Vapor Transport, Performance, and Design

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Introduction

Since the mid-1990s, the Nye County Nuclear Waste Repository Project Office (NWRPO) has conducted independent modeling studies to analyze the feasibility and potential benefit of long-term ventilation at the U.S. Department of Energy (DOE) high-level radioactive waste repository at Yucca Mountain, Nevada. As a part of this effort, Dr. George Danko from the University of Nevada at Reno was retained as a consultant to perform computer simulations of thermohydrology and ventilation.

Dr. Danko has developed a code called Multiflux, which applies the non-equilibrium, unsaturated-saturated, flow and transport (NUFT) model as a module for simulating heat and moisture flows in the rock domain (LLNL, 1999), and a computational fluid dynamics (CFD) module for the simulation of transport processes in the airway system, including the waste packages. The two modules are coupled on the rock/air interface until the heat and moisture flows are balanced at the common surface temperature and partial vapor pressure at each surface node and time instant. For integrated pre- and post-closure hydrothermal simulations, Multiflux applies a three-dimensional (3-D), combined canister- and mountain-scale rock mass model based on NUFT.

The purpose of this report is to briefly explain the relation and implications of Dr. Danko's recent model simulations on performance assessment and repository design.

Movement of Water Vapor During the Thermal Period

Deficiencies in Current Conceptual Model for Moisture Migration

The current DOE conceptual model for vapor flow is shown on Figure 1. A major feature of this conceptual model is the movement of vapor into the rock during the thermal period. The assumption that vapor moves into the rock is more important to total systems performance assessment (TSPA) and design than might initially be assumed.

An important first step in evaluating model results is to apply the test of reasonableness. Does it make sense that the system would act this way? If common sense and model results are in conflict, then either the model is producing counterintuitive results or there is an error. At a minimum, results that fail the common sense test should be subjected to greater initial skepticism and analysis.

Imagine a parcel of water in the rock near the drift/rock interface. As temperatures rise, the water will turn to vapor and the increased volume will increase pressure. The water vapor will now follow the path of least resistance. In comparison to the dense rock, the drift has effectively infinite permeability for the vapor, thus common sense says that the water vapor will move into the drifts, where it then moves to colder locations and condenses. Notice that the vapor direction in Figure 1 is into the rock, exactly the wrong direction according to the common sense test.

Next, examine the model assumptions and calculations of the vapor heading into the rock. The DOE (e.g., DOE, 2000; Andrews, 2004) initially modeled this system as a two-dimensional cross section running perpendicular to the drift (Figure 1). No-flux boundary conditions were placed in the drift direction, preventing the vapor from migrating along the drift. Because the drift was

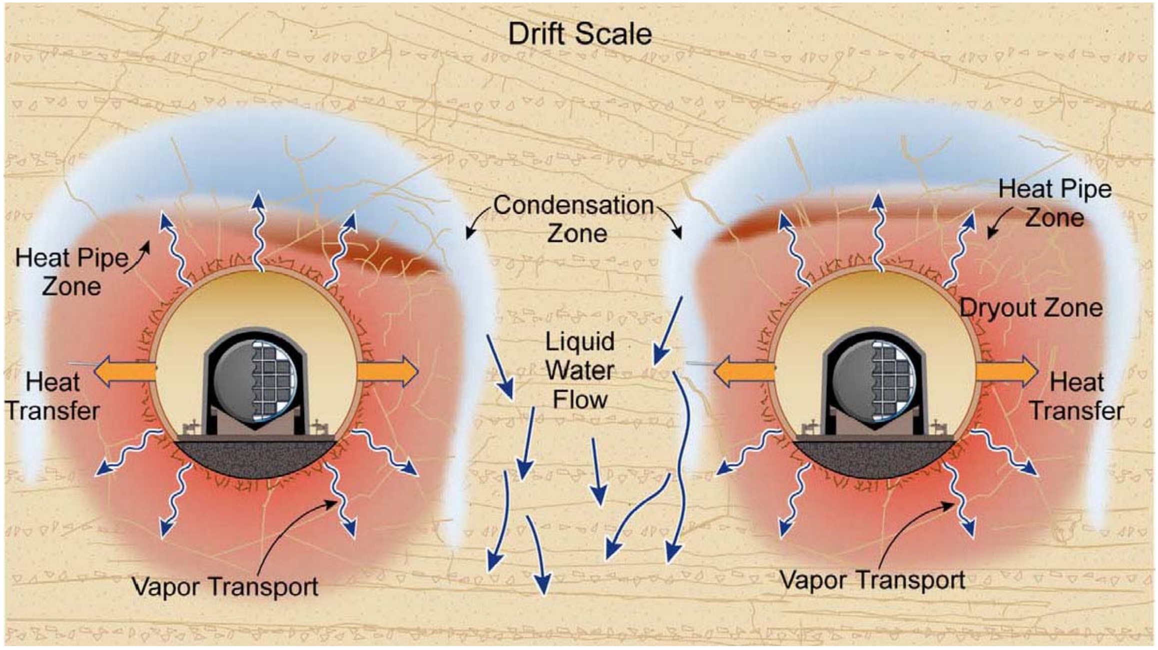

Figure 1
DOE conceptual model of liquid and vapor flux during the thermal period (Andrews, 2004).

artificially blocked, the vapor moved into the rock. From a thermodynamics perspective, an open system was modeled as a mostly closed system. In the completed repository, the drifts will not be artificially blocked.

As a third step, consider the results from 3-D models, such as Multiflux. Figure 2 shows the predicted net evaporation of water into the drift at different locations and times based upon a Multiflux simulation for the first 5,000 years (Danko and Bahrami, 2005). The evaporation rates shown on Figure 2 are great, especially for the first 1,500 years. These results predict that water and water vapor move towards the drifts for at least the first 5,000 years, although the rate of migration decreases significantly after 1,500 years.

Current DOE models (Andrews, 2004, Bodvarsson; 2004) also assume that the system is relatively static, with changes occurring slowly over time. Short-term fluctuations in relative humidity are assumed not to occur. Dr. Danko has examined how the effects of barometric pressure changes in the atmosphere can reach to the level of the repository and lead to a piston-like movement of the air along the drifts and then into or out of the rock. Periodic movement of air leads to periodic fluctuations in relative humidity on a time scale measured in days.

Revised Conceptual Model

The current conceptual model for moisture migration in the repository that forms the foundation of TSPA and design has substantial limitations and requires revision. During the thermal period, vapor moves predominantly out of the rock into the drift, as shown on Figure 3a. The condensation zone and movement of condensed water between the drifts (i.e., thermal shedding) shown on Figure 1 are likely modeling and experimental artifacts that will not be important during the thermal period in the repository as currently designed.

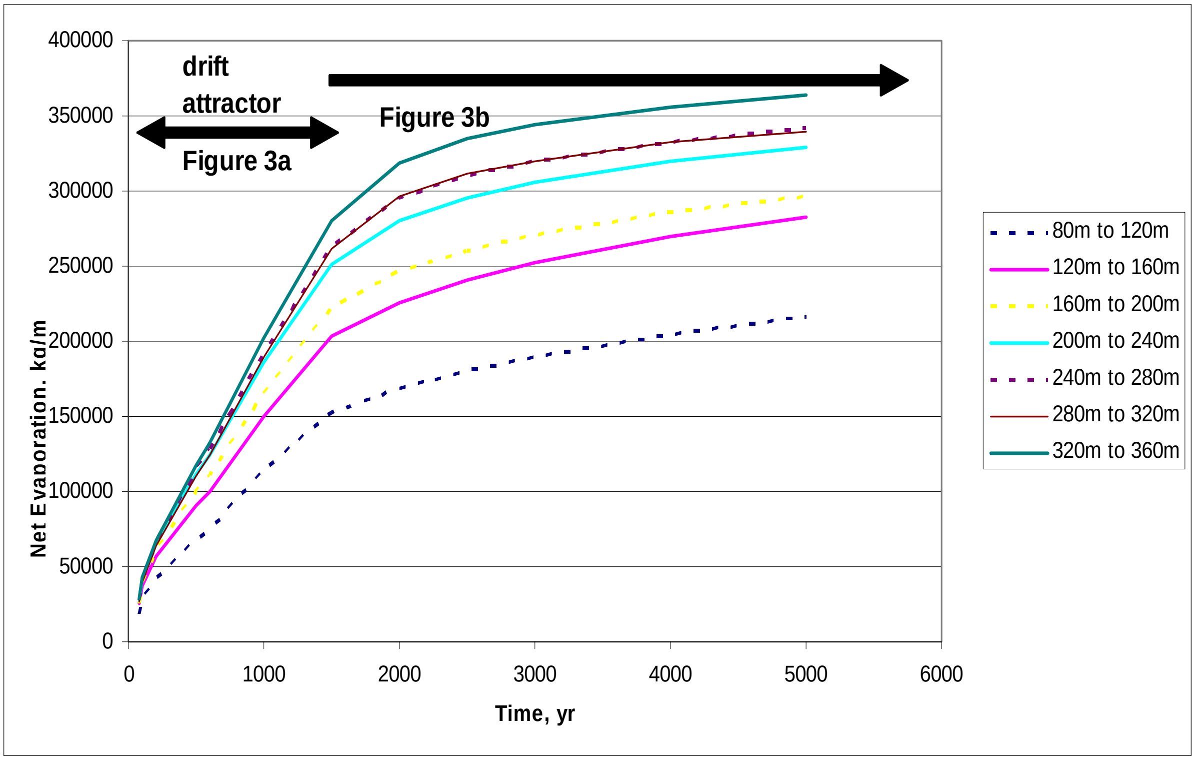

Figure 2
Net evaporation of water into the drifts

Once in the drifts, the vapor moves from warmer to cooler portions near the ends, where it condenses. Mass balance tells us that if most of the vapor moves into the drift it cannot also move into the rock, condense, and produce the flow system shown on Figure 1.

The dark blue portions of the arrows shown in Figure 3a represent liquid water moving toward the drift. As the liquid water approaches the drift, it is converted to vapor by thermal energy and continues to move into the drift as water vapor, as shown by the light blue portion of arrows on Figure 3a. We refer to this as "drift attractor" behavior. During this period, the drift attracts

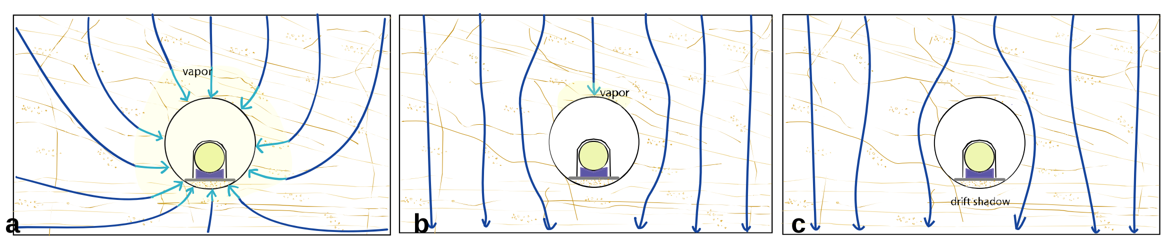

Figure 3
a) Moisture movement at 500 years showing drift attractor behavior.
b) moisture movement at 5,000 years. c) moisture movement at 20,000 years.

percolating water from a footprint larger than that of the drift. The infiltrating water moves into the drifts as water vapor and is transported in vapor form to the ends, where it condenses. In the simulation shown on Figure 2, the drift attractor period lasts for approximately 1,500 years. Although it is not shown on Figure 3a due to scale considerations, it should be noted that the migration of liquid water likely continues between the drifts, but not as a result of thermally driven shedding as suggested on Figure 1.

As the repository cools, the transport of moisture in the system gradually transitions from domination by water vapor movement to domination by liquid water flow. Figure 3b illustrates the repository at 5,000 years, where vapor transport is still important but now coexists with capillary diversion of liquid water around the drifts. By 20,000 years (Figure 3c), the thermal effects have become insignificant and moisture moves by capillary diversion around the drifts, with formation of a drift shadow below each drift.

At the same time, changes in barometric pressure lead to cycles in relative humidity in the drifts on a time scale of days. The amplitude of the cycles changes over time and may cause relative humidity to fluctuate by as much as plus or minus 25 percent during some periods (Danko and Bahrami, 2005). The simulation of relative humidity cycles is currently subject to significant uncertainty; further analysis will be required to ascertain their ultimate importance.

Water Chemistry

Movements of liquid water and water vapor along with associated evaporation and condensation are the most important factors controlling water chemistry during the thermal period. The water movement (i.e., thermal shedding) shown on Figure 1 causes most dissolved salts to be removed from the area of the drift by the movement of the condensed water downward between the drifts. The result of thermal shedding is that large amounts of precipitated salts do not accumulate near the drift according to the current conceptual model. This conclusion has led to the perception that tunnel and atmospheric dust represent the most significant sources of salts in the repository.

The revised conceptual model shown on Figure 3 leads to a paradigm shift in our understanding of the near field environment. During the drift attractor period (Figure 3a), large volumes of percolating water move into the drifts as water vapor. The extensive evaporation process leaves large quantities of precipitated salts in the rock near the drift and at the rock/drift interface. The approximate accumulation of salts is shown on Figure 4, which shows the product of the mass of water vapor entering the drifts at different locations along the drift multiplied by the concentration of chloride in pore water and integrated over time. This is an example from one Multiflux simulation; specific numbers change with the assumptions made in each simulation (Danko, G and D. Bahrami, 2005). The calculation does not account for the continuation of some liquid water flow paths where some, but not all, the water is evaporated or washing away of accumulated salts as the system rewets; and does not specify the exact location of salt deposition. As such, Figure 4 can be considered as an upper bound calculation for chloride accumulation. The point we are making is that the revised conceptual model is associated with large quantities of evaporated water and associated salt deposits.

Accumulation of chloride is rapid and significant. Three periods are evident in Figure 4. At time periods of less than 100 years, the initial moisture in the rock is evaporated and the curves are

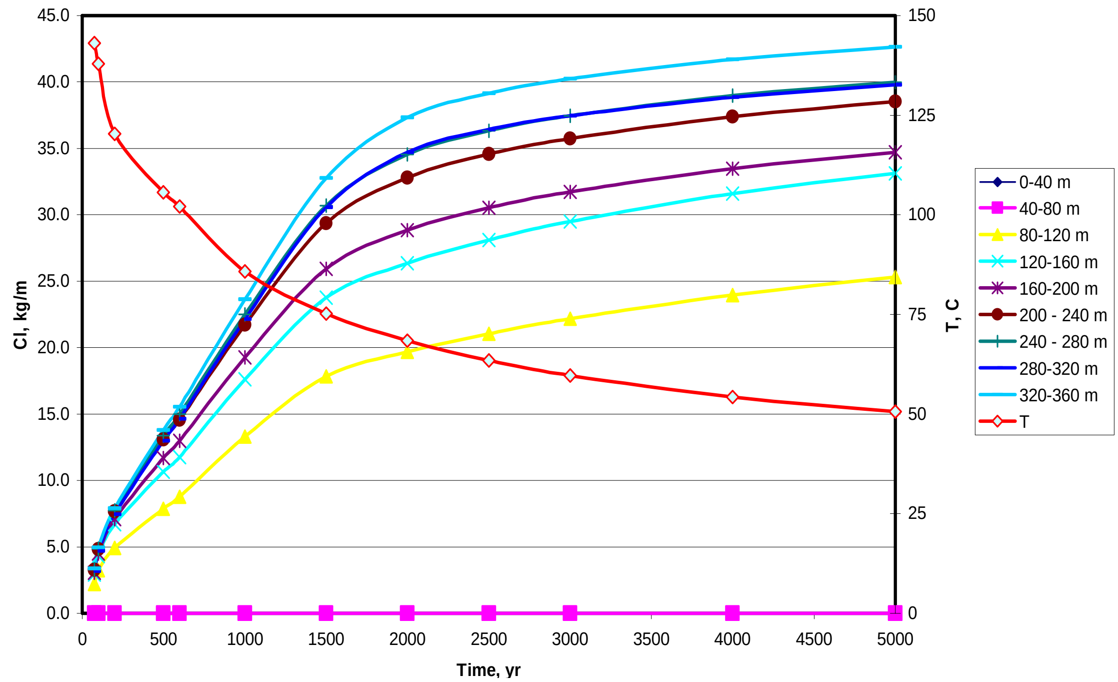

Figure 4
Upper bound chloride ion accumulation in the rock near and at the drift/rock interface according to time, wall temperature, and distance from the end of the drift.

very steep. Next, the slope (i.e., the rate of evaporation) remains nearly constant until approximately 1,500 years. This is the drift attractor period. Drift attractor behavior is still poorly understood, but does not require above boiling temperatures. In the simulation shown on Figure 3, drift attractor behavior ends only after the drift wall temperature drops below approximately 75 degrees Celsius.

The accumulated precipitates containing soluble salts may migrate as dust, fall from the top of the drift, deliquesce and drip onto the titanium drip shields or Alloy-22 waste containers, and/or be transported around the drifts in liquid water when relative humidity rises. At some point, a significant quantity of the dissolved salts deposited near the drift wall will deliquesce and potentially drip. This time period will depend on the specifics of design, emplacement of high and low thermal energy waste packages, location in the drift, and location within the repository.

Next consider the periodic fluctuations in relative humidity caused by changes in barometric pressure. Imagine a deposit of hydroscopic salts on the Alloy-22. The salts are initially dry. As relative humidity rises, the salts deliquesce, leading to the formation of an aqueous phase on the metal surface. Relative humidity then falls and the salts effloresce. Many variants of this scenario are possible and likely. For example, an aqueous phase may be present continuously and shift from more to less concentrated with the periodic changes in relative humidity. This cyclic behavior continues indefinitely, but will become less important as increasing relative humidity prevents the development of highly concentrated solutions.

An additional consideration is that the conditions described above match those anticipated to cause flow separation of salts (Hall and Walton, in press). Differential solubility of salts in flowing water can lead to precipitation of salts at different locations. Nitrate and chloride salts will not always be mixed in the repository.

Repository Design

The revised conceptual model of moisture migration and waste package environment presents significant challenges for design. However, the NWRPO believes that a creative design exercise can lead to improved repository performance and lower costs.

A primary design criterion, in addition to costs, must be to protect the Alloy-22 from localized corrosion. If localized corrosion can be realistically eliminated, the Alloy-22 will provide complete containment for many thousands of years. Even if the final container lifetime is less than the 1,000,000-year regulatory time frame, a longer lifetime allows many radionuclides to decay and spreads release over time, leading to lower peak dose.

The DOE currently minimizes localized corrosion by taking credit for a process of shedding water and salts during the thermal period (Figure 1), which does not appear to occur in the revised NWRPO conceptual model. The localized corrosion DOE tests and modeling are based on dust as a source of salts, a situation where total salts are few and flow separation does not occur. Simple tunnel and atmospheric dusts represent an insignificant source of salts and do not merit the degree of attention they have received.

The near-field environment is one with repeated wet/dry cycles, resulting in less or more concentrated chloride solutions, sometimes with and sometimes without nitrate. The NWRPO believes that, at above-boiling temperatures, these conditions may cause failure of the Alloy-22 by localized corrosion.

The NWRPO has been unable to find repository design alternatives that eliminate the large amounts of evaporation into the drifts with associated chloride accumulation. Thus, it has been concluded that the best approach for reducing the likelihood of localized corrosion is to lower temperatures to below boiling and possibly raise relative humidity. Corrosion tests have found that Alloy-22 is more corrosion-resistant at lower temperatures and high relative humidity precludes the formation of highly concentrated solutions.

Currently, between-drift spacing is based on distances required to promote shedding of water during the thermal period (Figures 1 and 5). Since this process does not occur in the revised conceptual model as currently conceived, it cannot form the logical basis for design. Capillary diversion after the thermal period and the resulting drift shadow are important processes that can probably be maintained with closer drift spacing. During at least the first 5,000 years of repository operation, the movement of moisture and salts in the repository will be closely associated with in-drift vapor phase transport. Repository design should be concerned with controlling temperature and humidity by managing the rate and movement of air and water vapor through the system.

A variety of options are available for lowering repository temperature without increasing repository size or reducing capacity. The options include one or more of the following:

Source: Andrews, 2004

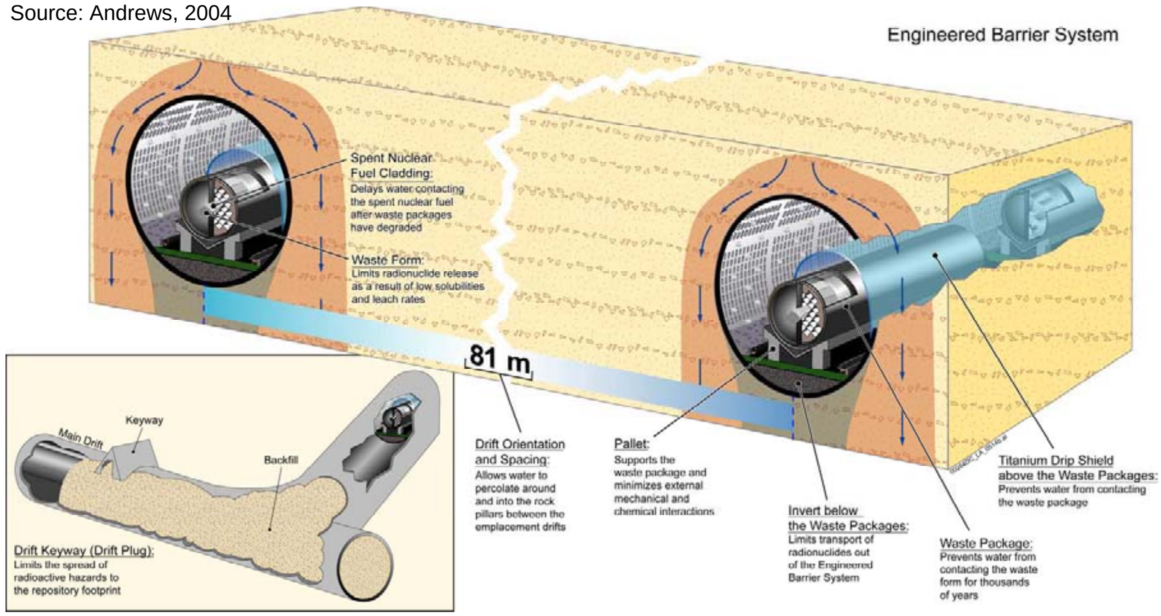

Figure 5
Drift spacing is based upon thermal shedding of salts between drifts during the thermal period.

a) Long-term forced ventilation.
b) Permanent natural draft ventilation.
c) Aging of waste.
d) Reprocessing.

The revised conceptual model of moisture migration during the thermal period raises a number of questions relevant to repository design that will require additional analyses to answer. For example, how do the following influence vapor transport, evaporation, and condensation?

a) Drift slope.
b) Drift connections and plugs.
c) Faults and fracture systems.
d) The presence or absence of bulkheads or drift seals.
e) The time variant failure of seals.
f) Localized collapse of drifts.
g) Mountain-scale buoyancy-driven circulation.
h) Barometric pressure fluctuations.
i) The distribution of thermal loading.
j) Lithophysal cavities.

Conclusions

Water vaporized during the thermal period is currently assumed to move predominantly into the rock, followed by gravity drainage between drifts. Both common sense and the most sophisticated models available predict that water vapor will instead move into the drifts. The movement of water vapor into the drifts is associated with the accumulation of large quantities of soluble salts in each drift.

The TSPA inadvertently takes great amounts of performance credit, in the form of eliminating localized corrosion, from a process of shedding of water during the thermal period that does not occur in the revised conceptual model presented herein. The current repository design is also based on the same conceptual model.

The design of the repository and the TSPA must be revised to reflect the correct direction of vapor transport along with associated issues such as the potential importance of relative humidity cycling and the accumulation of salts.

Lowering repository temperatures to below boiling while perhaps raising relative humidity will lead to greater confidence in predictions, true defense in depth, better performance, and lower costs.

References

Andrews, R. 2004. *Overview of U.S. Department of Energy Total System Performance Assessment for the Yucca Mountain Repository*. Presented to the Nuclear Waste Technical Review Board, September 20, 2004.

DOE (U.S. Department of Energy). 2000. *In-drift Thermal-Hydrological-Chemical Model*. Prepared by Bechtel SAIC Company, LLC. ANL-EBS-MD-000026 -REVW/ICN 1.

Bodvarsson, B. 2004. *Thermal Hydrologic Environment and Thermal Seepage*. Presented to the Nuclear Waste Technical Review Board, May 19, 2004.

DOE (U.S. Department of Energy). 2001. *Multiscale Thermohydrologic Model Report*. ANL-EBS-MD-000049 REV 00, ICN02, Las Vegas, Nevada.

Danko, G. and D. Bahrami. 2005. *Coupled Hydrothermal-Ventilation Studies for Yucca Mountain Annual Report For April 2004-March 2005*. NWRPO-2005-02. Prepared for the Nye County Department of Natural Resources and Federal Facilities. Pahrump, Nevada. September 2005.

Hall, D. and J. Walton. 2006. *Conceptual Model for Flow Separation Processes Affecting Waste Package Chemical Environment, Yucca Mountain, Nevada*. Applied Geochemistry, in press.

LLNL (Lawrence Livermore National Laboratory). 1999. *Flow and Transport Code Version 3.0s*. Software Configuration Management, Yucca Mountain Project – STN: 10088-3.0S-00. Prepared by Lawrence Livermore National Laboratory.