Evolution of the Conceptual Model of the Unsaturated Zone and other Observations at Yucca Mountain, Nevada

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Documenting our current understanding and how we got here

- National Research Council Panel (2001)
- Journal of Hydrology (2001)
- Reviews of Geophysics (2001)
PROBLEM: questions, goals, decisions

Available site-specific data, experience

Generic scientific knowledge: physics, chemistry, biology

CONCEPTUAL MODEL: features, processes, events

disciplinary bias

MATHEMATICAL MODEL computer code, verification

MODEL CALIBRATION (PARAMETER ESTIMATION) sensitivity analysis, parameter uncertainty

MODEL TESTING including peer review

PREDICTIONS with uncertainty

SOLUTIONS? decisions, regulations, policy, management

FIELD DATA collection analysis

data not used for calibration

(from Hsieh et al., 2001)
By 1990 TSPA estimated less than 1 percent chance that flux through the TS\textsubscript{w} was more than 3 mm/yr

80 percent chance the flux was less than 1 mm/yr
Early Data Collection
(by 1986 over 100 boreholes had been drilled)

- Deep boreholes
- Shallow neutron holes
- Surface geologic mapping
- Meteorology
- Geochemistry and hydrologic properties of rock core
Early Conceptual Models of Hydrology

- Identified water as a critical parameter
- Described geologic/hydrologic framework
- Identified relevant hydrologic processes
- Described consequences of hydrologic flow
Early Conceptual Models (Scott et al., 1983)
Early Conceptual Models (Roseboom, 1983)
Early Conceptual Models (Montazer and Wilson, 1984)

Diagram:

- A: Alluvium
- TC: Tiva Canyon Welded Unit
- P: Paintbrush Nonwelded Unit
- TS: Topopah Spring Welded Unit
- CH: Calico Hills Nonwelded Unit
- CF: Crater Flat Unit

Legend:
- Arrow with a line: Direction of liquid flow
- Arrow with a triangle: Direction of vapor movement
- Triangle: Perched water
Early Conceptual Models (DOE, 1984)
Four major concepts that strongly influenced further development of the conceptual model

- Fully saturated matrix was required for fracture flow
- Overall flux was low
- Only matrix flow occurred in the TSw
- Most net infiltration was diverted laterally by the PTn
Hypothetical relationship between effective permeability and matric potential for a double-porosity medium

(Montazer and Wilson, 1984)
Conceptual model of a partially saturated, fractured, porous medium

(Wang and Narasimhan, 1985)
Alternative conceptual models and their corresponding characteristic curves

(Altman et al., 1996)
Development of current conceptual and numerical models (mid 1990’s paradigm shift)

- Three-dimensional site-scale numerical model
- Spatially distributed high infiltration
- Little lateral flow in PTn
- Evidence of fast fracture flow
- Decoupled fracture flow (important modeling breakthrough)
Three-dimensional site scale model grid with early version of potential repository boundary

(Flint and Flint, 1994)
- Spatially distributed infiltration in bedrock units

(Flint and Flint, 1994)
Spatially distributed net infiltration at Yucca Mountain using (a) statistical analyses and (b) numerical modeling.

(a) Statistical analyses
(b) Numerical modeling

Hudson and Flint, 1995
Flint et al., 1996
Developing a Conceptual Model of Flow in the Near Surface
Net infiltration; a precursor to flux

- Infiltration is the process of water entering the soil surface.
- Net infiltration is the quantity of water that has moved below the zone of evapotranspiration.
- Knowing net infiltration is a critical precursor to knowing recharge.
- Percolation or drainage is the process by which net infiltration moves through the unsaturated zone.
- Recharge is quantity of net infiltration that reaches the regional water table (net infiltration today may be recharge 5,000 years from now).
Net infiltration at Yucca Mountain

- Factors controlling infiltration
  - Precipitation
  - Soil thickness
    - Soil porosity
    - Drainage characteristics
  - Bedrock permeability
  - Evapotranspiration
Net infiltration at Yucca Mountain

- Conceptual understanding
  - Arid conditions make net infiltration an infrequent occurrence
  - Particularly wet winters allow for near saturated conditions at the soil-bedrock interface which allows fracture flow and deep penetration of infiltrated water below the zone of evapotranspiration
  - Deep soils (non stream channels) have sufficient soil water storage capacity to retain most precipitation in the root zone for eventual evapotranspiration
  - Runoff accumulates and infiltrates enough water to overcome the storage capacity of the root zone in deeper soils allowing for deep penetration of infiltrated water below the zone of evapotranspiration
Mechanisms Controlling Net Infiltration (Recharge)
Precipitation + Change in Storage - Drainage - ET - Runoff = 0
Moisture monitoring in 99 neutron-access boreholes monthly for over 10 years became one of the most useful tools for evaluating the spatial processes contributing to net infiltration and percolation.
Infiltration at Borehole UZN #1

DEPTH, IN METERS


WATER CONTENT, IN METERS PER METER

0.05 0.15 0.25

bedrock
Infiltration at Borehole UZN-15

(75 cm soil over 2 m lower porosity fractured bedrock, underlain by 10 m high porosity fractured bedrock)
Calculation of Flux
Measuring Soil Water Potential Gradient using Heat Dissipation Probes

Probes are plotted for March, June, and September.

Probe depth is from ground surface

Depth to bedrock is 75 cm

Water Potential, in bars

7.0 cm 15.0 cm 36.5 cm 73.7 cm
Calculation of Flux

Selected Data
Change in Water Content
24-hr Data

Water Content, in m/m
Change in Water Content, in mm/day

Mar Jun Sep
Observations on Data Supporting Higher Fluxes

- Neutron hole data
- Darcy flux calculations in the PTn
- Tritium
- C-14
- Thermal profiles
- Chloride mass balance
- Other chemistry techniques
Temperature profiles: inverse modeling using various fluxes

(a) and (b) show graphs of temperature (degrees Celsius) against elevation (meters). The graphs display modeled temperature profiles for various fluxes, with measured temperatures indicated by diamond markers. The fluxes represented are 0.1 mm/a, 0.5 mm/a, 1.0 mm/a, 2.0 mm/a, 5 mm/a, 10 mm/a, and 15 mm/a.
Comparison of Flux from Thermal Modeling with Net Infiltration

\[ y = 0.64x - 0.36 \]

\[ R^2 = 0.47 \]
Schematic of North Ramp Alcoves used for Darcy flux calculations
Darcian Flux Calculations

- Darcy’s law, \( q = K(\theta) \left( \frac{d\psi}{dz} \right) \)
- Using *in situ* matric potential measurements from boreholes to estimate hydraulic gradient and core properties
  - 8-15 mm/yr vertical flux in 2 boreholes
  - < 1 mm/yr lateral flux in the PTn or the top of the welded Topopah Spring Tuff
Surface Fluxes over Trace of ECRB

- Potential Repository Boundary
- Boreholes used in large-scale analyses

Legend:
- 0 mm/year
- 0.1 - 1
- 1 - 3
- 3 - 5
- 5 - 10
- 10 - 20
- 20 - 50
- > 50
Cross Drift Moisture

The graph shows the relationship between matric potential and modeled net infiltration across cross drift stations. The x-axis represents the cross drift station in meters, ranging from 0 to 2600 m. The y-axis on the left represents matric potential in MPa, ranging from 0.01 to 1.0 MPa, and the y-axis on the right represents modeled net infiltration in mm/yr, ranging from 0.01 to 1000 mm/yr.

Key features of the graph include:
- Green circles indicating matric potential data points.
- Black line representing modeled net infiltration.
- Fault markers at specific cross drift stations.

The graph illustrates how matric potential and modeled net infiltration vary with distance and the presence of faults.
Comparison of Flux from Chloride Mass Balance with Net Infiltration

Flux, mm/yr

CMB Method
Bounds of Modeled Flux
Comparison of percolation fluxes estimated by various methods
Beyond Net Infiltration

- Unsaturated flow in the UZ is vertical (gravitational gradients dominate)
- Lateral flow in the UZ generally occurs under locally saturated conditions
- Fracture flow initiated in the near surface can move quickly toward the PTn (<50 year travel time)
- Matrix flow in the PTn dampens seasonal and decadal pulses of water (except for faults) and greatly increases travel time
- Vertical fracture flow in TSw
- Lateral flow above the zeolitic CHz
- Recharge occurs through major faults
Current (2000) conceptual model of flow in the unsaturated zone

Average annual precipitation: 170 mm

Infiltration: 5 mm/yr (ranging 0 - 80 mm/yr)

Surface

TCw

fracture flow

PTn

matrix flow

Welded Tiva Canyon Tuff

Paintbrush Group nonwelded tuff

Welded Topopah Spring Tuff

TPw

fracture flow

CHv

matrix flow

Nonwelded Calico Hills Formation

CHz

perched water

water table
ESF faults and Cl-36/Cl: evidence for fast pathways
Current (2001) site-scale unsaturated zone numerical model grid
Spatially distributed net infiltration at Yucca Mountain compared to flux estimates at the water table using a 3-D hydrologic model.
Observations on Lateral Diversion

- New analyses since the “Evolution” paper regarding the PTn
Paintbrush Tuff
nonwelded unit
(PTn)

- This unit has been targeted as the location of a capillary barrier mechanism for diverting downward percolation laterally
- Modeling exercises have repeatedly supported this concept
- Models have typically used idealistic geometry and large contrasts in properties
Diversion due to PTn

- Early observations of high saturation above the PTn suggested the potential for lateral diversion
- Core data, however showed the lack of strong property contrasts, except at the bottom of the PTn
- Analytical solution to the flow equation, using detailed measured properties, showed insignificant diversion
PTn Diversion: analytical estimates of Capillary Barrier Effects

\[ Q_{\text{max}} = \frac{K_s \tan \phi}{\alpha} \left[ \left( \frac{q}{K_s^*} \right)^{\alpha^*} - \left( \frac{q}{K_s} \right) \right] \]

\[ L = \frac{Q_{\text{max}}}{q} \]  
(Ross, 1990)

- Equations are based on Darcy’s law and applied to sloping interfaces between 2 media
- Includes contrast in pore sizes with upper layer having smaller pores
- Downward flux rate, degree of slope, and permeability of the 2 media influence diversion due to capillary barrier effects
Diversion above PTn:

Influence of number of layers representing the real properties of transitional units

![Graph showing the relationship between number of layers and Q_max (cm²/day)]
Diversion within PTn:
Analytical estimates using mean properties for each layer

<table>
<thead>
<tr>
<th>Hydrogeologic unit</th>
<th>Porosity (v/v)</th>
<th>Saturated Hydraulic Conductivity (m/s)</th>
<th>$\alpha$</th>
<th>Qmax (cm$^2$/d)</th>
<th>Fracture Density (F/m)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean</td>
<td>Geometric mean</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CNW</td>
<td>0.39</td>
<td>1.2E-08</td>
<td>0.009</td>
<td>0</td>
<td>0.5</td>
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<tr>
<td>BT4</td>
<td>0.44</td>
<td>5.8E-07</td>
<td>0.005</td>
<td>4.7</td>
<td>0.5</td>
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<tr>
<td>TPY</td>
<td>0.27</td>
<td>1.6E-07</td>
<td>0.016</td>
<td>0</td>
<td>1.0</td>
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<tr>
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<td>5.4E-07</td>
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<td>TPP</td>
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<td>0.0001</td>
<td>1.0</td>
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<td>BT2</td>
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<td>2.2E-06</td>
<td>0.005</td>
<td></td>
<td>0.5</td>
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</table>
Diversion at the Base of the PTn:
Representing transition of vitric tuff properties overlying vitrophyre fractures

<table>
<thead>
<tr>
<th>Matrix porosity (v/v)</th>
<th>Fracture aperture* (microns)</th>
<th>$\alpha$ (1/cm)</th>
<th>$K_s$ (cm/day)</th>
<th>Air entry of matrix (cm)</th>
<th>Total $Q_{\text{max}}$ (cm²/day)</th>
<th>$L$ (m)</th>
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</thead>
<tbody>
<tr>
<td>vitric tuff fractures</td>
<td>0.2</td>
<td>0.0248</td>
<td>1.9E-02</td>
<td>1423</td>
<td>2.8</td>
<td>207</td>
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<td>vitric tuff fractures</td>
<td>0.2</td>
<td>25</td>
<td>0.0007</td>
<td>1.8E-02</td>
<td>1423</td>
<td>3.2</td>
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<tr>
<td>vitric tuff fractures</td>
<td>0.1</td>
<td>125</td>
<td>0.1482</td>
<td>2.7E-01</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>vitric tuff fractures</td>
<td>0.1</td>
<td>25</td>
<td>0.0004</td>
<td>1.8E-02</td>
<td>0</td>
<td>0</td>
</tr>
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<td>125</td>
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<td>125</td>
<td>0.1482</td>
<td>2.7E-01</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

*Fracture properties from Kwicklis and Healy (1993)
Potential for Lateral Diversion?

- On the basis of analyses and interpretations, it seems clear that the early conceptual models of lateral diversion did not take into consideration the scale at which the mechanisms responsible for diversion operate in a natural system.

- Neither data nor field observations corroborate the existence of lateral diversion caused by a barrier effect due to the PTn.

- Calculations and field data support the conceptual model of small-scale localized lateral diversion, and generally large-scale vertical fluxes through the PTn.
Observations on Fracture Characteristics

- Detailed measurements in ESF benches provide unsaturated properties of fractures
- Fractures may exhibit multi-hump curves
- Small fractures may carry high fluxes and be in potential equilibrium with matrix
Fracture Permeability

![Fracture Permeability Graph]

- Conductivity (m/s) vs. Potential (-m)
- Lines represent different fracture sizes and types:
  - 25 um (Kwicklis)
  - 125 um (Kwicklis)
  - 250 um (Kwicklis)
  - Tptpmn Fracture (LBNL)
  - Tptll Fracture (LBNL)
  - Percolation

Legend:
- Blue: 25 um (Kwicklis)
- Pink: 125 um (Kwicklis)
- Green: 250 um (Kwicklis)
- Blue: Tptpmn Fracture (LBNL)
- Yellow: Tptll Fracture (LBNL)
- Orange: Percolation
ECRB Bench #4, 17+35, Tptpll
ECRB Bench #1, Fracture Permeability

![Graph showing conductivity vs. potential with different fracture sizes.](image-url)
ECRB Bench #4, Fracture Permeability

![Diagram showing conductivity vs potential with different labels and markers for different samples and sizes.](image-url)
Measured and Modeled Fracture Permeability

![Graph showing measured and modeled fracture permeability.](image)

- Measured and modeled permeability values are presented on a logarithmic scale for both potential and conductivity.
- Key markers and labels corresponding to different permeability values and scenarios are shown.
- The graph includes lines and markers for various permeability values, such as 25 um, 125 um, 250 um, and 2.5 um, among others.
- Different scenarios and fluxes are indicated through distinct markers and line styles.

**Legend:**
- 25 um (Kwicklis)
- Tptpmn matrix
- Tptpmn (air)
- Tptpmn B1 flux
- Tptpmn B4 flux
- Tptpmn Fracture (LBNL)
- 125 um (Kwicklis)
- Alcove 1 (water)
- Tptpl (air)
- Tptpl B2 flux
- Percolation
- 250 um (Kwicklis)
- Tptpl (air)
- Tptpl Niche 5 (air)
- Tptpl B3 flux
- 2.5 um (Kwicklis)
- Tptpmn matrix (LBNL)
Final Thoughts and Lessons Learned

- Model development must start with a clear statement of the problem and identify technical objectives
- A variety of alternative conceptual models should be formulated early on in the project
- Numerical models should be developed concurrently with conceptual models
- Evaluation of conceptual models should rely on consistency with independent lines of evidence
- Robust model development depends on an extensive high-quality dataset at different spatial and temporal scales
Summary

- The early models had low flux, extensive lateral flow in the PTn, and no fracture flow through the TSw.
- The current model has high flux (5 to 10 mm/yr) with over 80 mm/yr in some locations, vertical matrix-dominated flow in the PTn, fracture-dominated flow in the TSw, vertical matrix-dominated flow in the vitric rocks of the Calico Hills and Prow Pass, and extensive lateral flow above the zeolitic boundary in those units.
Summary

- Within these few concepts we have made significant strides in addressing the major issues regarding the behavior of Yucca Mountain as a potential nuclear waste repository.

- The conceptual model we have today has evolved over 20 years through an integrated scientific approach with highly motivated and creative scientists from a variety of disciplines and organizations that were provided a work environment that fostered quality technical interaction.
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