a cataloged loam soil (Carsel and Parrish, 1988), fitting of laboratory developed WRC data for tailings from Pond 3 using ASTM D6836 with field saturated (base case) and laboratory-measured saturated hydraulic
conductivity, and parameters generated using grain size distribution from Pond 3 and Rosetta Lite (Schaap, 2003) (Table 6).

Differences in cumulative atmospheric flux between material types drive the observed differences in cumulative drainage. Cumulative fluxes are closely tied to the flux limiting effect of \( K(\psi) \) during evaporative periods. During evaporative periods, the upper boundary condition is limited to 100 m suction (10^4 cm), for numerical solution considerations. Because precipitation events are fleeting and observed atmospheric suction are commonly higher than 100 m, a 100 m suction constant head boundary is the most persistent upper boundary condition. At 10^4 cm suction, \( K(\psi) \) for the Loam and \( K_s \) based tailings are 2-3 orders of magnitude below those for the \( K_{ts} \) based tailings and Rosetta tailings (Figure 31). Although \( K(\psi) \) also differ between the materials at saturation (Figure 31), \( K(\psi) \) is not a limiting factor for infiltration events, because \( K_s \) is generally greater than the precipitation rate.

The effect of the differences in hydraulic properties is that the \( K_{ts} \) based tailings and Rosetta tailings producing more drainage, while drainage is limited by increased upward evaporative flux during extended evaporation periods for the Loam and \( K_s \) based tailings (Figure 44). The change in storage was related both to the storage capacity of the tailings (Figure 31), and differences in cumulative drainage and atmospheric flux from the \( K(\psi) \) effects discussed above (Figure 44). Mass balance error was insensitive to material properties at the spatial and temporal discretization used. Results for varying hydraulic properties compared to the 1D base case simulation resulted differences of -.6 -.23 m, -.2 -.06 m and -.65 -.4 m in terms of cumulative drainage, cumulative atmospheric flux, and average water storage over the 15.4 year simulation period (Figure 44). Differences in material properties affected steady state drainage
rates by as much as .017 m/yr., or 128.6% increase with respect to the 1D base case simulation (Table 7, Figure 39).

**Sensitivity to Finite Element Discretization**

Sensitivity to finite element mesh sizing was tested using large element meshes consisting of ~3.7 m uniform sized elements, medium element meshes consisting of .6 m elements with a .2 m refinement along the surface of the tailings, and small element meshes consisting of .2 m meshes with .033 m (3.3 cm) refinement along the surface of the tailings (Figure 33, Figure 35). 1D models were parameterized with a node discretization equivalent to the small mesh. Relative to the base case (small mesh), model results for the larger mesh sizes showed higher evaporation rates, higher mass balance errors, lower water storage, and less percolation. Although infiltration behavior was similar for all element sizes, evaporation varied by a factor of 10 between the small, large and medium element mesh sizes (Figure 45).

The difference between the simulations is related to the ability of linear finite elements to accurately simulate steep, non-linear head gradients near the surface during late stage evaporation (Hayhoe, 1978) (Figure 35). Evaporation and infiltration events occur on length scales of 1-3 cm (Lehmann et al., 2008; White and Sully, 1987), and linear interpolation of non-linear head gradients with large elements allows high suctions present at the surface to extend further into the subsurface than observational studies suggest is reasonable (McCord, 1991; McCord et al., 1991; Sisson, 1987). The effect is similar to that of a rooting zone, and leads to conveyance of water to the surface. Infiltration events are less affected because they occur over shorter time scales and produce head gradients with a more linear character than those present during evaporation dominated periods. Differences in water storage are related to the
differences in atmospheric fluxes rather than the ability to simulate water storage with varying element sizes.

Results for varying finite element discretization period compared to the 2D base case simulation resulted in differences of -.15 m, .27 m and -.5 m in terms of cumulative drainage, cumulative atmospheric flux, and average water storage over the 15.4 year simulation (Figure 45). Differences in finite element discretization affected steady state drainage rates by as much as .0094 m/yr., or 98.7% decrease with respect to the 2D base case simulation (Table 7, Figure 39).

**Sensitivity to Temporal Data Resolution**

Sensitivity to temporal data resolution was tested with hourly, daily (base case), monthly, and yearly climate data. For each simulation, maximum time steps were set the temporal resolution of input data (e.g. one day for daily input data). For increasing temporal resolution (smaller time periods) infiltration increased, which resulted in increased drainage (Figure 46). Infiltration events occur when the precipitation rate is greater than the evaporation rate and a downward gradient is present. Accordingly, the time interval over which the rates are averaged can have large impacts on the behavior at the upper boundary. As temporal resolution decreases (larger time periods), the number of instances where precipitation rate exceeds the evaporation rate decreases, culminating with yearly rates always being net evaporative (Figure 41). Results for varying temporal data resolution compared to the 2D base case simulation resulted in differences of -.14 -.07 m, -.14 -.16 m and -.2 -.04 m in terms of cumulative drainage, cumulative atmospheric flux, and average water storage over the 15.4 year simulation period (Figure 46). The hourly steady state drainage rate was greater than the base case drainage rate by .005 m/yr, or a 54.1% increase, while the monthly model was less than the
base case rate by .009 m/yr, an 89.5% decrease (Table 7, Figure 39). The yearly simulation drainage rates exhibit an exponential decline, and will eventually decline to zero as a result of perpetual evaporative conditions with no precipitation at the atmospheric boundary (Figure 37, Figure 41).

Although the results of the temporal resolution sensitivity group clearly show that finer temporal resolution of input data significantly impacts drainage results, multiple considerations factor into the feasibility of a modeling project. For instance, computation time was significantly increased for the hourly simulation in comparison to the 2D base case (daily) simulations. The hourly simulations required a smaller finite element mesh (.2 m global with 1.3 cm refinement at the atmospheric boundary) in order to achieve convergence, which, along with the requirement of hourly time steps, significantly increased computation time for that simulation. The computational time for the hourly steady state model was 11.6 days, while it was only .8 days for the base case (daily) model. Additionally, cumulative mass balance error for the hourly simulation was quite high at 10.3%, compared to .19% for the daily model (Table 7).

Because model construction and calibration is a highly iterative process, long simulation times can inhibit progress severely. However, there are several ways to improve the rate of progress while retaining model accuracy. For example, choosing an alternative hydraulic property model such as the van Genuchten – Mualem with 2 cm air entry pressure or the Brooks and Corey model may mitigate some of the computation expenses of the hourly simulation. Another approach is to construct initial models with more coarse temporal and spatial resolution, and then increase the resolution toward the end of the modeling process. Finally, initial models can be constructed in 1D, and then extended to 2D models to answer questions related to more complex geometries.
**Sensitivity to Lower Boundary Condition**

Sensitivity to selection of lower boundary condition was evaluated with free drainage, seepage face, and material interface boundary conditions. Out of all sensitivity groups, atmospheric boundary and cumulative drainage fluxes were most sensitive to lower boundary condition (Figure 39). Cumulative drainage totals for the transient models in the lower boundary condition sensitivity group were highest for the material boundary lower boundary, and lowest for the seepage face lower boundary (Figure 47). High drainage and low water storage develop in the material boundary simulation due to development of equilibrium conditions with the 245 m column of alluvium. Equilibrium suction at the lower boundary of the tailings for the material interface lower boundary model are ~15.4 m, while they are ~3 m in the free drainage model. The higher suctions in the material boundary model are transmitted upwards into the tailings, resulting in water storage ~.1 m lower relative to the 1D base case (free drainage). Water storage in the seepage face model is higher than the 1D base case by ~.2 m because positive pore pressure must develop at the lower boundary before water can drain.

Varying lower boundary condition compared to the 1D base case simulation resulted in differences in cumulative drainage of up to .64 m for the material boundary over the 15.4 year simulation period of the transient model. Varying choice of lower boundary condition affected steady state drainage rates by as much as .039 m/yr., or 315% decrease with respect to the 1D base case simulation (Table 7, Figure 39).

**Sensitivity to Model Dimensionality and Geometry**

Sensitivity to model dimensionality and geometry was tested with HYDRUS 1D and 2D simulations of varying geometry. HYDRUS 2D simulations were conducted with both realistic channel geometry and a rectangular idealized cross section. The depth of the rectangular simulation was equal to the 1D simulation (4.6 m) with width equal to the approximate upper
width of the channel geometry (114 m). Atmospheric and lower boundary fluxes were normalized to 1D fluxes by division with boundary widths for the upper and lower tailings surfaces, respectively. The 2D models were equivalent in terms of cumulative drainage, cumulative atmospheric flux, and water storage, suggesting that differences in 2D geometry may not cause significant changes in results if fluxes are normalized to achieve direct comparison (Figure 48). The 1D model produced more infiltration and drainage (Figure 48) than the 2D models, due to decreased evaporation rates over time (Figure 49) suggesting that dimensionality has a measurable effect on results. Cumulative drainage in the 1D model was .18 m (Figure 48), compared to approximately .15 m in the 2D models, a difference of .03 m. Atmospheric fluxes were within .1 m between the 1D and 2D models. Storage increases appeared to be greater subsequent to large infiltration events in the 1D model, although differences in storage between 1D and 2D models diminished between large infiltration events. 1D steady state drainage were greater than the 2D base case rates by .004 m/yr., or 39.4% increase with respect to the base case simulation (Table 7, Figure 39).

Comparison of Mechanistic Models to HELP Models in EECA

The discussion in the preceding sections focuses on the transient differences between various mechanistic models, in order to determine if model predictions are consistent with expected physical reality. These simulations also investigate the sensitivity of transient responses to various uncertain model inputs and assumptions. For long term management, an important modeling outcome for assessing potential impacts to groundwater resources is steady state drainage rate.

Steady state drainage rates from the HELP model (Dynamac Corporation, 2010) were less than the 2D base case model by .006 m/yr., a 66.5% decrease (Table 7, Figure 39). The relative
agreement of the HELP model is surprising, considering the significant differences in hydraulic properties between the HELP simulation and laboratory derived properties (Table 6, Figure 31), the simplification of governing processes in the HELP model (e.g. no simulation of matric gradients), and the use of monthly data from a climate generator. However, due to the non-unique nature of unsaturated hydrologic models, many different combinations of model parameters can arrive at similar solutions. The non-unique nature of unsaturated hydrologic models implicates the need for experimental validation of as many physically based model parameters as possible, and the verification that parameters related to the numerical solution (e.g. element sizing) are chosen appropriately. The main differences in the hydraulic definition used in the HELP model are a lower $K_s$, and higher $n$ parameter, which indicates a broader grain size distribution. The effect is that $K_s$ forces $K(\Psi)$ lower at low suctions, and $K(\Psi)$ decreases more slowly at higher suctions due to increased water retention. Additionally, average climate data does not incorporate climate variability such as the extended precipitation seen in the winters of 2005 and 2011.

In summary, simplified models such as HELP can be useful to capture the average behavior of the system, but are not adequate if more detailed information such as fate and transport analysis is required. This is because the mechanistic models can simulate the dynamic transport characteristics of the tailings which are dependent on governing factors beyond percolation rate.

**Comparison of Model Results to Field Observations**

During an investigation in 2000, and during the November, 2015 site visit, two excavated pits, one in Pond 3 and one in Pond 4 contained appreciable amounts of standing water (Figure 24). During a site visit in August, 2016, the pits contained substantially less water
than during the November, 2015 site visit. However, the only modeling scenario at the Caselton Tailings impoundment that predicted fully saturated tailings material, was the seepage face model, which must produce saturated media at the lower boundary by definition.

The presence of ponded water in the pits presents an opportunity to analyze model results in the context of field observations. There are a few possible explanations for the ponded water. First, the ponded water could be a reflection of the phreatic surface within the tailings, implying that the lower depths of the tailings are saturated (Figure 50) and the models have incorrectly captured water balance on the tailings. This scenario can be developed further by analyzing the tailings along a longitudinal cross section, where the elevation of ponded water within the upstream tailings impoundment contributes to a hydraulic gradient that induces flow through to downstream tailings ponds (Figure 50). Second, the ponded water in the pits could be a result of run-on from the surrounding tailings and alluvial pediment, and the transiently ponded water could be infiltrating into the tailings and evaporating to the atmosphere at variable rates throughout the year. Third, the ponded water could arise from a combination of scenarios 1 and 2, with the phreatic surface near the lower portions of the pits. The upper pit shows evidence of significant run-on, presenting significant channelization of the tailings in the area surrounding the upper pit. While the lower pit shows less channelization, some run-on combined with flow through from the upper pit could be contributing to the ponded water in the lower pit.

Positive determination of which scenario is occurring in the field using only predictive models for hypothesis testing is unlikely. However, several models utilizing the van Genuchten, (1980) hydraulic property model predict pore pressures greater than field capacity (-33 kPa or -337 cm water), which could induce seepage to the pits (Figure 52). Increased evaporation in the
alternative hydraulic property models result in pore pressures less than field capacity (-3.37m). Should future data collection indicate model inaccuracy, disagreement with field data could be due to any combination of incorrect assumptions pertaining to material homogeneity, boundary conditions, or occlusion of processes not adequately captured by field data or modeling implementation (e.g. inclusion of osmotic potential could lead to a reduction in simulated evaporation, or hysteresis effects). In order to determine which conditions are occurring in the field, additional data collection is warranted. Tensiometers or water content sensors installed at depth in the tailings, proximal and distal to the ponded water could help to confirm or reject the hypothesis that the tailings are saturated at depth.
Summary, Conclusions, and Recommendations

Six computer codes that are currently in use for simulation of water balance processes were compared in a series of simple hypothetical column experiments to compare the degree of similarity between code outputs for a simple and identical model setup. The simulations presented in this Chapter 1 are identical in terms of geometry, initial conditions and boundary conditions between codes. It follows that the slight differences between solutions for each code are due to differences in how the Richards equation is implemented in each code. The HELP model does not solve Richards equation, and so the results for that model differ more than the Richards equation based codes do from each other. The main difference between HELP and the remaining simulations is that the HELP model does not simulate matric gradients, which allows drainage to occur sooner than the other models, which initially partition more water to storage. For the Chapter 1 simulations, matric gradients do not play a large role once the soil columns are wetted to field capacity. However, steep upward matric gradients near the soil surface are present in many arid and semiarid climates. Upward matric gradients can have a large impact on water balance, and ignoring them is inappropriate for most semiarid to arid climates. Matric gradients are also common near material interface boundaries, and can alter the water balance of natural or engineered structures. Another significant difference is the ability to simulate time periods smaller than 1 day. The HELP and UNSAT-H models used in this study were not capable of hourly outputs, and thus could not be compared to the other models on this time scale. This inability to simulate smaller time periods may produce inaccurate results for climates with convective storms that produce precipitation events that last < 1 hour.

Additionally, a literature review of vadose zone model comparison studies was conducted. While the model comparisons presented in Chapter 1 are valuable in highlighting
that the Richards equation based codes are based on the same governing equations and should produce similar outcomes for simple, well defined problems, the literature provides a starting point for evaluating the performance of the codes and divergence of results under more complicated scenarios including complex geometries, time varying boundary conditions, and field scale heterogeneity. The reviewed model comparison studies were conducted under a variety of climactic conditions and included field observations to validate model results. A common conclusion of the model comparison studies and of this model comparison study is the recommendation that hydrologic modelers should exercise careful consideration regarding meteorological input data, site-specific hydraulic parameters, site specific vegetation parameters, and select computer codes based on matching of the strengths and weaknesses of a particular model to the dominant processes occurring at a particular site.

Finally, background research, on-site data collection, laboratory testing and characterization, and predictive numerical modeling of percolation was conducted at the Caselton Tailings impoundment. Field and laboratory characterization included measurement of field saturated hydraulic conductivity, bulk density determination, and unsaturated tailings characterization via a variety of methods. Predictive modeling of percolation through the Caselton Wash Tailings was conducted utilizing HYDRUS 1D and HYDRUS 2D under a range of expected conditions and predicted steady state annual drainage rates spanning 0 mm/yr. for the yearly temporal discretization simulation to 51 mm/yr. for the material boundary lower boundary condition simulation. Sensitivity analysis indicated that the hydrologic models were most sensitive to material properties and lower boundary condition, with up to a 435% increase (41.5 mm/yr.) in steady state drainage rates for the material boundary lower boundary condition with respect to the 2D base case simulation. This range is of note, as all selected
parameterizations are reasonable approaches considering the paucity of data for this site. This study highlighted the importance of model parameterization techniques, as well as appropriate selection of boundary conditions, and spatial and temporal discretization. In order to more fully assess the risks to groundwater resources, future efforts should include further characterization of field scale heterogeneity in the tailings and alluvium, tailings chemistry, model calibration and transient parameter inversion with infiltration columns or on-site observational data, and an application of the findings in this study to the assessment of POC migration from the tailings to impact groundwater resources.
Chapter 2 Tables

Table 4. Physical Parameters for Caselton Sulfide Tailings

<table>
<thead>
<tr>
<th>Tailings</th>
<th>Field Dry Density (g/cm³)</th>
<th>Lab Dry Density (g/cm³)</th>
<th>Field Water Content Wt./Vol.</th>
<th>Field Water Content Wt. Wt.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sulfide (Pond 3)</td>
<td>1.3</td>
<td>1.2</td>
<td>1.21</td>
<td>0.19</td>
</tr>
<tr>
<td>Carbonate (Pond 7)</td>
<td>1.3</td>
<td>1.3</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 5. Saturated Hydraulic Conductivities for Caselton Sulfide Tailings

<table>
<thead>
<tr>
<th>Tailings</th>
<th>Saturated Hydraulic Conductivity (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Field Depth = 1.1 m</td>
</tr>
<tr>
<td>Sulfide (Pond 3)</td>
<td>1x10⁻⁴</td>
</tr>
<tr>
<td>Carbonate (Pond 7)</td>
<td>-</td>
</tr>
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</table>
Table 6. van Genuchten Parameters for Materials in Caselton Simulations

<table>
<thead>
<tr>
<th>Material</th>
<th>( \theta_r )</th>
<th>( \theta_s )</th>
<th>( \alpha ) (1/m)</th>
<th>n</th>
<th>( K_s ) (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rosetta tailings</td>
<td>0.046</td>
<td>0.34</td>
<td>0.83</td>
<td>1.53</td>
<td>1.32x10^{-4}</td>
</tr>
<tr>
<td>Rosetta alluvium</td>
<td>0.028</td>
<td>0.46</td>
<td>0.73</td>
<td>1.63</td>
<td>1.65x10^{-3}</td>
</tr>
<tr>
<td>Loam</td>
<td>0.078</td>
<td>0.43</td>
<td>3.6</td>
<td>1.56</td>
<td>2.89x10^{-4}</td>
</tr>
<tr>
<td>Lab tailings, ( K_{fs} )</td>
<td>0.044</td>
<td>0.53</td>
<td>5.75</td>
<td>1.26</td>
<td>1.52x10^{-3}</td>
</tr>
<tr>
<td>Lab tailings, ( K_s )</td>
<td>0.044</td>
<td>0.53</td>
<td>5.75</td>
<td>1.26</td>
<td>1x10^{-4}</td>
</tr>
<tr>
<td>Lab Tailings, ( K_{fs}, B.C.$^1$ )</td>
<td>0.00001</td>
<td>0.53</td>
<td>10.98</td>
<td>0.18</td>
<td>1.52x10^{-3}</td>
</tr>
<tr>
<td>EECA Tailings</td>
<td>0.077</td>
<td>0.48</td>
<td>1.78</td>
<td>1.15</td>
<td>1.8x10^{-5}</td>
</tr>
</tbody>
</table>

1. Parameters are for the (Brooks and Corey, 1964) hydraulic property model.
Table 7. Caselton Simulations – Descriptions and Results

<table>
<thead>
<tr>
<th>Code</th>
<th>Hyd. Model</th>
<th>Geometry</th>
<th>Lower b.c.</th>
<th>Mesh Size</th>
<th>Data Period</th>
<th>Material</th>
<th>Min. Δt(s)</th>
<th>SSRD (m/yr.)</th>
<th>Pct. Inc. (%)</th>
<th>Cum. Mass Bal. (%)</th>
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<td>H2D</td>
<td>V.G.M.</td>
<td>Channel</td>
<td>Free drainage</td>
<td>Hourly (2D)^6</td>
<td>Hour</td>
<td>Lab tails, Kfs</td>
<td>1x10^{-12}</td>
<td>1.47x10^{-2}</td>
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<td>H2D^7</td>
<td>V.G.M.</td>
<td>Channel</td>
<td>Free drainage</td>
<td>Small (2D)^1</td>
<td>Day</td>
<td>Lab tails, Kfs</td>
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<td>9.54x10^{-3}</td>
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<td>V.G.M.</td>
<td>Channel</td>
<td>Free drainage</td>
<td>Small (2D)^1</td>
<td>Month</td>
<td>Lab tails, Kfs</td>
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<td>1.00x10^{-3}</td>
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<td>Channel</td>
<td>Free drainage</td>
<td>Small (2D)^1</td>
<td>Year</td>
<td>Lab tails, Kfs</td>
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<td>-100.0</td>
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<td>V.G.M.</td>
<td>Channel</td>
<td>Free drainage</td>
<td>Med. (2D)^3</td>
<td>Day</td>
<td>Lab tails, Kfs</td>
<td>8.6x10^{-4}</td>
<td>3.21x10^{-3}</td>
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<td>V.G.M.</td>
<td>Channel</td>
<td>Free drainage</td>
<td>Large (2D)^2</td>
<td>Day</td>
<td>Lab tails, Kfs</td>
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<td>1.25x10^{-4}</td>
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<td>V.G.M.</td>
<td>Channel</td>
<td>Free drainage</td>
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<td>Day</td>
<td>Lab tails, Kfs</td>
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<td>Corey</td>
<td>Channel</td>
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<td>1D</td>
<td>Free drainage</td>
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<td>Rosetta tails</td>
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</table>

1. Small (2D) - .2 m global element size, with 3.3 cm refinement along tailings surface
2. Large (2D) - 3.7 m global element size
3. Med. (2D) - .6 m global element size, with .2 m refinement along surface
4. Small (1D) - .2 cm element size along surface, transitioning to .18 m near bottom boundary
5. Long (1D) - .5 cm element size along surface, transitioning to .5 m near bottom boundary
6. Hourly(2D) - .2 m global element size with 1.5 cm refinement along surface
7. Serves as the base case for the 2D simulations
8. Serves as the base case for the 1D simulations, pct. increase from 2D base case is 119.8%
9. Steady-state drainage rate
10. Refers to percent increase with respect to 2D base case
Figure 21. Location Map for the Caselton Tailings impoundment.
Figure 22. Plot of minimum and maximum average monthly temperature at Pioche, NV.

Figure 23. Average monthly precipitation at Pioche, NV as total precipitation (liquid cm), snowfall (cm), and snow depth (cm).
Figure 24. Ponded water in pit (Pond 3).

Figure 25. Regional surface water hydrology.
Figure 26. Flexible Wall Permeameter schematic diagram. The pictured device is for falling head rising tail permeability tests.
Figure 27. WRC characterization methods and applicable pressure ranges (Decagon Devices, Inc., 2016c).
Figure 28. Hanging column schematic diagram (ASTM D6836, 2008).

Figure 29. Pressure-plate schematic diagram (ASTM D6836, 2008).
Figure 30. Chilled mirror hygrometer schematic diagram.

Figure 31. H-K(Ψ) and H-Ψ relationships for materials used in simulations. Suctions observed in model range from 0 to 100 m.
Figure 32. WRCs regressed from measured equilibrium water content data. $K_f$ was used as the base hydraulic conductivity.

Figure 33. Cross section geometry across Pond 2, showing finite element discretization for the small and large meshes.
Figure 34. Hydraulic properties for varying hydraulic property model. $K_b$ is used as the base hydraulic conductivity for $K(\Theta)$ in this figure.

Figure 35. Vertical profile of final head distributions for daily simulations of varying element size.
Figure 36. Steady state drainage rate regressions for HYDRUS 1D models.
Figure 37. Steady state drainage rate regressions for HYDRUS 2D models.
Figure 38. Calculated hourly Penman potential evaporation (August, 1999)
Figure 39. Steady state drainage rates for all models and all sensitivity group.
Figure 40. Results for 2D base case simulation. Negative atmospheric flux indicates infiltration.
Figure 41. Potential evaporation and precipitation rates for varying temporal resolution.
Figure 42. Results for simulations of varying hydraulic property model. Negative atmospheric flux indicates infiltration.

Figure 43. Cumulative surface fluxes for varying hydraulic property model.
Figure 44. Results for simulations of varying material property. Negative atmospheric flux indicates infiltration.
Figure 45. Results for simulations of varying finite element size. Negative atmospheric flux indicates infiltration.
Figure 46. Results for simulations of varying temporal data resolution. Negative atmospheric flux indicates infiltration.
Figure 47. Results for simulations of varying lower boundary condition. Negative atmospheric flux indicates infiltration.
Figure 48. Results for simulations of varying dimensionality and geometry. Negative atmospheric flux indicates infiltration.

Figure 49. Comparison of surface fluxes for 1D and 2D simulations.
Figure 50. Schematic cross-sections of tailings impoundment, showing hypothetical phreatic surfaces.
Figure 51. Photograph showing the channelization of Caselton tailings near Pond 2.

Figure 52. Cross section of pore pressures in base case model plotted with field capacity (3.37 m).
References


USGS National Elevation Dataset, 2013. US Geol. Surv. NED n38w115 1/3 arc-second 2013 1 x 1 degree GridFloat.


