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Earth Sciences Division

August 1998



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**Two-Phase Unsaturated Flow at Yucca Mountain, Nevada  
- A Report on Current Understanding**

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# **Two-Phase Unsaturated Flow at Yucca Mountain, Nevada - A Report on Current Understanding**

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## **1. Introduction**

Most countries plan to dispose of high-level nuclear wastes in tight geologic formations below the water table, in the saturated zone (SZ; Witherspoon, 1996). The chief pathway through which radionuclides could escape from a geologic repository is through dissolution and transport in groundwater. Various mechanisms have been recognized that could cause a gas phase to appear in an otherwise saturated environment; these include gas generation by corrosion, radiolysis, or microbial degradation, as well as exsolution of naturally present gas due to depressurization near the repository excavations. The presence of two-phase (water-gas) conditions could alter groundwater flow and solute transport, as well as affect the chemical environment of the waste packages. In addition, gas flow could conceivably promote the release of volatile radionuclides. A sound understanding of two-phase flow and gas migration in geologic media, and in engineered barrier materials, is needed for design and performance assessment of a saturated-zone repository.

The U.S. civilian nuclear waste program is unique in its focus on disposal of high-level wastes in the unsaturated zone (UZ), above the water table. The potential repository site currently under investigation is located in a semi-arid region of the southwestern U.S. at Yucca Mountain, Nevada (Fig. 1). The geology of the site consists of layered sequences of faulted, fractured, and bedded tuffs (Fig. 2). The groundwater table is approximately 600 m beneath the land surface, while the proposed repository horizon is at a nominal depth of approximately 375 m. In this kind of environment, two-phase flow is not just a localized perturbation to natural conditions, as in the saturated zone, but is the predominant mode of water and gas flow.

The purpose of this report is to review the current understanding of gas and water flow, and mass transport, in the unique hydrogeologic environment of Yucca Mountain. Characteristics of the Yucca Mountain site are examined, and concepts and mathematical modeling approaches are described for variably saturated flow in thick unsaturated zones of fractured rock. The paper includes a brief summary of the disposal concept and repository design, as developed by a team of

engineering contractors to the U.S. Department of Energy (DOE), with strong participation from the DOE National Laboratories.

## **2. Disposal Concept at Yucca Mountain**

Thick unsaturated zones in desert environments of the southwestern U.S. were proposed as possible host media for high-level nuclear waste disposal more than thirty years ago (National Academy of Sciences - National Research Council, 1966). Much of the credit for suggesting the suitability of thick unsaturated zones for nuclear waste disposal belongs to scientists from the U.S. Geological Survey. Winograd (1974) pointed out that such zones have a number of favorable hydrogeologic and logistical characteristics, including “(1) the probable absence of an effective mechanisms to dissolve and transport the radionuclides to a deep water table under present climatic conditions, (2) probable protection from exhumation by erosion in a time frame of several thousands of years, (3) availability of remote federally owned lands with suitable unsaturated zones, and (4) relative ease of placement and retrieval” (Winograd, 1974). These aspects were further elaborated by Roseboom (1983) who emphasized specific advantages of unsaturated as compared to saturated zone waste disposal. Roseboom noted that even strong episodic infiltration will drain away rapidly because of the high fracture permeability. This would tend to keep waste packages dry and minimize the possibility of groundwater contact and leaching (the so-called “storm sewer” concept). He also pointed out that site characterization through boreholes would be easier in the unsaturated zone because there would be less concern about compromising site integrity. Winograd (1974) also cautioned about “potentially serious liabilities of unsaturated zone storage [that] include (1) the necessity and difficulty of guaranteeing that the wastes will not be exhumed during the next several hundred thousands of years ...; (2) the necessity and difficulty of predicting the effects of a return of pluvial climate ...; (3) the complexity of processes in, and difficulty of *in situ* measurements of unsaturated flow parameters for, an unsaturated stratified medium; (4) evaluation of stresses created by the radiogenic heat ...; and (5) necessity of protecting the surface of the burial area.” Discussing potentially adverse conditions, Roseboom (1983) mentioned the presence of perched water bodies, as well as heightened concerns about containment of gaseous radionuclides.

For a period of time, the U.S. nuclear waste disposal program considered different hydrogeologic settings and rock types, including granite, basalt, salt, and tuff. With the 1987 amendment to the Nuclear Waste Policy Act of 1982, the U.S. Congress established Yucca Mountain as the sole candidate site for hosting a high-level nuclear waste repository. In its most recent update (DOE, 1998), the repository safety strategy at Yucca Mountain relies “on the natural attributes of the unsaturated zone for primary protection by providing a setting where waste

packages assisted by other engineered barriers are expected to contain wastes for thousands of years. ... Four key attributes of an unsaturated repository system ... are critical to meeting the objectives: [1] Limited water contacting the waste packages, [2] long waste package lifetime, [3] slow rate of release of radionuclides from the waste form, [4] concentration reduction during transport through engineered and natural barriers” (DOE, 1998). In developing the case for safe disposal at Yucca Mountain, DOE is also addressing issues of future climate change, and a number of potentially disruptive scenarios, including tectonics and seismicity, volcanism, nuclear criticality, and human interference (DOE, 1998).

## 2.1 Hydrogeologic Setting

A general framework for hydrogeologic characteristics and conditions at the Yucca Mountain site was presented by Montazer and Wilson (1984). This built on extensive earlier work by USGS scientists, and was subsequently elaborated and refined by contributions from many investigators. Precipitation at Yucca Mountain is highly spatially and temporally variable, and has been estimated at approximately 150 mm/yr on average (Montazer and Wilson, 1984; Flint et al., 1997). Potential evapotranspiration is several times larger than precipitation, and net infiltration is believed to be small, on the order of 1 - 10 mm/yr on average (Flint et al., 1997). Temporal variability has also been documented, which correlates with ENSO (El Niño Southern Oscillation) recurrences of high-precipitation Pacific storm seasons (Flint et al., 1997).

Topographic elevations at Yucca Mountain range from 1200 - 1400 m (RIB, 1996). The geology is characterized by thick alternating layers of densely welded to non-welded tuffs which gently dip to the east at angles of 6 - 7.5 ° and are intersected by a number of primarily north-south trending faults (Figs. 2, 3). The welded tuffs have appreciable porosity, of order 10 %, but very low matrix permeability, of the order of microdarcies ( $10^{-18}$  m<sup>2</sup>). They have on the order of 10 fractures per m<sup>3</sup>, with average permeabilities of the fracture network of order  $10^{-11}$  m<sup>2</sup> (10 darcy). The non-welded tuffs have larger porosity of order 30 %, are more sparsely fractured, and have matrix permeability of order  $10^{-13}$  m<sup>2</sup>. The potential repository horizon is located in the unsaturated zone, approximately 200 m above the water table. While nuclear waste isolation beneath the water table generally needs to rely on host rocks with low permeability and sparse fracturing, Yucca Mountain was proposed as a candidate site chiefly because of the presumed low rates and velocities of water movement in a thick unsaturated zone (Winograd, 1974; Montazer and Wilson, 1984).

Site characterization activities and repository design and performance assessment studies have been conducted at Yucca Mountain since the late 1970s. Early studies employed borehole-based sampling, monitoring and testing. During the last 5 years an “exploratory studies facility”

(ESF) was constructed, consisting of a 7.8 km long tunnel with a diameter of 7.62 m, which provides direct access to the proposed repository horizon. Intensive site characterization efforts are underway in the ESF, including geologic mapping, hydrogeologic and pneumatic testing, heater experiments on a range of space and time scales, and programs for chemical sampling and mineralogic characterization. Recent field observations have produced some surprising results, challenging the "conventional" view of water seepage in a thick, unsaturated, fractured-porous medium (see below).

## **2.2 Current Repository Design**

The current repository layout as shown in Fig. 4 was developed on the basis of geological constraints imposed by the Solitario Canyon and Ghost Dance Faults (DOE, 1998). It has a capacity to store 70,000 metric tons of uranium (MTU), or heavy metal equivalent. Waste packages containing commercial spent nuclear fuel (SNF) will be horizontally emplaced on pedestals in the centers of drifts with 5.5 m diameter. The waste packages have cylindrical shape with a diameter slightly less than 2 m and length of approximately 5.5 m (Fig. 5). Based on a number of thermal goals, such as maximum rock temperatures not exceeding 200 °C (Saterlie et al., 1996), an areal mass loading of 85 MTU/acre (21 kg/m<sup>2</sup>) has been established. (The mass loading in units of MTU/acre is approximately equal numerically to initial heat loading in units of kw/acre; 1 acre ≈ 4,047 m<sup>2</sup>.) One hundred and five emplacement drifts with a total length of approximately 108 km are to be constructed in an area of 747 acres (3.02 x 10<sup>6</sup> m<sup>2</sup>). The drifts will have a sub-horizontal grade of 0.5 % for drainage. The ESF facility, consisting of the North Ramp, East Main, and South Ramp sections, constitutes an integral part of the repository layout (Fig. 4). A number of auxiliary excavations, such as performance confirmation drifts, are also planned.

## **2.3 Issues for Site Suitability**

The main pathway by which radioactive contaminants could escape from a repository at Yucca Mountain and reach the accessible environment is through dissolution and migration in groundwater. The major concern for site suitability then is with rates and velocities of water flow, no different than for saturated-zone repositories. Additional issues arise at Yucca Mountain from unsaturated-zone flow between land surface, repository, and water table, and from potential gas phase migration of volatile radionuclides, such as C-14 and I-129. Depending on thermal loading, host rock temperatures may rise beyond the boiling point of water at ambient pressures. This could lead to large-scale redistribution of moisture, with vaporization and partial drying of the host rock in some regions, condensation effects in others. In addition to understanding water and gas migration at ambient conditions, there is a need to understand heat-driven flows accompanied by



phase change effects. Elevated temperatures and phase change processes could also significantly impact the geochemical environment, affecting performance of waste package materials and engineered barriers, the mobilities of dissolved species, and sorptive properties of the host rocks. A comprehensive summary of technical issues relevant to high-level nuclear waste disposal at Yucca Mountain was presented by Narasimhan and Wang (1994).

### **3. Unsaturated Flow Concepts and Issues**

Measurement and modeling of unsaturated flow requires a quantitative understanding of the physical processes involved on “appropriate” scales, and a characterization of the hydrogeologic conditions under which these processes are being played out at a given field site. The latter involves determination of the relevant hydrogeologic parameters and constitutive relationships, and of initial and boundary conditions. Issues of space and time scale, intrinsic variability, uncertainty and averaging become paramount in practical applications. Here we summarize physical processes and modeling issues in unsaturated flow to provide background and context for a discussion of the Yucca Mountain site.

#### **3.1 Physical Processes in Unsaturated Flow**

From a fluid dynamics viewpoint, seepage of water through partially saturated media can be classified as a process of immiscible displacement in which water flows primarily downward under gravity force, invading previously gas-filled pore spaces. (Strictly speaking, pore invasion and phase occupancy changes would only occur for transient flow conditions, while for steady flows phase distributions would be time-independent. It is doubtful, however, whether the mathematical idealization of steady flow is useful in connection with unsaturated flow at Yucca Mountain; see below.) The gas phase in variably-saturated fractures and rock matrix pores is mostly air, but also contains some water vapor, and numerous trace constituents such as CO<sub>2</sub>. The aqueous phase is mostly water, but generally also contains dissolved solids and non-condensable gases.

The immiscible displacement of one phase by another in porous media has been studied in a number of engineering disciplines, including petroleum and geothermal reservoir engineering, chemical engineering, civil engineering, and soil science. The conventional approach for describing immiscible displacement processes has employed “macroscale continuum concepts” which are based on sound principles and well-established continuum field theories of classical theoretical physics (see appendix; Morse and Feshbach, 1953; Narasimhan, 1982a, b). Conservation of the active system components (water, air, heat, additional chemical constituents) is expressed by means of integral or partial differential equations (PDEs) for space-and-time varying fields of phase

saturations, pressures, temperatures, solute concentrations, etc. Mass and heat fluxes are given by phenomenological relationships between intensive variables that drive flow, such as multiphase extensions of Darcy's law for phase fluxes, Fick's law for mass diffusion, Scheidegger's hydrodynamic dispersion, and Fourier's law for heat conduction. For water flow under unsaturated conditions, it is often admissible to invoke approximations that consider air to be a passive spectator at constant pressure, requiring only water flow to be modeled explicitly (Buckingham, 1907; Richards, 1931; see Eq. A.15).

While there is an extensive literature on empirical observations and mathematical modeling concepts for multiphase flow, on scales ranging from pore level (Lenormand and Zarcone, 1985, 1989) to megascopic (kilometers), there are also serious limitations in the range and scope of phenomena that can be addressed by existing methods. Water seepage in partially saturated media involves an interplay of gravity, capillary, viscous, and inertial forces. Chaotic flow behavior on small scales can have significant impacts on large-scale fluid mixing and tracer dilution (Weeks and Sposito, 1997). On larger scales, the governing PDE's for unsaturated water flow become parabolic (diffusion-like) when capillary forces are dominant, indicating the presence of physical mechanisms for dampening spatial and temporal variability, and making conditions favorable for application of volume averaging. However, the governing PDEs become hyperbolic when gravity effects are dominant, as is the case for brief, localized infiltration events in highly permeable fractures. Under these circumstances the flow system lacks internal averaging mechanisms, and spatial and temporal averages become artificial constructs of the theoretical analysis, whose validity for a mechanistic description of the flow system is uncertain at best. Indeed, if localized preferential flow bypasses much of the flow system volume, then volume averages may be completely meaningless (see below).

Variably-saturated flow systems are highly non-linear. They are driven by the gravitational instability of denser water overlying and invading less dense air, and by non-linear feedback between flow and hydraulic conductivity. This gives rise to uneven displacement fronts, especially in media with fracture-dominated permeability. Unsaturated seepage may not proceed as smooth areally extensive plumes or (in fractures) sheets, but often occurs in localized "fingers" that are separated by regions with no water flow. Instability-driven fingering is a well-understood phenomenon that occurs even in (nearly) homogeneous media (Chuoque et al., 1959; Glass et al., 1989; Glass and Nicholl, 1996). Heterogeneities of the permeable medium provide an alternative mechanism for focusing distributed seepage into localized preferential pathways. In field-scale systems, heterogeneity-driven preferential flow effects tend to be much more important than those caused by instabilities. This is especially true for fractured media, where asperity contacts and

geometric features such as fracture intersections and terminations may divert water seepage from certain regions while funneling it into others. In regions with poorly connected fractures, perched water bodies may form with locally water-saturated or "satiated" conditions (see below). Capillary barrier effects with lateral flow diversion can arise at sloping contacts between layers of different permeability (Ross, 1990; Oldenburg and Pruess, 1993).

Laboratory studies have shown that unsaturated seepage is subject to intermittent flow, even when great care is taken to maintain time-independent conditions at the infiltration boundary (Prazak et al., 1992; Geller and Pruess, 1995; Su et al.; 1998). Field observations of seepage in unsaturated fractured rocks have also shown temporal variability on different time scales (Faybishenko et al., 1998). Flow intermittency may be caused by an interplay of different flow mechanisms, such as gravity or pressure-driven flow on the one hand, capillary-driven flow on the other (Persoff and Pruess, 1995; Su et al., 1998). It often entails an active participation of the gas phase, which locally may become surrounded and entrapped by water (Faybishenko, 1995). Thunvik and Braester (1990) presented a numerical model which demonstrated mechanisms for development of time-varying two-phase flows for time-independent boundary conditions.

Significant flow and transport effects may occur in the gas phase. These include "barometric pumping" where, in response to barometric pressure changes, atmospheric air may be pushed into the subsurface or, conversely, soil (or rock) gas may be discharged into the atmosphere. This process can have considerable impact on the moisture status in the subsurface, especially in semi-arid regions, where the relative humidity of atmospheric air can be much lower than that of soil gas which typically is close to 100 %. Exchange of soil gas and atmospheric air can be enhanced in regions with topographic relief, due to thermal and compositional buoyancy effects, as soil gas usually is (slightly) less dense than atmospheric air due to higher temperature and humidity (see below).

Heat transfer in unsaturated zones occurs not only by conduction, but also through sensible heat transport by advection of water and gas, and by means of vapor diffusion, driven by vapor pressure gradients. Soil science studies have demonstrated that vapor diffusion in porous media can be considerably enhanced compared to diffusion of non-condensable gases due to pore-level phase change effects (Cass et al., 1984). These effects may approximately cancel the added resistance to gas diffusion normally present in porous media, where the solid skeleton reduces the gas volume and increases diffusive path lengths.

Emplacement of heat-generating high-level nuclear wastes in unsaturated media may give rise to strongly heat-driven flows with extensive vaporization and condensation phenomena. As formation temperatures approach or exceed the boiling temperature at ambient pressures, formation waters will vaporize at increasing rates. The vapor will be driven away from the heat source by pressure gradients, primarily through fractures, and will condense in cooler rock. The condensate may drain downward and/or flow back towards the heat source under capillary and gravity effects, setting up a vapor-liquid counterflow process known as "heat pipe." Strong hydrothermal alteration effects are expected to occur in the region surrounding a strong heat source in unsaturated rock. Rock-fluid interactions involve dissolution and precipitation of minerals, and associated changes in formation porosity and permeability.

### **3.2 Unsaturated Flow in Fractured Media**

"Conventional" methods for modeling unsaturated water flow in fractured-porous media emphasize volume-averaged, macro-scale continuum concepts (Wang and Narasimhan, 1985, 1993; Pruess and Narasimhan, 1985; Peters and Klavetter, 1988; Nitao and Buscheck, 1991). Water seepage down steeply dipping fractures is viewed as proceeding in piston-like manner as smooth sheets, and subject to strong imbibition effects from the capillary suction of partially-saturated matrix rock. These conceptualizations would suggest that water in fractures can flow neither far nor fast, as matrix imbibition will quickly establish approximate capillary equilibrium between fractures and matrix rock. Under partially saturated conditions, capillary effects would essentially confine water to the rock matrix, so that the high permeability of the fracture network would not be available for water flow.

Recent field observations at a number of sites in semi-arid regions with thick unsaturated zones in fractured rock have not only shown the presence of "old" (10,000 yr or more) slowly moving waters, but have also demonstrated that water can flow rapidly through fracture networks along localized preferential pathways (Nativ et al., 1995; Yang et al., 1995; Fabryka-Martin et al., 1996; Eaton et al., 1996). The most compelling evidence is provided by man-made environmental tracers that were observed to migrate across thick unsaturated zones with velocities of order 10 m/yr, several orders of magnitude larger than would be expected if flow proceeded in volume-averaged manner. Several mechanisms and conditions have been proposed to explain this kind of flow behavior, including (a) non-uniform infiltration at the land surface boundary, (b) flow focusing due to medium heterogeneities (fracture terminations, capillary barriers), (c) episodic and intermittent flow, and (d) film flow along rough fracture walls. Some of these mechanisms (a, b) reduce matrix imbibition by reducing the rock surface area that is wetted by water, others (c) by making water available for imbibition only episodically. Pervasive flow focusing and intermittency

were observed in flow visualization experiments on transparent replicas of natural fractures (Su et al., 1998). Laboratory experiments on rock specimen have demonstrated that water films held by capillary force on rough surfaces may provide a mechanism for fast flow (Tokunaga and Wan, 1997).

Areally distributed seepage in fractured rocks can be funneled into localized pathways by means of sub-horizontal obstacles of low permeability, such as asperity contacts or fracture terminations (Fig. 6). It is rather obvious that obstacles of greater length will be more effective in funneling flow. At the same time, average fracture permeability in the vertical direction, as would be measured by means of gas pressure tests, becomes smaller for longer obstacles. These concepts have been confirmed in numerical simulation experiments, which demonstrated that downward water seepage may actually proceed faster in fractured media of lower average permeability (Pruess, 1998b). This seemingly paradoxical result emphasizes features that are unique to unsaturated fractured rocks, and suggests that "average permeability" may not be a meaningful concept for describing water seepage in such systems.

#### **4. Ambient Conditions**

Important issues for repository performance under ambient conditions include the percolation flux at the repository level, seepage into drifts that could contact waste packages, seepage behavior below the repository, flow partitioning between fractures and rock matrix, and the scale dependence of hydrogeologic parameters (Ho and Wilson, 1998).

##### **4.1 Water Flow**

Unsaturated water flow at Yucca Mountain occurs at rates that are so small that they cannot be directly observed, but must be inferred through indirect methods. Available methods include monitoring of water saturation changes in situ (Flint et al., 1997), measurements of natural geothermal gradients which are affected by sensible heat transport from downward water seepage (Sass et al., 1988), and measurements of radioisotope and solute concentrations, such as H-3, Cl-36, and Cl- (Yang et al., 1995; Fabryka-Martin et al., 1996). Our ability to determine water seepage rates and travel times from these methods is limited, because interpretation of the field data requires model assumptions (about spatial variability, mixing, boundary conditions, etc.) which typically have considerable ambiguity and uncertainty. The DOE recently conducted a formalized process of expert elicitation to review the status of percolation flux determination at Yucca Mountain (CRWMS, 1997). A general consensus seems to be emerging that mean net infiltration is in the range of 5 - 10 mm/yr, with considerable spatial variability, perhaps as large as 20 mm/yr in

some regions, and near zero in others. Substantial infiltration may only take place at time intervals of several years (Flint et al., 1997).

Matrix permeabilities of the welded tuff formations are small, on the order of a few microdarcies ( $10^{-18}$  -  $10^{-17}$  m<sup>2</sup>; Peters et al., 1984; RIB, 1996), corresponding to saturated hydraulic conductivities of  $10^{-11}$  -  $10^{-10}$  m/s, or 0.3 - 3 mm/yr. The welded tuffs have generally been found to be partially saturated, with water saturations typically in the range of 60 - 90 %, and moisture tension in the range from -3 to -6 bars (Rousseau et al., 1997). These observations have sometimes been taken as evidence that net infiltration must be less than saturated hydraulic conductivity of the matrix, based on the reasoning that, if infiltration were in fact exceeding saturated matrix conductivity, then some water seepage should occur in the fractures and consequently, because of strong capillary suction effects, the matrix rock should be fully saturated.

From observations of environmental isotopes we now have compelling evidence that an as yet unknown fraction of total infiltration at Yucca Mountain occurs with rapid velocities of the order of 10 m/yr or larger. Recent net infiltration estimates in the range of 5 - 10 mm/yr exceed matrix hydraulic conductivity, which in and of itself provides strong evidence for water flow in the fractures. Evidence for significant fracture flow in unsaturated rocks has also been found at Rainier Mesa, which is located approximately 50 km north-northeast of Yucca Mountain, and has been suggested as an analog site for Yucca Mountain due to its similar lithology of alternating welded and non-welded tuffs (Cook et al., 1991). Cook (1991) remarks "At this stage, it is not known how fractures could remain sufficiently saturated to act as fast paths in the face of high matrix suction."

The non-welded units have larger porosities of 20 - 40 % and matrix permeabilities mostly in the range of  $10^{-13}$  -  $10^{-16}$  m<sup>2</sup>, corresponding to saturated hydraulic conductivities of  $10^{-6}$  -  $10^{-9}$  m/s (Peters et al., 1984; RIB, 1996). These units have less fracture permeability which, together with the larger matrix permeability, suggests less of a tendency for development of fast preferential flow than in the welded units. There is some evidence that this is true, although observations of environmental tracers in the ESF also clearly indicate that some seepage is able to penetrate the non-welded Paintbrush tuff unit rapidly, possibly related to migration along faults (Bodvarsson et al., 1998).

Drilling at Yucca Mountain has encountered a number of perched water zones which are believed to be associated with local barriers to flow, such as low fracture permeability, or capillary barrier effects (Wu et al., 1998a). Pressure-transient testing has shown that "satiated zones," i.e.,

regions with positive water potential that may or may not contain trapped air, have a wide range of apparent volumes, from  $3 \times 10^4 - 1 \times 10^9 \text{ m}^3$ . Inferred formation permeabilities were typically in the range of a few hundred millidarcies (Wu et al., 1998a).

In situ experiments on water seepage and tracer migration on a scale of order 1 m were recently carried out in niches excavated from the ESF (Wang et al., 1998). Water with tracer was released from boreholes located above a niche, and subsequent seepage into the mined openings was monitored. Timing and quantity of water arrival could be described surprisingly well by homogeneous continuum models, building confidence in such models on the scale investigated.

## 4.2 Gas Flow

Boreholes penetrating the unsaturated zone at Yucca Mountain, and left open to the atmosphere, show interesting phenomena of gas discharge or (less frequently) intake of atmospheric air. These effects arise from barometric pressure fluctuations and from buoyancy due to temperature and humidity-induced density differences between formation gas and atmospheric air (Weeks, 1987). Considerable work has been done to monitor the propagation of barometric pressure fluctuations through the unsaturated zone at Yucca Mountain, and continuous high-resolution pressure records over time scales of several years are now available from many locations throughout the mountain (LeCain, 1997). Detailed analyses using conventional single-phase gas flow theory have led to excellent matches between observed and simulated pressures (Ahlers et al., 1996). Construction of the ESF facility has altered barometric pressure conditions at newly exposed rock faces. This change in boundary conditions produced well-resolved signals in a number of gas pressure monitoring locations, which allowed more detailed calibration of gas flow models.

Ongoing programs of transient gas pressure and gas tracer testing are underway from boreholes as well as in the ESF. These tests have provided valuable determinations of permeabilities and porosities of fracture networks on different scales (LeCain, 1997; Wang et al., 1998; Freifeld, private communication, 1998). Gas permeabilities of fractured units are typically in the range from 0.1 - 10 darcies ( $10^{-13} - 10^{-11} \text{ m}^2$ ), while typical fracture porosities are in the range of  $10^{-4}$  to  $10^{-2}$ .

## 4.3 Heat Flow

Formation temperatures at Yucca Mountain increase with depth by approximately  $3 \text{ }^\circ\text{C}$  per 100 m, which is a typical value for continental crust, and corresponds to a conductive heat flux of approximately  $60 \text{ mW/m}^2$  (Sass et al., 1988). Local variations in the geothermal gradient may be

caused by variations in the thermal conductivities of the rocks, and by cooling effects from non-uniform water seepage. Downward percolating water absorbs heat to maintain temperature equilibrium with the formations; the heat flux removed from the vadose zone is approximately 2.5 mW/m<sup>2</sup> per 1 mm/yr of percolation flux. Current estimates for percolation flux at Yucca Mountain are in the range of 1 - 10 mm/yr, with larger values in some regions (Flint et al., 1997), indicating that heat removal by percolating water may constitute a substantial fraction of total heat flux, and suggesting that careful temperature monitoring may be able to resolve spatial variations in downward seepage rate. However, temperature measurements are affected by gas flow and evaporation effects in boreholes and, furthermore, upward heat flux in the vadose zone is non-uniform at the water table boundary because of flow processes in the saturated zone. Both effects limit the ability to make inferences about water seepage from temperature data. Natural geothermal gradients are associated with vapor pressure gradients and an upward diffusive flux of vapor which has been estimated at a water-equivalent rate of .03 - .04 mm/yr (Ross, 1984).

#### **4.4 Modeling Approaches**

Most numerical modeling of water and gas flow at Yucca Mountain has used macroscale continuum approaches. Rates of liquid and gas flow are calculated from a multi-phase extension of Darcy's law, in which relative permeability and capillary pressure concepts are used to represent interaction between two fluid phases (see Eq. A.5). In addition to the "process complexity" of multi-phase flow, a very significant problem is posed by the heterogeneities of the rock formations, consisting of lithologic units with spatially variable permeability and porosity, intersected by numerous fractures on different scales, as well as a number of major faults. Most workers have adopted continuum approximations for modeling flow in fractured-porous media that are largely borrowed from geothermal and petroleum reservoir engineering. Approaches used include the (single) "effective continuum" model (ECM), and multiple-continua methods such as double-porosity (DPM), dual-permeability (DKM), and multiple interacting continuum (MINC) approaches (see Figures 7 - 9; Barenblatt et al., 1960; Warren and Root, 1963; Kazemi, 1969; Pruess and Narasimhan, 1985).

Early work employed schematic one and two-dimensional models (Wang and Narasimhan, 1985, 1993; Peters and Klavetter, 1988). Current flow and transport models for the unsaturated zone have become very elaborate (Robinson et al., 1995; Bodvarsson, et al., 1996, 1997; Wu et al., 1998b). Finite difference or finite element grids with on the order of 50,000 grid blocks or more are used for a detailed three-dimensional representation of natural and man-made hydrogeologic features (layers, faults, drifts), with spatial resolution of order 100 m, and finer sub-gridding to better resolve the ESF and potential repository region (Fig. 10). These models



address fracture-matrix interactions and employ sophisticated inverse modeling techniques for calibration against diverse laboratory and field data, including formation permeabilities and porosities, water saturations in the rock matrix, water potentials, presence of perched water bodies, variations in formation temperatures, and groundwater travel time and dilution effects (Bandurraga and Bodvarsson, 1998). Sensitivity studies have been performed to evaluate effects of parameter uncertainty, and to explore seepage behavior under future possibly more pluvial climatic conditions.

In spite of the sophistication of the large-scale volume-averaged models, serious questions and uncertainties remain about their conceptual basis and validity. It is not clear at the present time to what extent volume-averaged approaches can describe water seepage in unsaturated fractured systems. Propagation of gas pressure pulses is a diffusive process that will be subject to volume averaging in a well-connected fracture network. Water seepage on the other hand may be dominated by spatially highly localized preferential pathways. It lacks averaging mechanisms intrinsic to the medium, and is described by a PDE that is essentially hyperbolic in character. If important components of flow are localized in preferential pathways, then much of the system volume would not participate in these flows, and volume averages may be completely meaningless. Mechanistic process models that are based on macroscale continuum concepts do have a sound basis as long as formation heterogeneities and flow phenomena are described in full explicit detail on "sufficiently" small scales. This can be accomplished by means of finite difference approaches using high-resolution grids. Although such approaches are not practical for site-scale modeling at Yucca Mountain, they have been successfully employed for drift-scale tests (Birkholzer et al., 1998), as well as for more fundamental studies of unsaturated seepage in heterogeneous and fractured media (Birkholzer and Tsang, 1997a; Pruess, 1998a). High-resolution finite difference models have shown that the episodic nature of seepage, together with reduced fracture-matrix interface areas from localization of flow into preferential paths, severely limits water uptake into the matrix by imbibition (Pruess, 1998b). This offers an explanation for the conundrum succinctly stated by Cook (1991), "how fractures could remain sufficiently saturated to act as fast paths in the face of high matrix suction."

Growing field evidence for fast preferential flow, and the conceptual difficulties of large-scale continuum models to represent such phenomena, have prompted the development of alternative modeling approaches. Gauthier et al. (1992) introduced the bold hypothesis that, somehow, capillary mechanisms were of limited effectiveness in removing water from the fractures, and proposed a model which ignored matrix flow altogether and considered seepage to occur only in the fractures (Fig. 11). The "weeps" model of Gauthier et al. does not attempt to

explain unsaturated flow in terms of physical mechanisms. Instead it proposes a phenomenological parametrization of unsaturated flow as a collection of fast paths. It is well-suited for repository performance assessment, because it allows the direct parametrization of flow in terms of its temporal and spatial distribution and variability (Wilson et al., 1993). Conceptually, this approach is closely related to transfer function and transit time distribution models, which have been successfully applied to a wide range of subsurface flow and transport processes, including water flooding of oil reservoirs, migration of contaminants in the unsaturated zone, and water inflow into tunnels and drifts (Chesnut et al., 1979, 1992, 1994a, b; Jury, 1982; Jury and Roth, 1990).

Strengths and weaknesses of alternative modeling approaches for unsaturated flow in fractured media were recently reviewed by Pruess et al. (1997). These authors argued that “no single approach can be expected to provide a “complete” and “truthful” model of a complex subsurface system. Different approaches emphasize and approximate different aspects of flow system behavior, and have different strengths and weaknesses. The selection of a particular approach, or a combination of approaches, needs to be closely tied to the objectives of the modeling study. Clearly defined objectives are perhaps the single most important factor in the selection of a proper modeling approach. Space and time scales of interest, and present and future availability of site characterization data, are also important considerations.” Pruess et al. (1997) recommended that several different modeling approaches should be pursued simultaneously, to achieve a robust basis for engineering design and repository performance assessment.

## **5. Strongly Heat-Driven Flows**

Emplacement of a strong heat source in a partially saturated fractured medium gives rise to boiling and condensation phenomena with a potential for large-scale redistribution of moisture. Water will be vaporized in the rock matrix, the vapor will be pressurized and flow towards the fractures where it will condense upon encountering cooler wall rocks. The condensate may drain downward or may in part return towards the heat source under capillary and gravity forces. An intriguing possibility is the development of water-vapor counterflow systems, generally referred to as “heat pipes” in the heat transfer and geothermal literature. Because of their very efficient heat transfer characteristics, heat pipes would keep rock temperatures lower than in purely conductive regimes, and would also cause liquid water to persist in regions that otherwise would be subject to dry-out. This could have considerable impacts on waste package and repository design. Simple heat balance considerations indicate that the amount of condensate that could be generated from the waste heat is huge, on the order of thousands of cubic meters of water per waste package (Pruess and Tsang, 1994). This suggests that for several thousand years following waste emplacement, condensate may be a more significant source of water seepage than infiltration from the land

surface. In addition to conduction and advection, significant contributions to heat transfer could arise from vapor diffusion, especially if enhancement effects known to be present in soils (Cass et al., 1984) also occur in rocks (Tsang and Pruess, 1990). However, in preliminary laboratory experiments on tuff samples from the Topopah Spring unit at Yucca Mountain no enhanced vapor diffusion was observed (Wildenschild et al., 1998).

Heat-driven flow at a Yucca Mountain repository has been extensively studied through computer simulation, employing standard multiphase flow and heat transfer concepts borrowed from geothermal reservoir and petroleum engineering (see appendix). More recently, useful insight was gained through laboratory flow visualization experiments, and through field tests in the ESF facility at Yucca Mountain.

### **5.1 Laboratory and Field Experiments**

Laboratory flow visualization experiments on assemblies of artificial or natural rock fractures were performed by Kneafsey and Pruess (1998). This allowed direct observation and confirmation of many of the multi-phase fluid and heat flow phenomena that had been hypothesized in mathematical modeling studies, including vaporization-condensation cycles, heat pipes, formation of dry-out zones and condensation halos, penetration of liquid seepage in regions above the nominal boiling point, and flow funneling and bypassing. The experiments also showed frequent highly transient "rapid evaporation events" (REE) whose significance for field-scale processes is unclear at this time.

An important recent development is the performance of heater testing in the ESF facility for examining thermo-hydrologic behavior over a range of space and time scales (Birkholzer and Tsang, 1997b; Tsang and Birkholzer, 1998). The field experiments include a "single heater test" (SHT; typical scales of order 5 m, 1 yr) and a "drift-scale heater test" (DST; scales of order 50 m, 10 yr). The tests are instrumented with numerous sensors to monitor changes in temperatures, water saturations, and formation (gas) permeabilities. The SHT showed formation of a dry-out zone around the heaters which is surrounded by a condensation halo. Evidence for gravity drainage of condensate was also seen.

### **5.2 Modeling Approaches**

Modeling of the complex thermo-hydrologic phenomena induced by strong heat sources placed in fractured, partially saturated rock is a challenging task. Beginning in the early 1980s, different groups have carried out numerical simulations of fluid and heat flows with phase change at increasing levels of sophistication (Pruess and Wang, 1984; Pruess et al., 1985, 1990a, b;

Buscheck and Nitao, 1992, 1993; Ryder, 1993; Pruess and Tsang, 1993; Haukwa et al., 1998). While different numerical simulation programs were used in these studies, a review (Pruess and Tsang, 1994) has shown general agreement among investigators on the underlying mathematical model. Capillary pressure and relative permeability concepts are used to represent two-phase flow of aqueous and gaseous phases that are composed of varying mixtures of water vapor and air. Issues addressed by the modeling include spatial and temporal changes of temperatures and water saturations, peak temperatures at the repository level, formation of dry-out zones, time scale and spatial patterns of re-wetting, matrix-fracture interactions, and thermally-buoyant gas flow (Tsang and Pruess, 1987). Minor differences in predicted thermo-hydrologic conditions are attributable to different parameter choices (Pruess and Tsang, 1994). The highly non-linear equations describing multi-phase fluid and heat flow admit a semi-analytical similarity solution under certain conditions, which does not require any simplifications in process descriptions (O'Sullivan, 1981). Comparison with the similarity solution has helped build confidence in the numerical simulators (Doughty and Pruess, 1992).

Modeling studies using volume-averaged continuum models have predicted formation of a dry-out zone around the waste packages, prompting the Livermore group to advocate an "extended dry" repository concept, in which high thermal loading would be used to effectively protect waste packages from being contacted by liquid water (Ramspott, 1991; Nitao et al., 1992; Wilder, 1993; Buscheck and Nitao, 1993). However, critics have pointed out that exclusion of liquid water from hot rocks is not absolute, and that large repository heat loads would increase rates of vaporization and condensate formation. This could promote non-equilibrium matrix-fracture flow effects, and could conceivably even enhance localized and intermittent water flow near the waste packages (Pruess and Tsang, 1994). High-resolution finite difference modeling has shown that liquid water can migrate considerable distances through fractured rock that is at above-boiling temperatures and be only partially vaporized (Pruess, 1997). Modeling of thermal testing in the ESF showed the dominance of heat conduction, but also revealed important multiphase hydrogeologic processes, such as vaporization, vapor flow, condensation, and condensate migration (Birkholzer and Tsang, 1997b; Tsang and Birkholzer, 1998). Reactive chemical transport simulations have been initiated to model the complex chemical transformations that accompany the hydrothermal processes (Sonnenthal et al., 1998).

## **6. Discussion and Conclusions**

Yucca Mountain presents an unusual hydrogeologic environment, with many features that are favorable to the safe, long-term isolation of high-level nuclear wastes. Net infiltration is low, and has been estimated in the range of 5 mm/yr on average at current climatic conditions. Thick

layers of fractured, welded and non-welded tuffs provide large-scale permeability which easily accommodates natural water percolation rates, causing development of a very thick (approximately 600 m) unsaturated zone. Water seepage in this zone is complex and difficult to characterize, as had been anticipated in early discussions of unsaturated waste storage (Winograd, 1974). It has become clear that low average values for infiltration do not necessarily translate into slow migration of aqueous solutes. Seepage behavior is highly variable both temporally and spatially. There is now a large body of field data that demonstrates the presence of fast preferential flow paths, where aqueous solutes can travel downward with average flow velocities of 10 m/yr or more. Slowly moving "old" waters, with ages of several thousand years or more, have also been documented.

Early work at Yucca Mountain had to rely on sampling and observation from boreholes. The recent completion of the Exploratory Studies Facility (ESF) has provided direct access to the proposed repository host formations. Ongoing programs of ESF-based sampling and testing have led to rapid progress in our understanding of fluid flow and mass transport at the site.

The possibility of fast solute travel as such is obviously not a desirable feature for a geologic waste disposal system. However, it appears to indicate seepage conditions that on the whole enhance, rather than diminish, the waste isolation capabilities of the Yucca Mountain site. If water seepage would occur mostly in the form of spatially-averaged percolation, groundwater travel across the unsaturated zone would be slower, but the probability that any one waste package may be contacted by water would also be larger. If most seepage indeed occurs as episodic flow in highly localized pathways, then most waste packages would be bypassed, and the probability of mobilizing water-soluble contaminants would be low. Thus, as far as waste isolation capabilities are concerned, there is a tradeoff between water seepage being fast and spatially localized, versus seepage being slow and widely distributed.

The prevalence of localized preferential flow in fracture networks also suggests considerable robustness of the Yucca Mountain hydrogeologic system. It is expected to be able to cope well with larger seepage rates, as may occur under future more pluvial climatic conditions (the "storm-sewer" concept suggested by Roseboom, 1983).

Average permeability of the fracture systems in the welded units at Yucca Mountain is high, of order 1 darcy or more, as indicated by the propagation of barometric and artificially induced gas pressure changes. Mathematical models of pressure diffusion have been very successful at matching gas pressure data from the field. Together with gas tracer tests, they have furthered our understanding of subsurface flow conditions at Yucca Mountain, and have provided fracture

porosity and permeability data that are valuable for repository design and performance analysis. The success of "macroscale continuum models" in describing gas flow at Yucca Mountain is very gratifying; it was not unexpected, however, because gas flow, being described by a parabolic PDE, is subject to strong internal averaging mechanisms.

Modeling of water flow in the unsaturated zone is much more difficult than modeling of gas flow. Most modeling of water seepage at Yucca Mountain has employed large-scale volume-averaged approaches, such as finite difference or finite element-based flow and transport models with typical spatial averaging over 10 - 100 m or more. These models have reached a very high level of sophistication, employing comprehensive multi-phase, multi-component process models, and on the order of 100,000 grid blocks in three dimensions for a detailed representation of natural and man-made hydrogeologic features in a fractured rock mass. Yet, in spite of their sophistication, serious questions and uncertainties remain about the conceptual basis and validity of these large-scale volume-averaged models. It has not been established whether or not they can properly represent the physics of partially saturated flow in fractured media, especially the fast preferential flow component. Water seepage in conditions where average hydraulic conductivity of the fracture network is much larger than net infiltration, and where rock matrix permeability is low, is dominated by gravity effects and medium heterogeneities. It lacks averaging mechanisms intrinsic to the medium, and is described by a PDE that is essentially hyperbolic in character. If important components of flow are localized in preferential pathways, then much of the system volume would not participate in these flows, and volume averages may be completely meaningless.

Macroscale continuum approaches for water seepage have a much firmer basis when applied for conceptual studies of processes on a limited range of scales. Some of the earlier work on Yucca Mountain had emphasized the role of capillary effects, which presumably would provide a mechanism for removing mobile water from the fractures through imbibition into the rock matrix, thus making the large fracture permeability unavailable for water flow. High-resolution finite difference models of water seepage in heterogeneous fracture systems have clarified the conditions under which the presence of an unsaturated rock matrix at strong suction is compatible with fast preferential water flow in fractures. It now appears that a conceptual model of episodic seepage along highly localized, preferential pathways, as suggested by field observations, is consistent with known physical mechanisms of flow.

Introduction of a strong heat source, as would be provided by high-level waste packages, gives rise to additional complexities of flow and transport. Heat transfer mechanisms tend to be diffusive in nature, and involve a considerable degree of spatial averaging, providing favorable

conditions for predicting temperature distributions. Modeling of thermal testing in the ESF showed the dominance of heat conduction, but also revealed subtle multiphase flow effects. Mobilization and fate of condensate is highly dependent on geometric details of the fracture network. Characterization of fractured rock masses in the field at a spatial resolution that would be needed for predictive modeling of condensate pathways seems impractical. High-resolution numerical simulation studies have provided insight into water seepage through fractured rocks at temperatures above the nominal boiling point. Water flowing down hot fractures is subject to vaporization, but vaporization rates are limited by the relatively slow conductive heat supply from the wall rocks. The interplay between vaporization and cooling of the rock enables localized seepage to persist through nominally superheated zones of significant thickness (many meters).

Alternative, more phenomenologically oriented modeling approaches have been developed. Notable examples are the "weeps" model (Fig. 11) of Gauthier et al. (1992), and closely related transit time distribution models (Chesnut, 1992), that seek to directly parametrize seepage behavior at Yucca Mountain in terms of parameters that can be related to repository design and performance issues, such as spatial and temporal distributions of preferential pathways. These approaches avoid the complexities and conceptual difficulties of the mechanistic process models; however, their calibration may be difficult (Ho and Wilson, 1998). Given present conceptual uncertainties, it appears prudent to pursue several alternative modeling approaches simultaneously (Pruess et al., 1997). Different models and concepts are needed to describe unsaturated flow and transport behavior on different scales. Through a combination of different approaches, including numerical, field, and laboratory studies, it should be possible to achieve a high degree of robustness in the engineering analysis and design, and thereby establish the confidence that is so vital for a successful repository project.

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## Appendix A. Mass and Energy Balances

The basic mass- and energy balance equations for multi-phase flows of multicomponent fluid mixtures can be written in the general form (Pruess, 1991)

$$\frac{d}{dt} \int_{V_n} M^\kappa dV_n = \int_{\Gamma_n} \mathbf{F}^\kappa \cdot \mathbf{n} d\Gamma_n + \int_{V_n} q^\kappa dV_n \quad (\text{A.1})$$

The integration here is over an arbitrary subdomain  $V_n$  of the flow system under study, which is bounded by the closed surface  $\Gamma_n$ . The quantity  $M$  appearing in the "accumulation term" denotes mass or energy per volume, with  $\kappa = 1, \dots, NK$  labeling the mass components (water, air,  $H_2$ , solutes, ...), and  $\kappa = NK + 1$  the heat "component."

The general form of the mass accumulation term is

$$M^\kappa = \phi \sum_{\beta} S_{\beta} \rho_{\beta} X_{\beta}^{\kappa} \quad (\text{A.2})$$

The total mass of component  $\kappa$  is obtained by summing over the fluid phases  $\beta$  (= liquid, gas).  $\phi$  is porosity,  $S_{\beta}$  is the saturation of phase  $\beta$  (i.e., the fraction of pore volume occupied by  $\beta$ ),  $\rho_{\beta}$  is the density of phase  $\beta$ , and  $X_{\beta}^{\kappa}$  is the mass fraction of component  $\kappa$  present in phase  $\beta$ . Similarly, the heat accumulation term in a multi-phase system is

$$M^{NK+1} = (1 - \phi) \rho_R C_R T + \phi \sum_{\beta} S_{\beta} \rho_{\beta} u_{\beta} \quad (\text{A.3})$$

where  $\rho_R$  and  $C_R$  are, respectively, grain density and specific heat of the rock,  $T$  is temperature, and  $u_{\beta}$  is specific internal energy in phase  $\beta$ .

Advective mass flux is a sum over phases,

$$\mathbf{F}^{\kappa} \Big|_{\text{adv}} = \sum_{\beta} X_{\beta}^{\kappa} \mathbf{F}_{\beta} \quad (\text{A.4})$$

and individual phase fluxes are given by a multi-phase version of the Darcy-Buckingham law:



$$\mathbf{F}_\beta = \rho_\beta \mathbf{u}_\beta = -k \frac{k_{r\beta} \rho_\beta}{\mu_\beta} (\nabla P_\beta - \rho_\beta \mathbf{g}) \quad (\text{A.5})$$

Here  $\mathbf{u}_\beta$  is the Darcy velocity (volume flux) in phase  $\beta$ ,  $k$  is absolute permeability,  $k_{r\beta}$  is relative permeability to phase  $\beta$ ,  $\mu_\beta$  is viscosity, and

$$P_\beta = P + P_{c\beta} \quad (\text{A.6})$$

is the fluid pressure in phase  $\beta$ , which is the sum of the pressure  $P$  of a reference phase (usually taken to be the gas phase), and the capillary pressure  $P_{c\beta}$ .  $\mathbf{g}$  is the vector of gravitational acceleration. Heat flux includes conductive and convective components

$$\mathbf{F}^{\text{NK}+1} = -\lambda \nabla T + \sum_{\beta} h_{\beta} \mathbf{F}_{\beta} \quad (\text{A.7})$$

where  $\lambda$  is thermal conductivity, and  $h_{\beta}$  is specific enthalpy in phase  $\beta$ .

Absolute permeability of the gas phase depends on pressure according to the relation given by Klinkenberg (1941)

$$k = k_{\infty} \left( 1 + \frac{b}{P} \right) \quad (\text{A.8})$$

where  $k_{\infty}$  is the permeability at "infinite" pressure, and  $b$  is the "Klinkenberg parameter." In addition to Darcy flow, mass transport can also occur by diffusion and hydrodynamic dispersion, as follows (Scheidegger, 1974; de Marsily, 1986).

$$\mathbf{F}^{\kappa} \Big|_{\text{dis}} = - \sum_{\beta} \rho_{\beta} \bar{\mathbf{D}}_{\beta}^{\kappa} \nabla X_{\beta}^{\kappa} \quad (\text{A.9})$$

The hydrodynamic dispersion tensor is given by

$$\bar{\mathbf{D}}_{\beta}^{\kappa} = D_{\beta,T}^{\kappa} \bar{\mathbf{I}} + \frac{(D_{\beta,L}^{\kappa} - D_{\beta,T}^{\kappa})}{u_{\beta}^2} \mathbf{u}_{\beta} \mathbf{u}_{\beta} \quad (\text{A.10})$$

where

$$D_{\beta,L}^{\kappa} = \phi S_{\beta} \tau_{\beta} d_{\beta}^{\kappa} + \alpha_{\beta,L} u_{\beta} \quad (\text{A.11a})$$

$$D_{\beta,T}^{\kappa} = \phi S_{\beta} \tau_{\beta} d_{\beta}^{\kappa} + \alpha_{\beta,T} u_{\beta} \quad (\text{A.11b})$$

are longitudinal and transverse dispersion coefficients, respectively.  $d_{\beta}^{\kappa}$  is the molecular diffusion coefficient for component  $\kappa$  in phase  $\beta$ ,  $\tau_{\beta}$  is the tortuosity, and  $\alpha_L$ ,  $\alpha_T$  are the longitudinal and transverse dispersivities. The mass flux from molecular diffusion alone is obtained by setting  $\alpha_L = \alpha_T = 0$  in Eq. (A.9 - A.11); diffusive flux of component  $\kappa$  in phase  $\beta$  is given by

$$\mathbf{F}_{\beta}^{\kappa}|_{\text{dis}} = -\phi S_{\beta} \tau_{\beta} \rho_{\beta} d_{\beta}^{\kappa} \nabla X_{\beta}^{\kappa} \quad (\text{A.12})$$

By applying Gauss' divergence theorem, Eq. (A.1) can be converted into the following PDE

$$\frac{\partial M^{\kappa}}{\partial t} = -\text{div} \mathbf{F}^{\kappa} + q^{\kappa} \quad (\text{A.13})$$

which is the form commonly used as the starting point for deriving finite difference or finite element discretization approaches. Of special interest is a simplified version of Eq. (A.13) for an approximate description of water seepage in the unsaturated zone. Neglecting phase change effects and assuming that the gas phase acts as a "passive bystander" with negligible gas pressure gradients, the following equation for liquid phase flow is obtained

$$\frac{\partial}{\partial t} \phi S_1 \rho_1 = \text{div} \left[ k \frac{k_{r1}}{\mu_1} \rho_1 \nabla (P_1 + \rho_1 g z) \right] \quad (\text{A.14})$$

Neglecting variations in liquid phase density and viscosity, as is appropriate for (nearly) isothermal conditions, Eq. (A.14) simplifies to Richards' equation (1931)

$$\frac{\partial}{\partial t} \theta = \text{div} [K \nabla h] \quad (\text{A.15})$$

where  $\theta = \phi S_1$  is specific volumetric moisture content,  $K = k k_{r1} \rho_1 g / \mu_1$  is hydraulic conductivity, and  $h = z + P_1 / \rho_1 g$  is the hydraulic head.

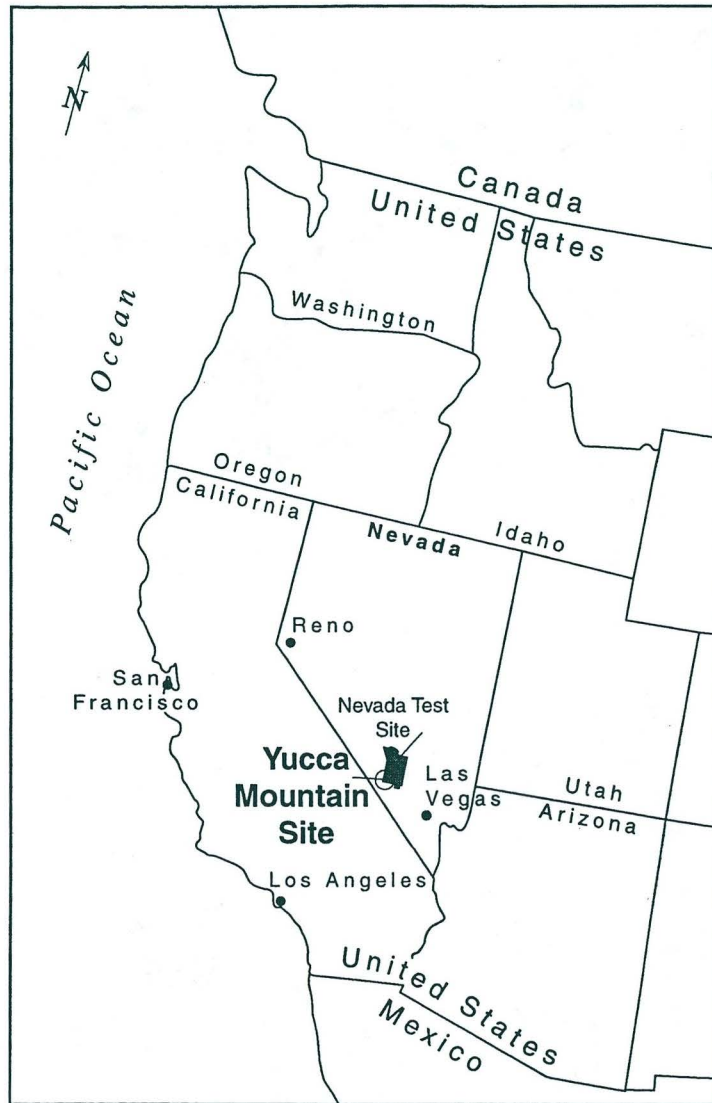


Figure 1. Location of the Yucca Mountain site.

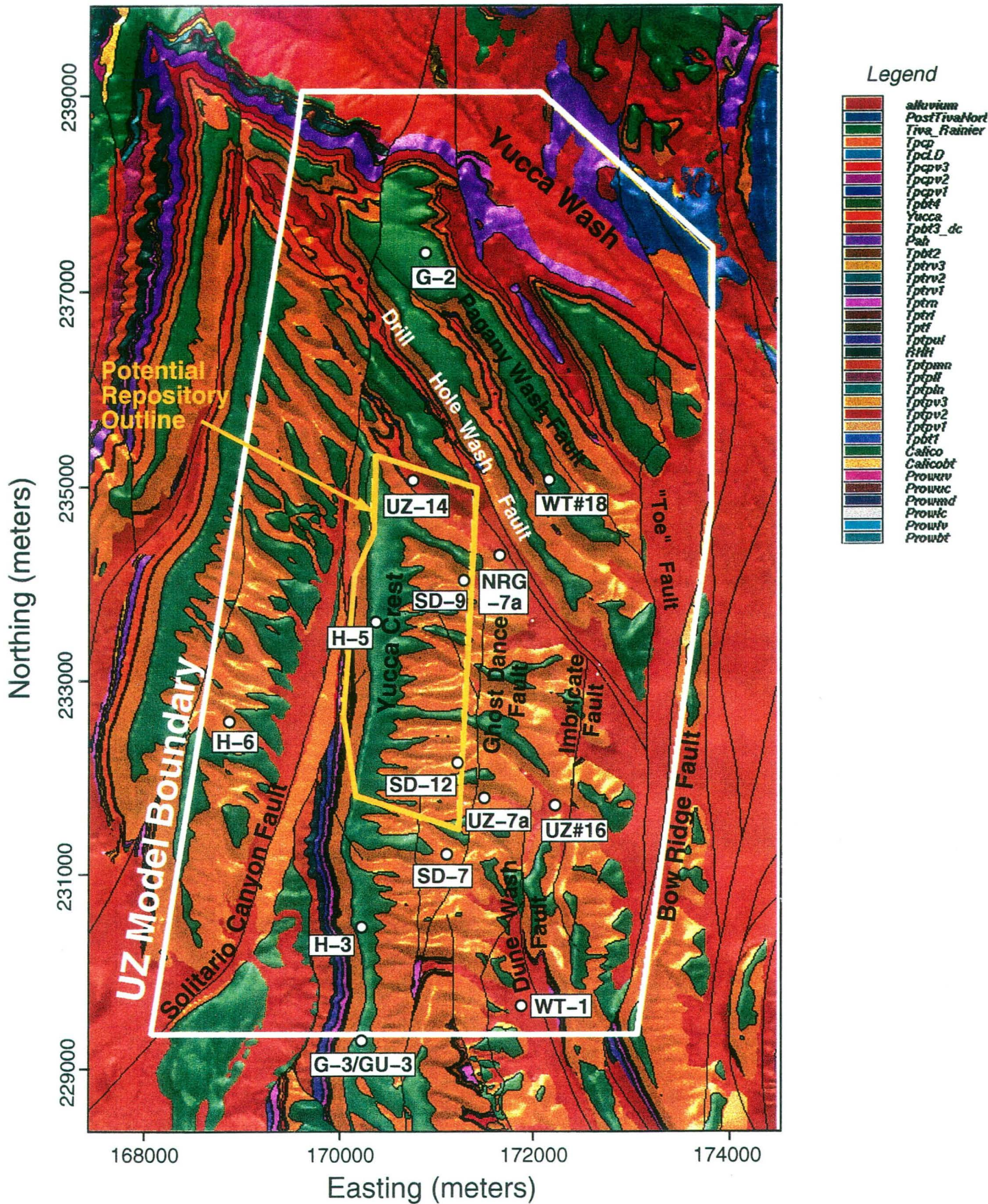


Figure 2. Surface geology with shaded relief of Yucca Mountain (J. Hinds, private communication, 1998). Selected borehole locations, the outline of the proposed repository, and the region included in current hydrogeologic models are also shown.

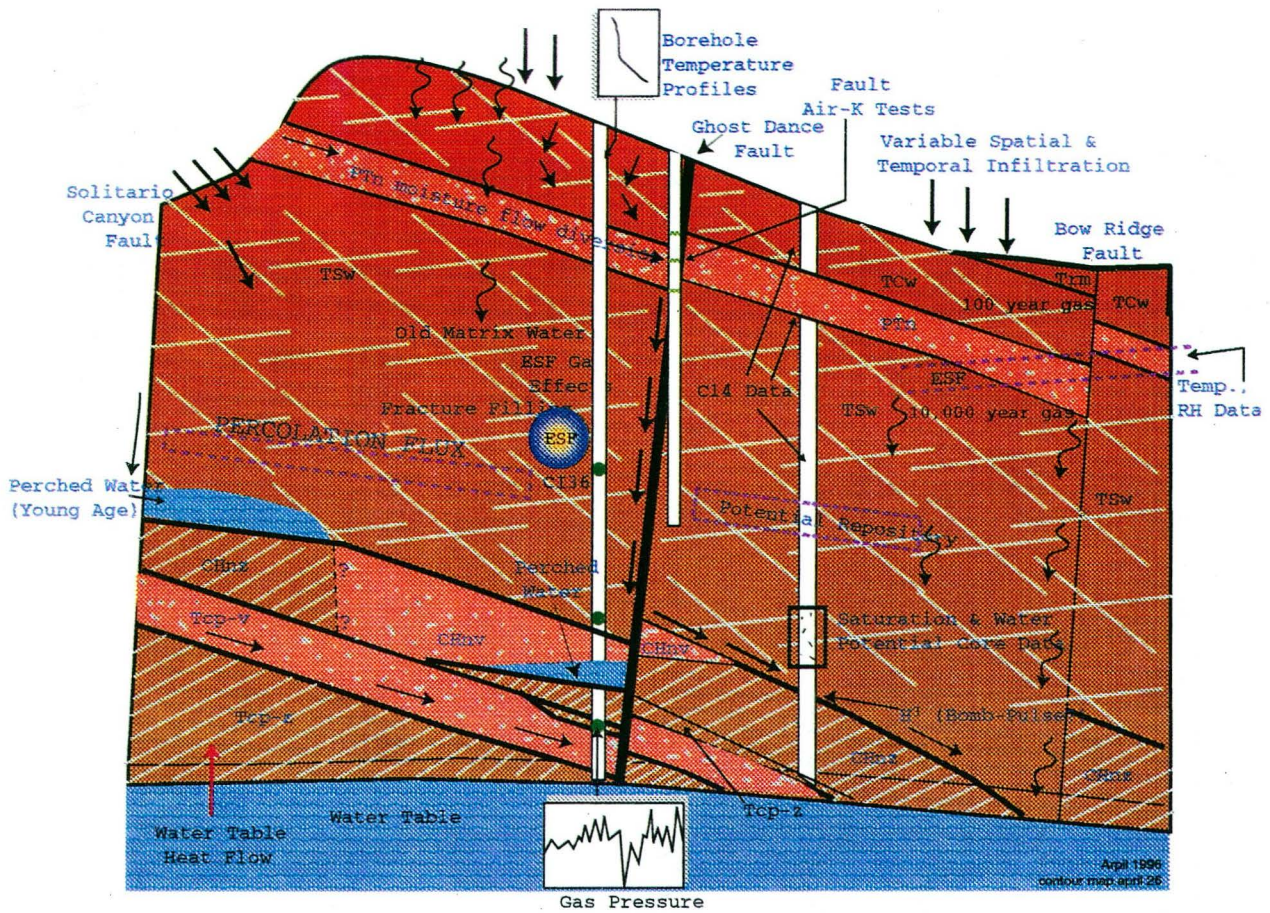
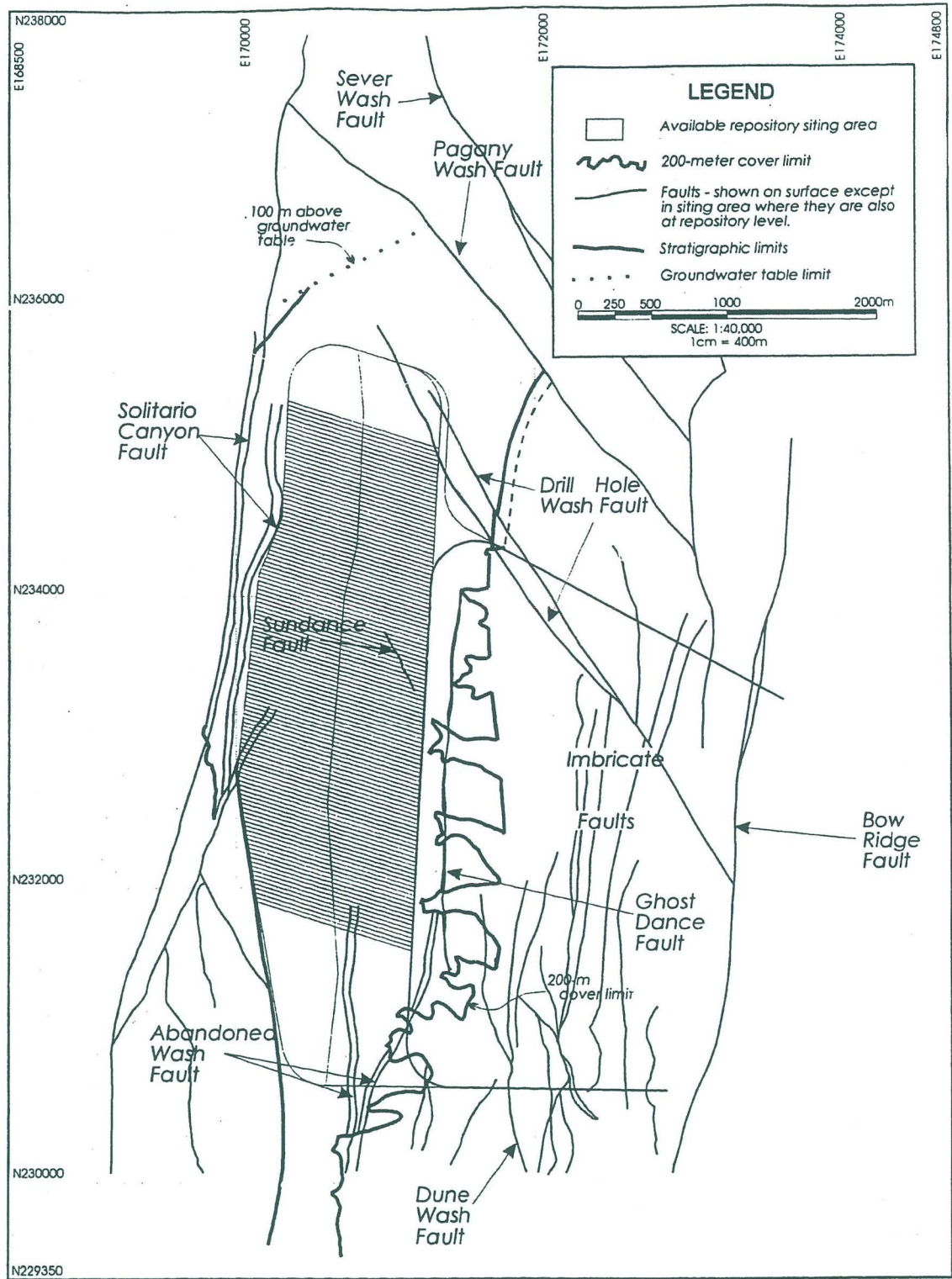


Figure 3. Schematic west-east cross section through Yucca Mountain, showing major hydrogeologic features and processes (from Bodvarsson et al., 1996).



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Figure 4. Plan view of proposed repository layout (from TRW, 1998).

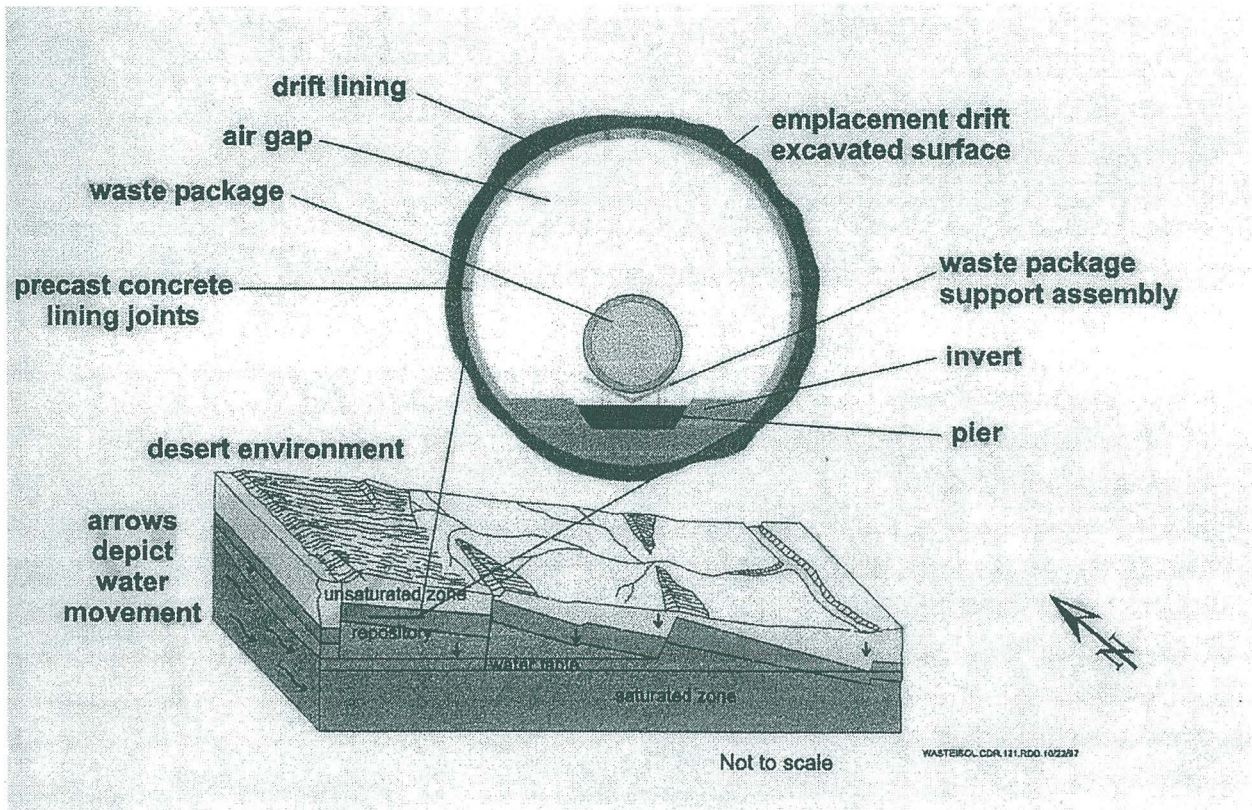
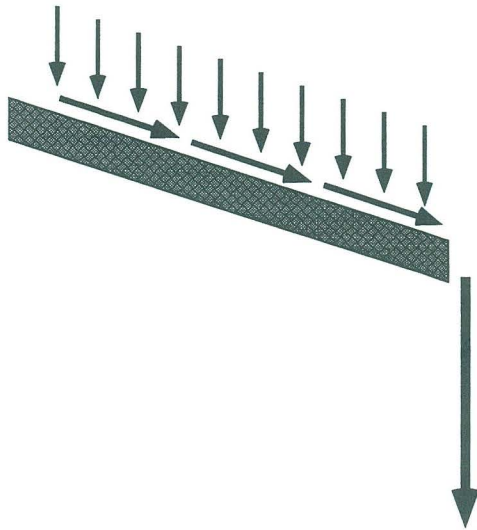
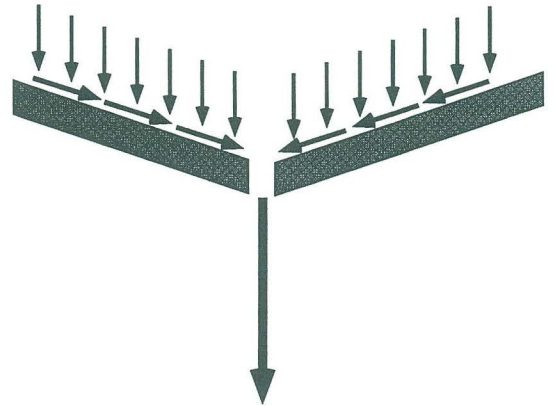


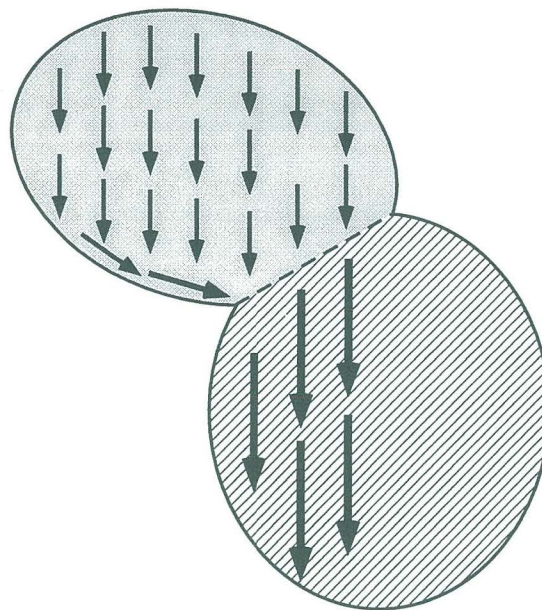
Figure 5. Proposed design for emplacement of large waste packages in drifts (from DOE, 1998).



(a) one-sided funnel



(b) two-sided funnel



(c) fracture intersection/termination

Figure 6. Schematic of heterogeneity structures that can give rise to focusing of spatially distributed flows into localized pathways (after Pruess, 1998b).



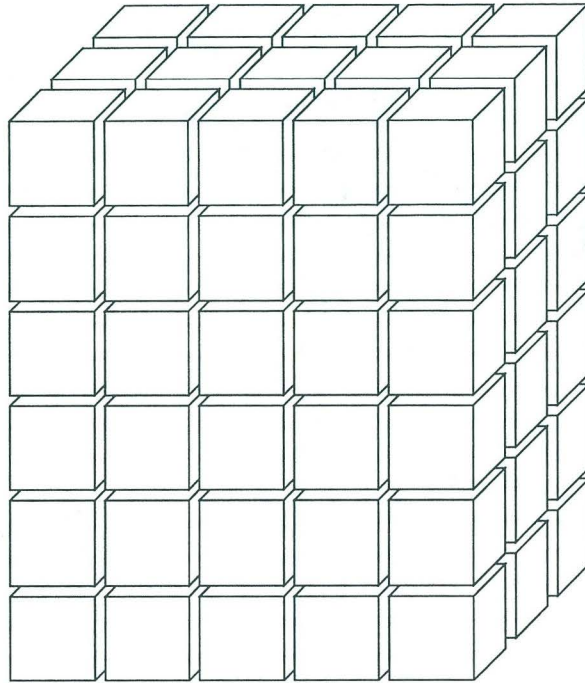


Figure 7. Schematic of the double-porosity concept (DPM; after Warren and Root, 1963). Global flow occurs exclusively through a network of interconnected fractures, which may interact with embedded matrix blocks of low permeability locally.

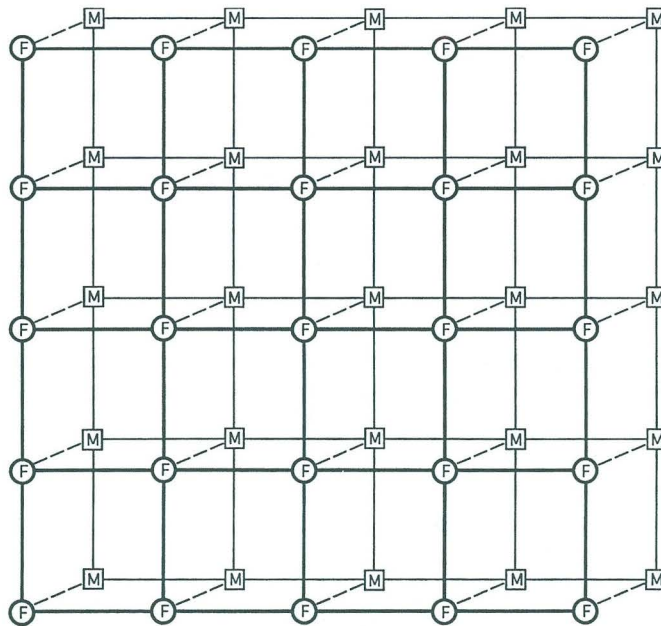


Figure 8. Most general flow connections in the dual permeability model (DKM; after Pruess, 1991). Fracture network and matrix rock both have large-scale connectivity and contribute to global flow, as well as exchanging fluid (and heat) locally.

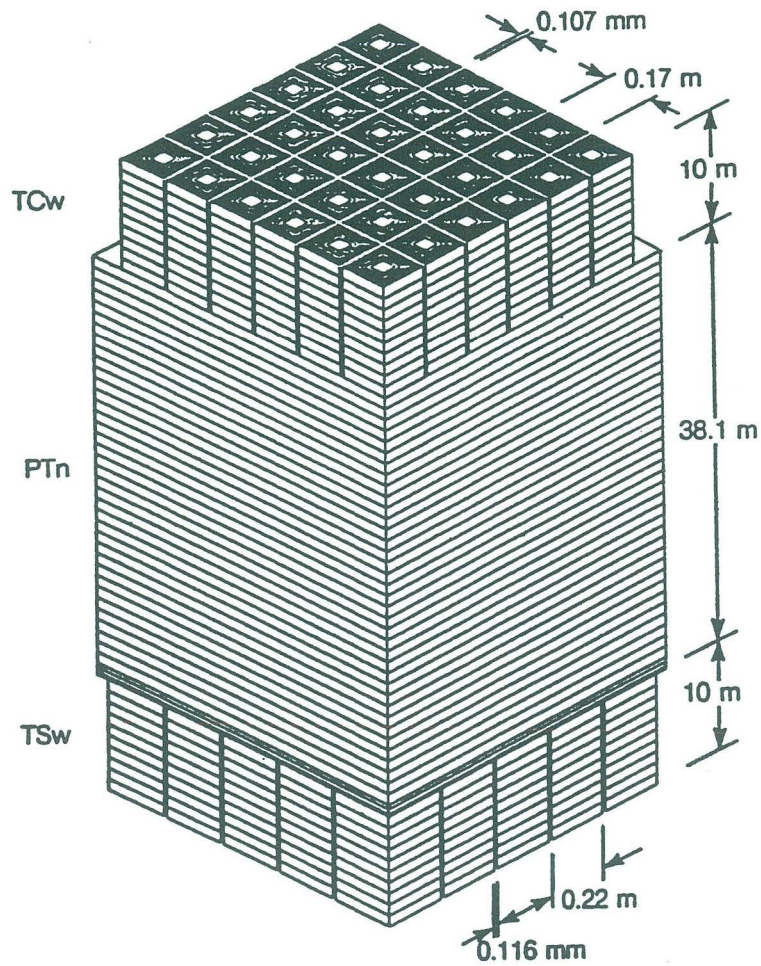


Figure 9. Three-dimensional mesh used by Wang and Narasimhan (1993) for studying propagation of infiltration pulses at Yucca Mountain. The fractured TCw and TSw units are modeled with the MINC approach, while the sparsely fractured PTn unit is modeled as a single porous medium.

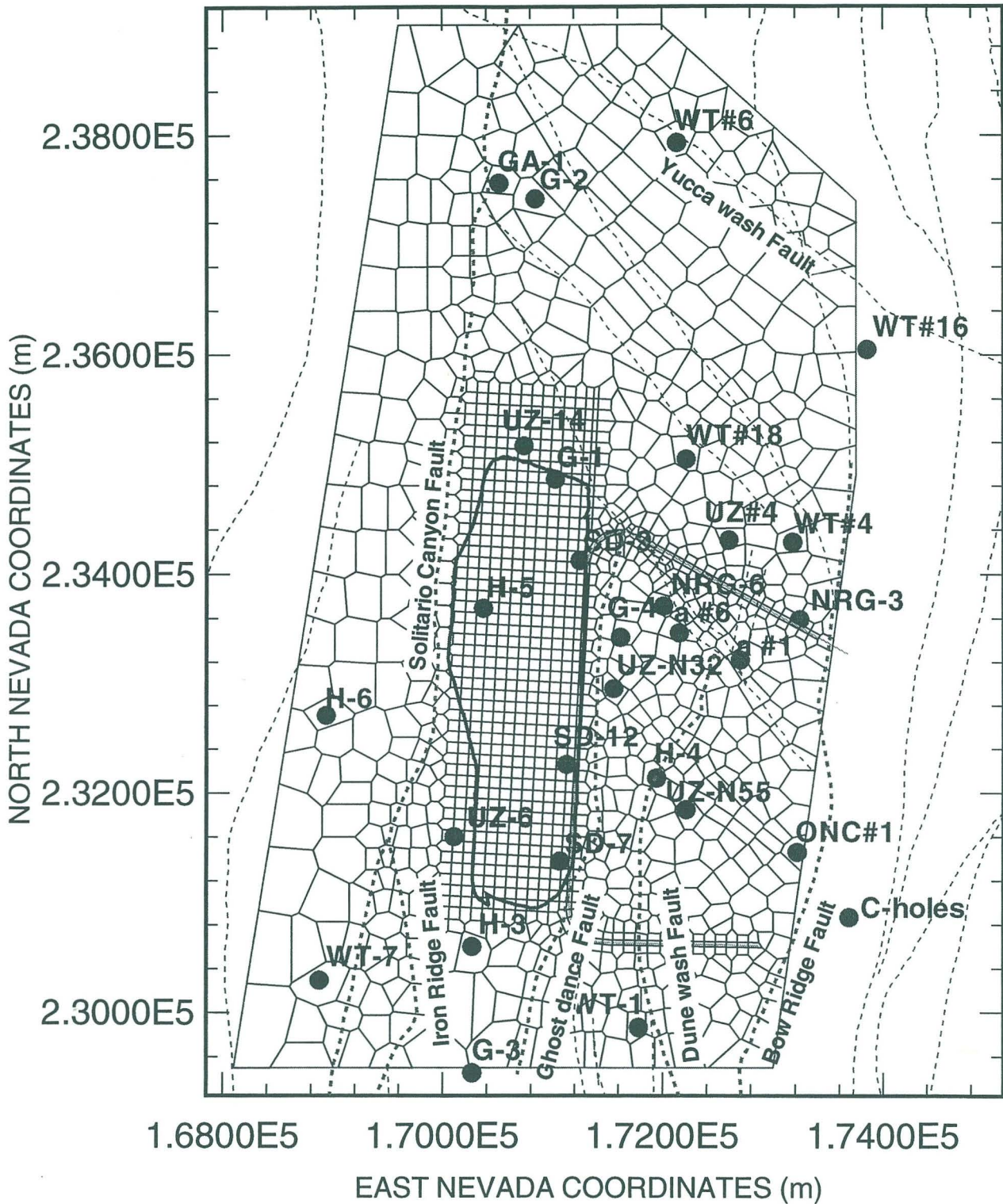


Figure 10. Plan view of computational grid used by the LBNL group for modeling flow in the unsaturated zone. A number of boreholes are also shown. The grid has 1470 blocks and 27 layers, for a total of 39,690 blocks (Wu et al., 1998b). The number of grid blocks is doubled when a dual-permeability model is used.

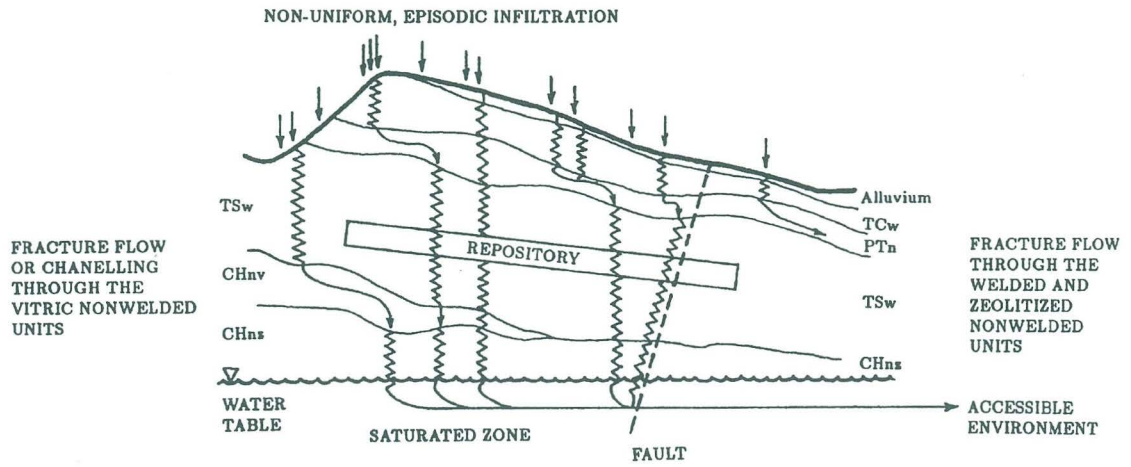


Figure 11. Schematic of the weeps model for significant fracture flow at Yucca Mountain, from Gauthier et al. (1992).

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