U.S. DEPARTMENT OF ENERGY
OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

NUCLEAR WASTE TECHNICAL REVIEW BOARD FULL BOARD MEETING

SUBJECT: NUMERICAL MODELING OF PROPOSED YUCCA MOUNTAIN REPOSITORY UNDER VARIOUS THERMAL LOADS

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Key Issues about Yucca Mountain Thermo-hydrological Performance

The critical concern is water contacting a waste package (WP), accelerating its failure rate, and transporting radionuclides to the water table

The only credible means of getting water to WPs and transporting radionuclides to the water table is by nonequilibrium fracture flow, originating from

- Episodic infiltration of meteoric water
- Condensate drainage due to repository-heat-driven
  - Boiling conditions
  - Small-scale and mountain-scale, buoyant vapor flow

Preferential fracture pathways do not need to be connected to overlying meteoric sources

Three Fundamental Questions about Thermo-hydrological Performance of the Mined Geological Disposal System (MGDS)

- Can the thermal load be limited and distributed in such a way that the hydrological impact of repository heat is negligible?

- For the reference SCP-CDR thermal load, will the thermal impacts on the hydrological system and the understanding of those impacts demonstrate that the MGDS meets regulatory compliance?

- For higher thermal loads, which have the potential of generating extended-dry conditions, will the thermal impacts on the hydrological system and the understanding of those impacts demonstrate that the MGDS meets regulatory compliance?

Status of Modeling Repository-Heat Driven Hydrothermal Flow

Past calculations addressed averaged thermo-hydrological performance

- Considered a limited range of bulk permeability, k_b
- Impact of heterogeneous properties, nonequilibrium flow, and spatially variable heating conditions was not emphasized

More recent calculations include complementary models and analyses in order to address impact of heterogeneity and nonequilibrium flow

Status of Modeling Repository-Heat-Driven Hydrothermal Flow

(Continued)

Recent calculations consider a very broad range of thermal-loading parameters, thermo-hydrological properties (e.g., k_b), and boundary conditions to

- Identify distinct regimes of thermo-hydrological performance
- Identify critical dependencies
- Evaluate the impact of the assumptions
- Develop fundamental hypotheses addressing thermo-hydrological performance
- Identify the parameter space for which the hypotheses are invalidated

Based on this understanding, a comprehensive strategy is being developed for testing and analysis

Model Assumptions

- V-TOUGH code (LLNL's version of LBL's TOUGH code)
- Equivalent Continuum Model (ECM)
- Hydrostratigraphic units are horizontal and have constant thickness
- Repository-scale R-Z model
- Drift-scale X-Z model
- Initial vertical temperature, saturation, and pressure profiles correspond to geothermal and pneumatistatic pressure gradients and assumed recharge flux
- Thermal loading history with all WPs emplaced at t = 0 yr

Modeling Statistical Variability in Condensate Drainage

- Analytical models for performance assessment
- Condensate flow idealized as a log-normal random field
- Estimates variability about the mean of the condensate flux computed from numerical models
- Transient fracture flow
- Focusing of condensate

There are various time and length scales involved in how repository heat influences the three major potential sources of fracture flow

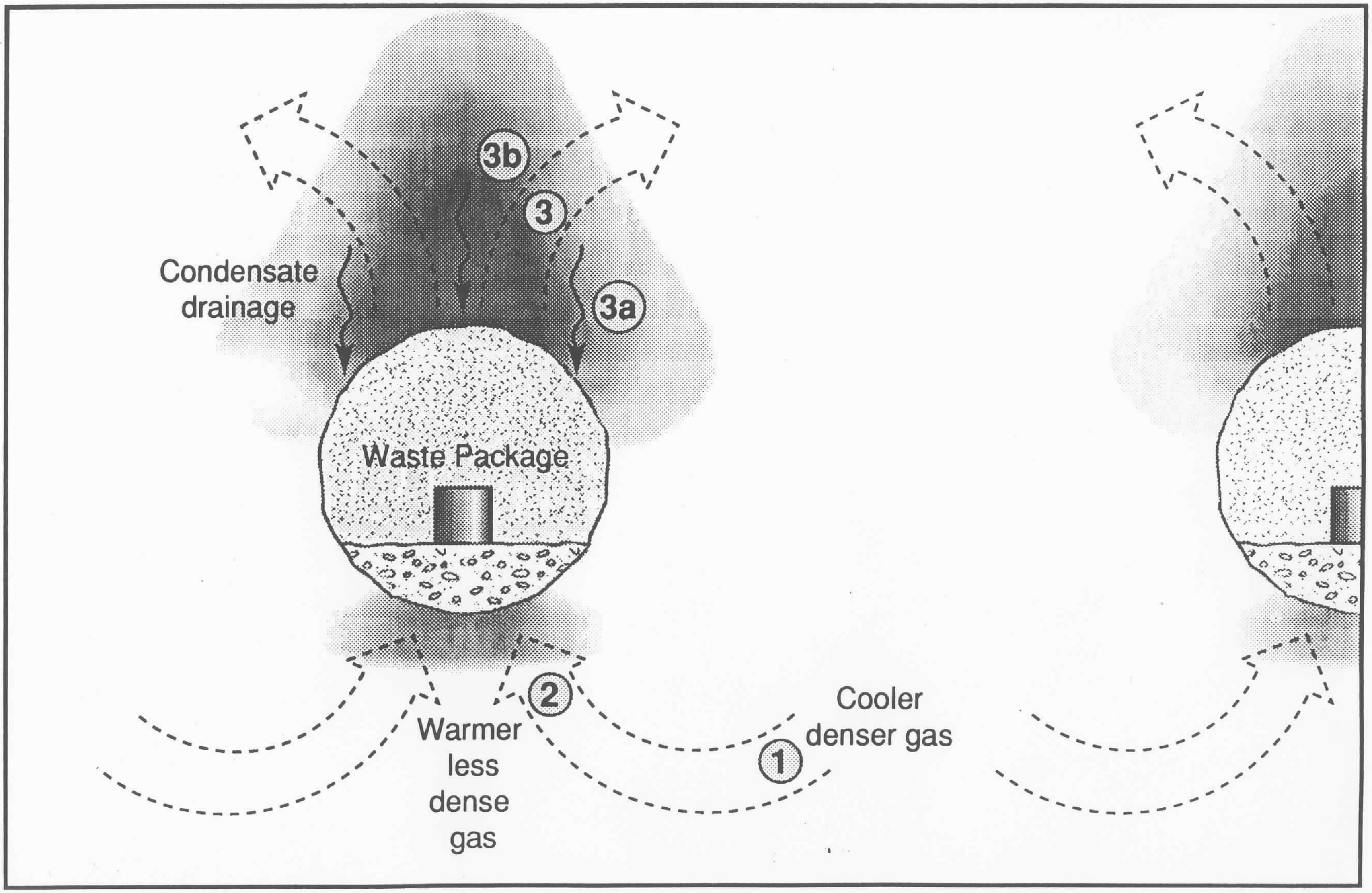
Natural infiltration

Affected by repository-heat-driven changes to the

- moisture distribution
- intrinsic hydrological, geochemical, and geomechanical properties

Buoyant, gas-phase convection and condensate drainage		Boiling and condensate drainage	
Small-scale	Mountain-scale	Small-scale	Mountain-scale
Local heating conditions WP/EBS/repository design	Global heating conditions Areal Mass Loading AML (MTU/acre)	Local heating conditions WP/EBS/repository design	Global heating conditions Areal Mass Loading AML (MTU/acre)
Near-field hydrological properties	UZ-scale hydrological properties	Near-field hydrological properties	UZ-scale hydrological properties
t < 1000 yr	1000 < t < 100,000 yr	t < 50 yr for 27 MTU/acre t < 1000 yr for 49 MTU/acre t < 50 yr for 155 MTU/acre	t < 1000 yr t < 100,000 yr for residual effects

Small-Scale, Buoyant, Gas-phase Convection and Condensate Drainage



Small-Scale, Buoyant, Gas-phase Convection and Condensate Drainage

(Continued)

- **Occurs within fracture networks having a connectivity with length scale comparable to the distance between the hot and cold regions of the repository**

  ① **Buoyant convection cells develop as the warmer, less dense column of gas within the footprint of the hot WPs is displaced by the cooler, denser column of gas in adjacent areas (areas without WPs or with cooler WPs)**

  ② **As the initially cooler gas is heated up, its relative humidity is lowered, causing it to evaporate water from the rock matrix below the hot regions of the repository**

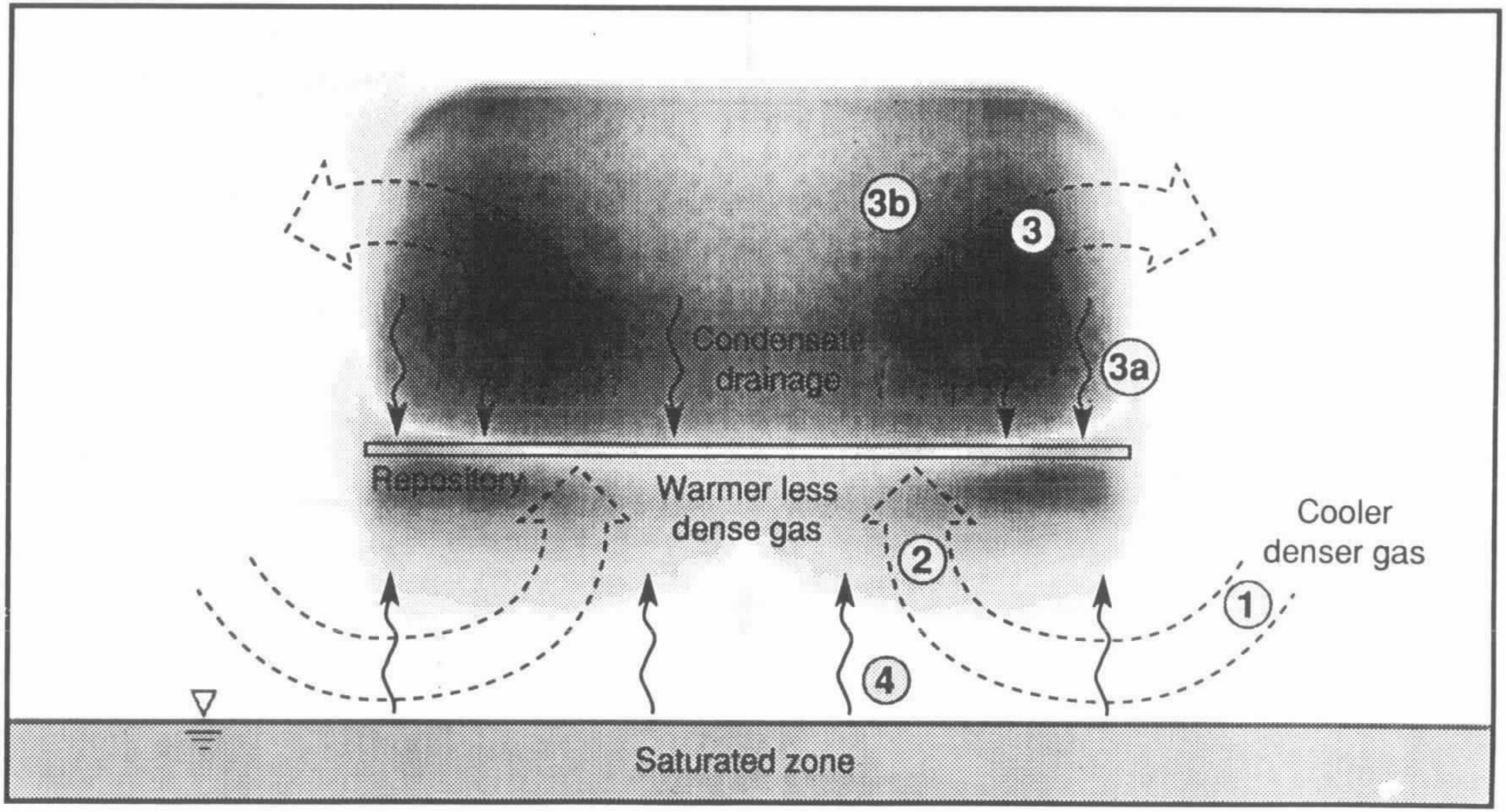
  ③ **This warm moist air is convected upward to where it cools above the repository, generating condensate that:**

    (3a) **Drains down fractures back towards the repository horizon, and/or**

    (3b) **Is imbibed by the matrix, causing a saturation buildup above the repository horizon**

      - Small-scale, buoyant, gas-phase convection continues as long as significant temperature differences persist within the repository
      - Given sufficiently large fracture connectivity, large-scale, buoyant, gas-phase convection may eventually replace small-scale convection

Mountain-Scale, Buoyant, Gas-phase Convection and Condensate Drainage



Mountain-Scale, Buoyant, Gas-phase Convection and Condensate Drainage

(Continued)

- Occurs within fracture networks having a connectivity with length-scale comparable to the UZ thickness and repository width

① Buoyant convection cells develop as the warmer, less dense column of gas within the footprint of the repository is displaced by the cooler, denser column of gas outside of the repository footprint

② As the initially cooler gas is heated up, its relative humidity is lowered, causing it to evaporate water from the rock matrix below the repository

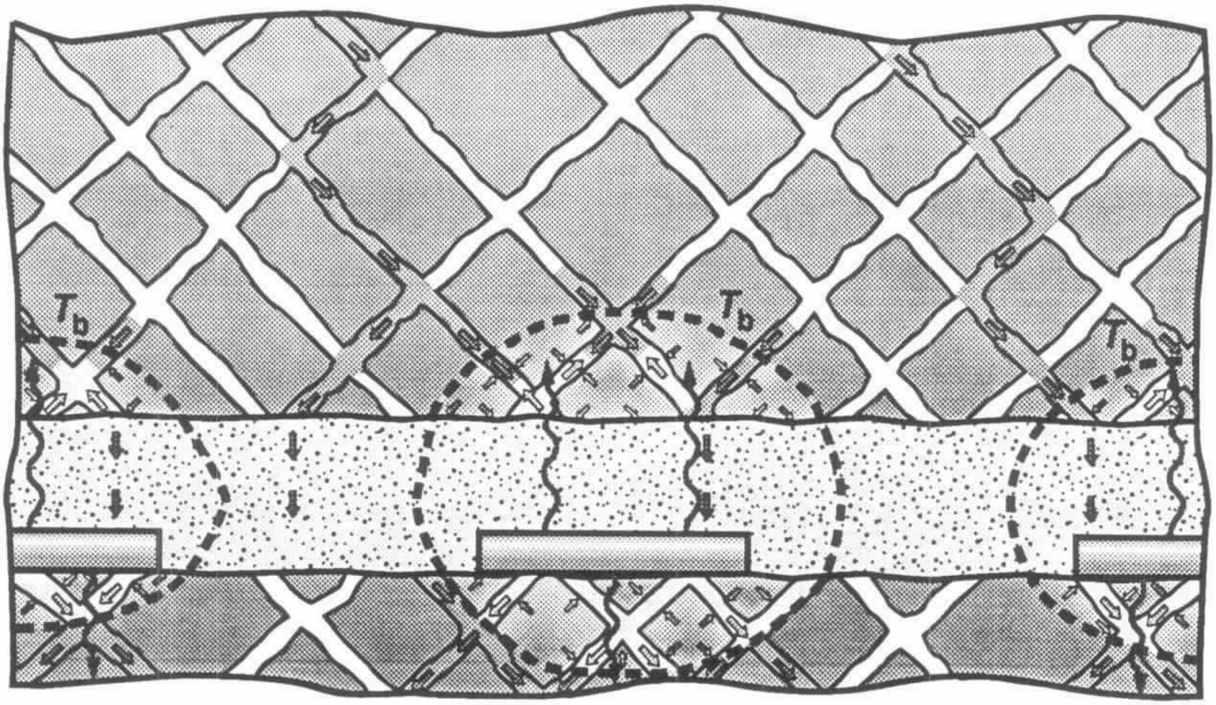
③ This warm moist air is convected upward to where it cools above the repository, generating condensate that:

  (3a) Drains down fractures back towards the repository horizon, and/or

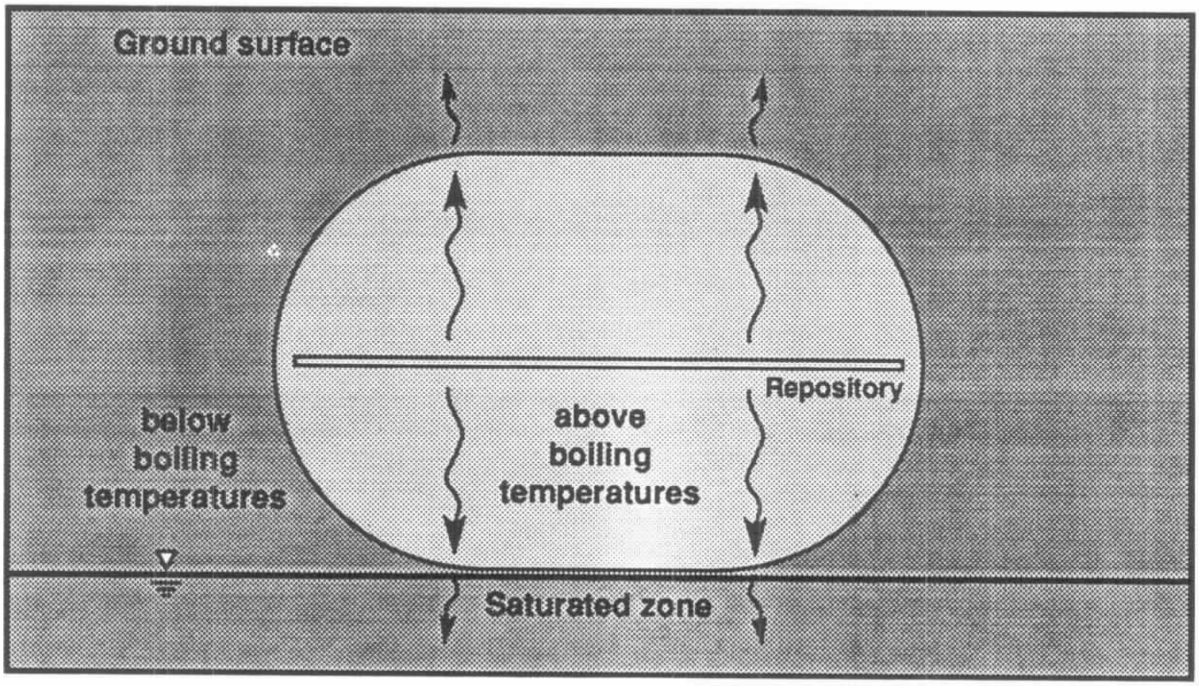
  (3b) Is imbibed by the matrix, causing a saturation buildup above the repository horizon

④ Because water removed below the repository may be replenished by water imbibed from the SZ, this process can result in a net saturation increase in the UZ

Small-Scale and Mountain-Scale Boiling & Condensate Drainage Effects



Small-scale boiling and condensate drainage



Mountain-scale boiling and condensate drainage

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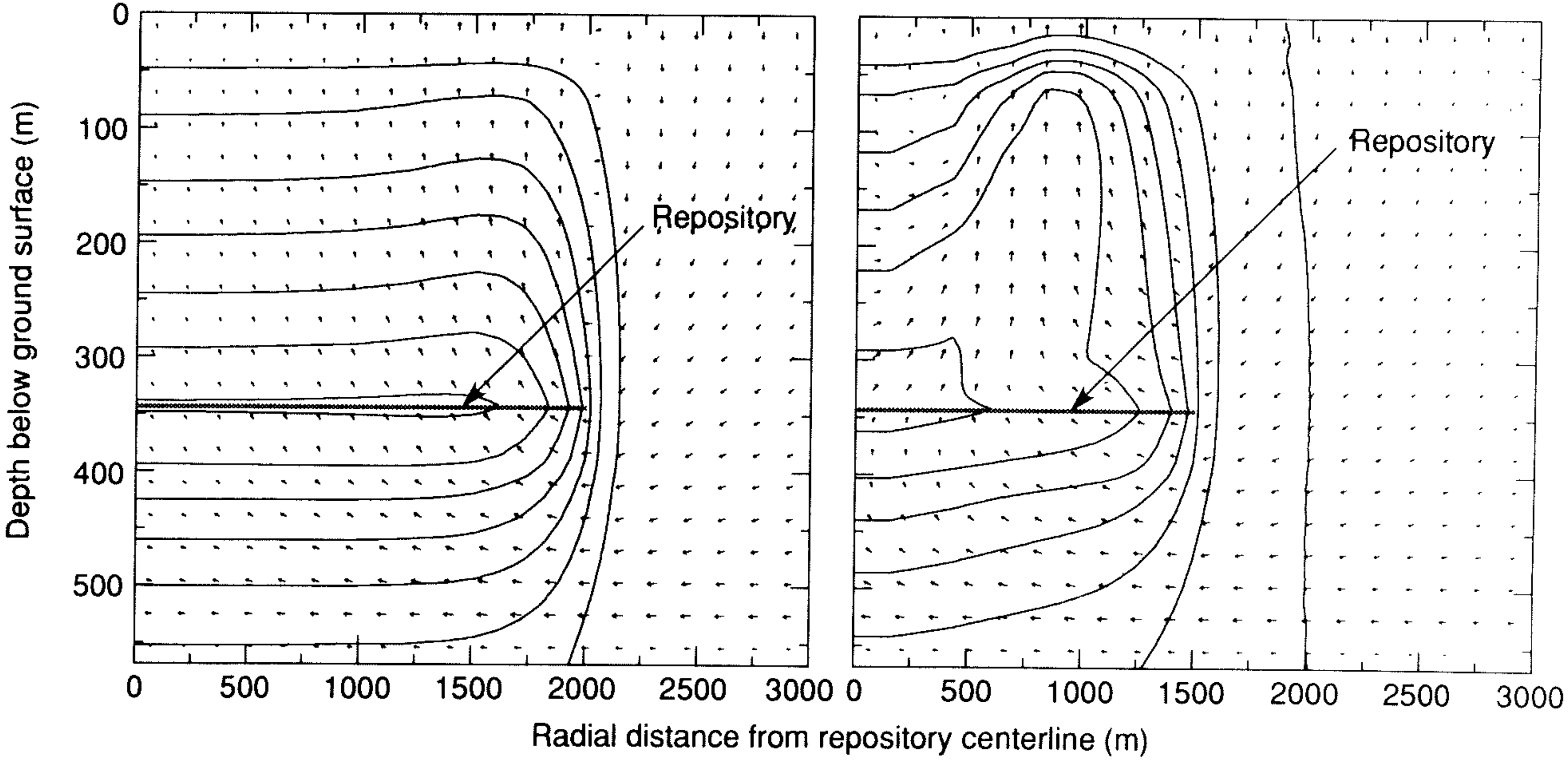
Small-Scale and Mountain-Scale Boiling & Condensate Drainage

- Small-scale boiling and condensate drainage effects occur as long as sub-boiling conditions persist at the repository

- For sufficiently large Areal Mass Loading (MTU/acre), the effects of boiling and condensate drainage begin to occur at the scale of the mountain

Mountain-Scale, Buoyant Vapor Flow and Condensate Drainage

Temperature Buildup Contours and Gas-phase Velocity Vectors at t=1000yr for $k_b = 40$ darcy



20 kW/acre
30-yr-old SNF
27.1 MTU/acre

57 kW/acre
10-yr-old SNF
49.2 MTU/acre

Mountain-Scale, Buoyant Vapor Flow and Condensate Drainage

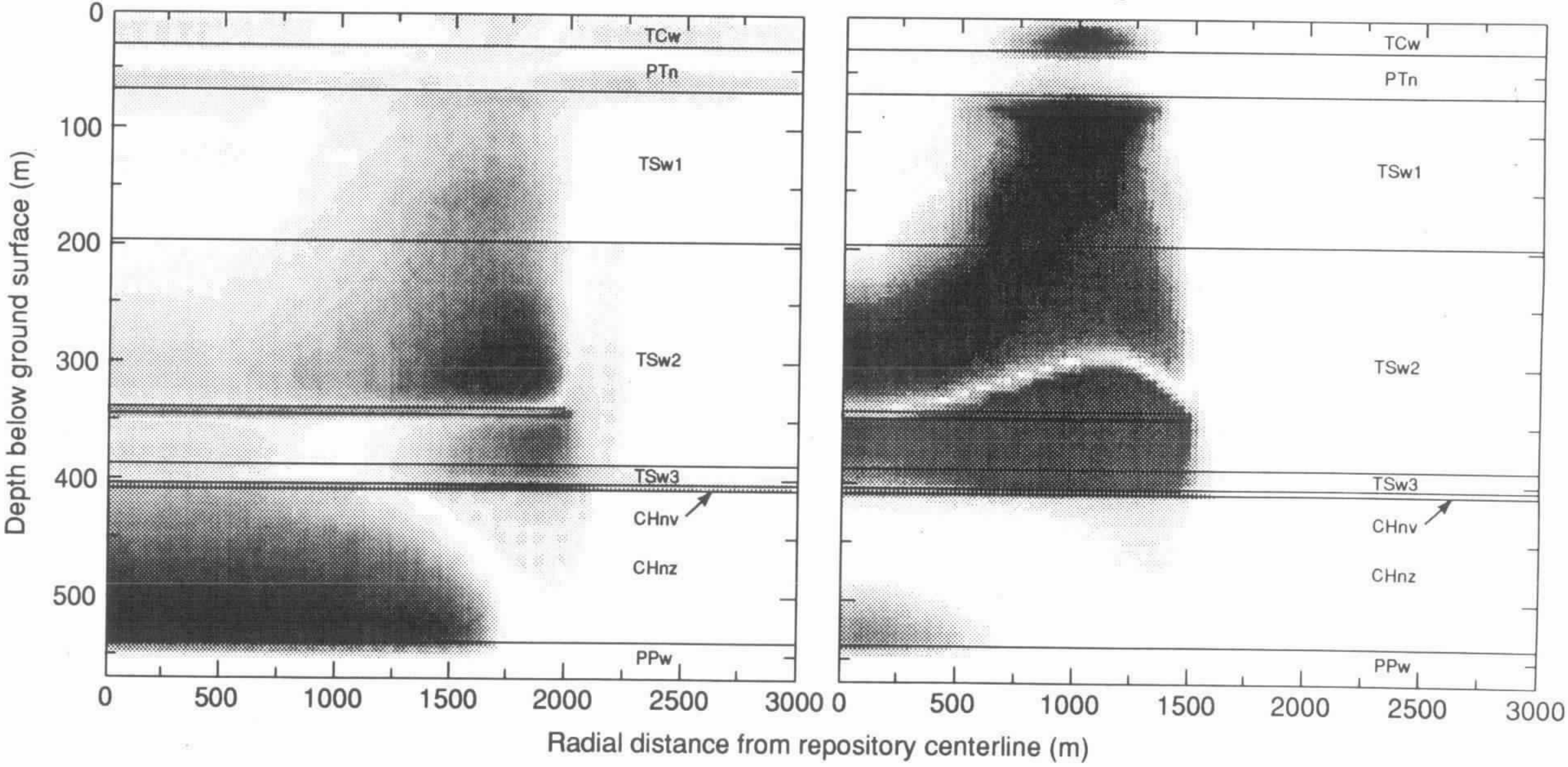
(Continued)

- Given sufficiently large connected bulk permeability, k_b, mountain-scale, buoyant vapor flow begins to dominate moisture movement in the unsaturated zone (UZ) 1000 yr after waste emplacement
- Given sufficient magnitude, buoyant convection can also dominate heat flow

Mountain-Scale, Buoyant Vapor Flow and Condensate Drainage

(Continued)

Dimensionless Liquid Saturation Contours at t = 1000yr for k_b = 40 darcy



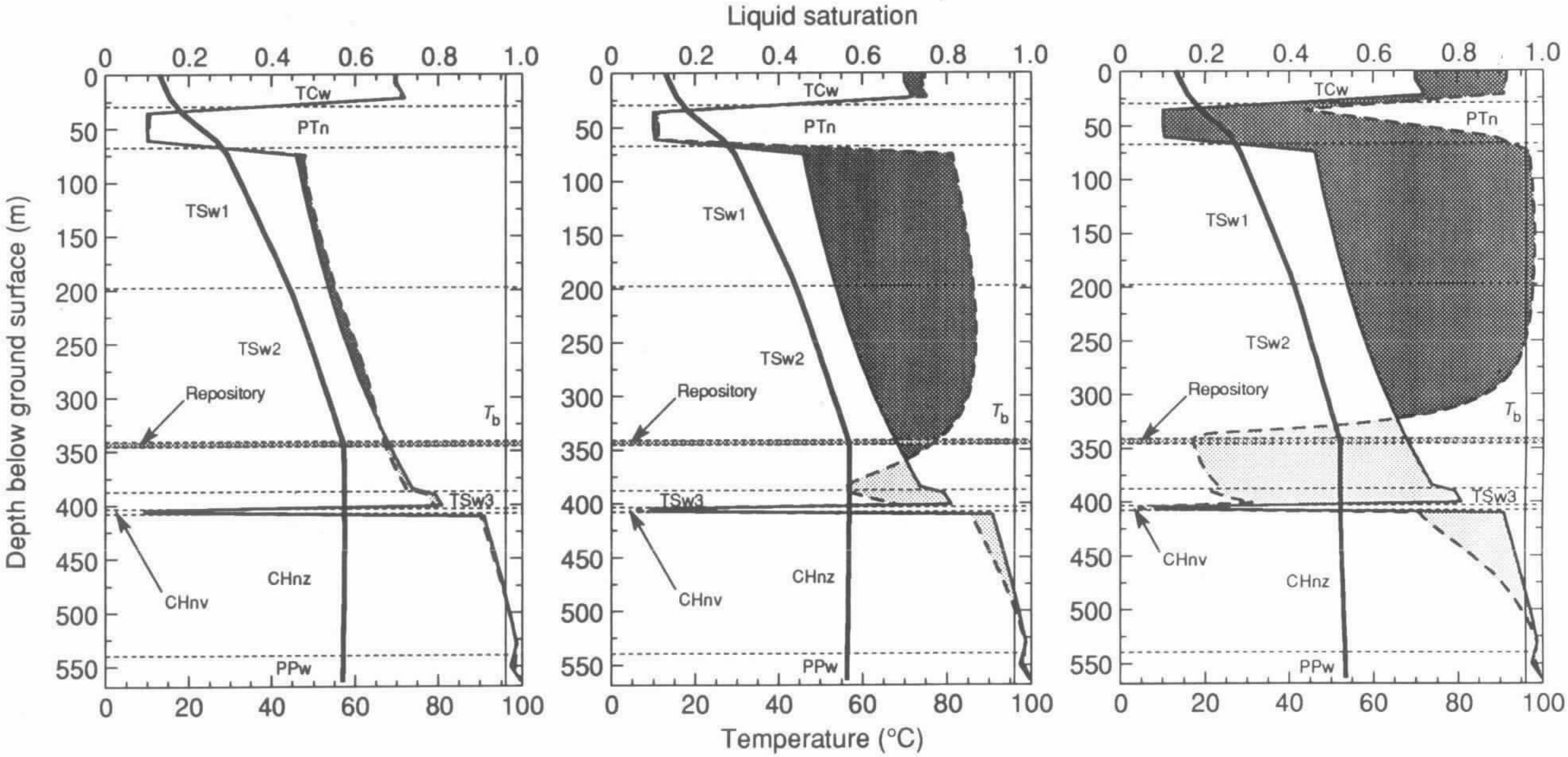
20 kW/acre
30-yr-old SNF
27.1 MTU/acre

57 kW/acre
10-yr-old SNF
49.2 MTU/acre

Mountain-Scale, Buoyant Vapor Flow and Condensate Drainage

(Continued)

Vertical Temperature and Saturation Profiles at t = 10,000yr for 10-yr-old SNF, an APD of 57 kW/acre, and an AML of 49.2 MTU/acre



k_b = 280 millidarcy at r = 0 m

k_b = 10 darcy at r = 800 m

k_b = 84 darcy at r = 0 m

Mountain-Scale, Buoyant Vapor Flow and Condensate Drainage

(Continued)

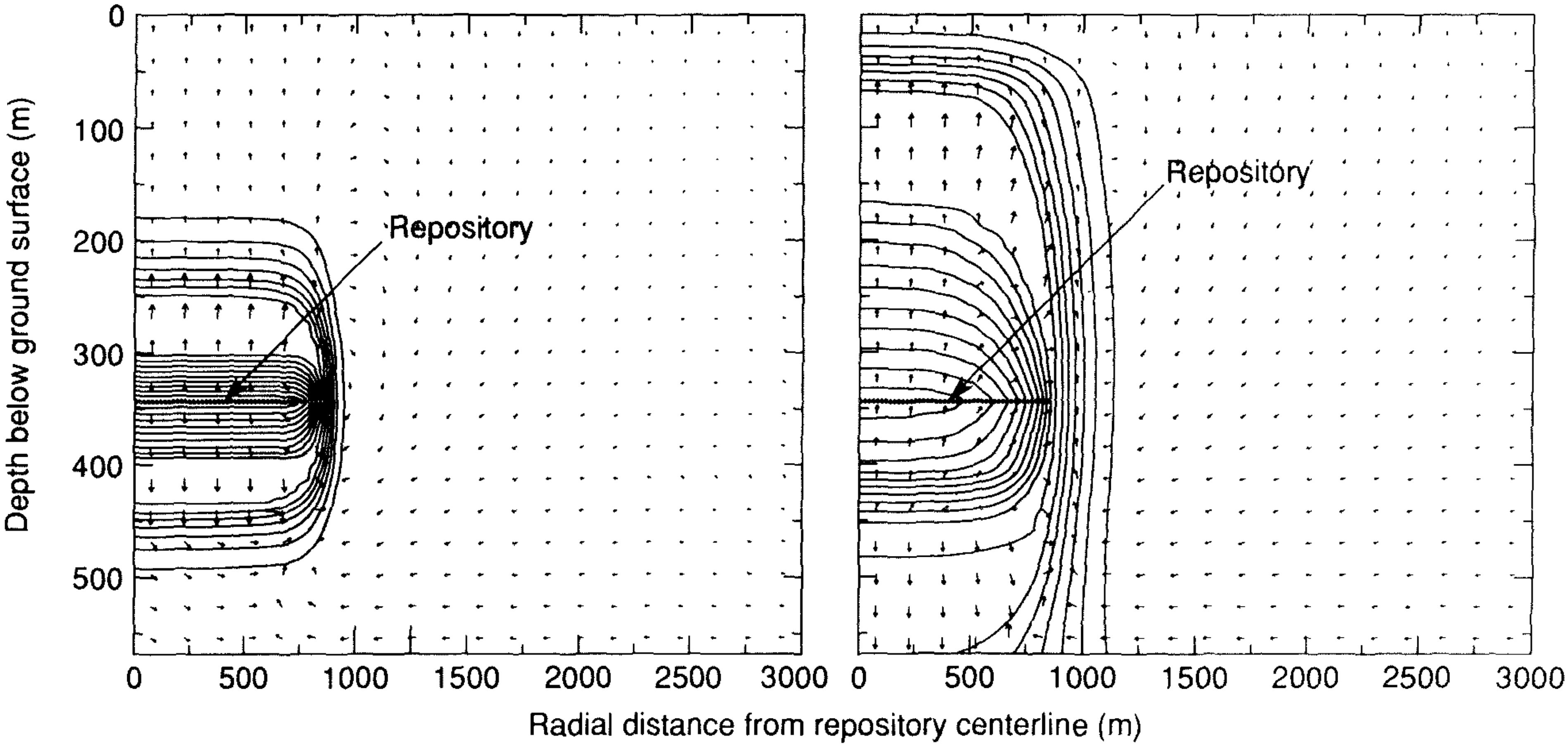
- Given sufficiently large connected bulk permeability, k_b, mountain-scale, buoyant vapor flow begins to dominate moisture movement in the unsaturated zone (UZ) 1000 yr after waste emplacement

- Given sufficient magnitude, buoyant convection can also dominate heat flow

- Given sufficiently large connected k_b, mountain-scale, buoyant vapor flow can cause the saturation in the upper half of the unsaturated zone to approach 100%

The development of a large, persistant region of above-boiling temperatures can suppress mountain-scale, buoyant vapor flow for thousands of years

Temperature Buildup Contours and Gas-Phase Velocity Vectors for
30-year-old SNF, an APD of 114 kW/acre, and an AML of 154.7 MTU/acre

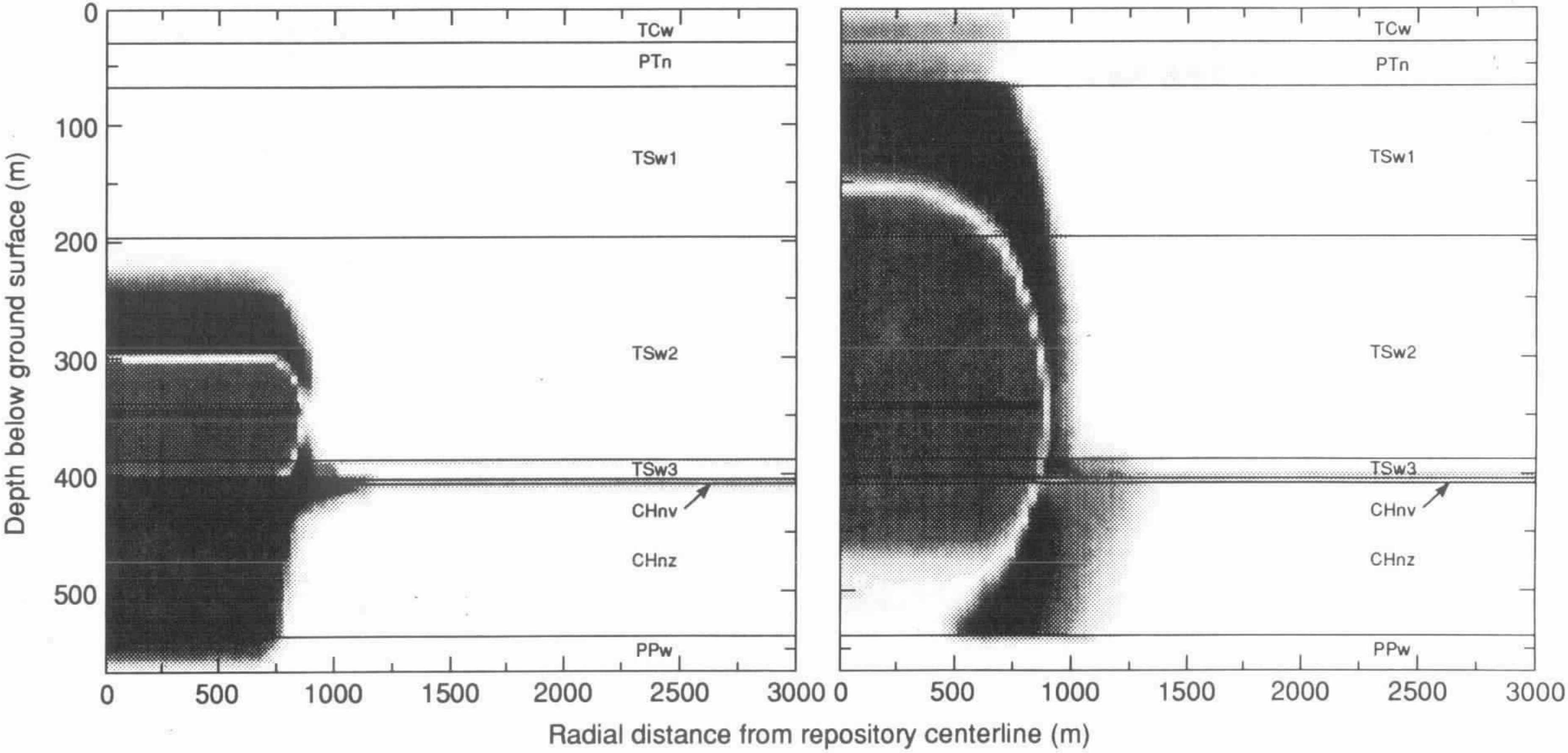


t = 100 yr

t = 1000 yr

About 90% of the total dry-out due to boiling occurs within the first 1000 yr

Dimensionless Liquid Saturation Contours for 30-year-old SNF,
an APD of 114 kW/acre, and an AML of 154.7 MTU/acre

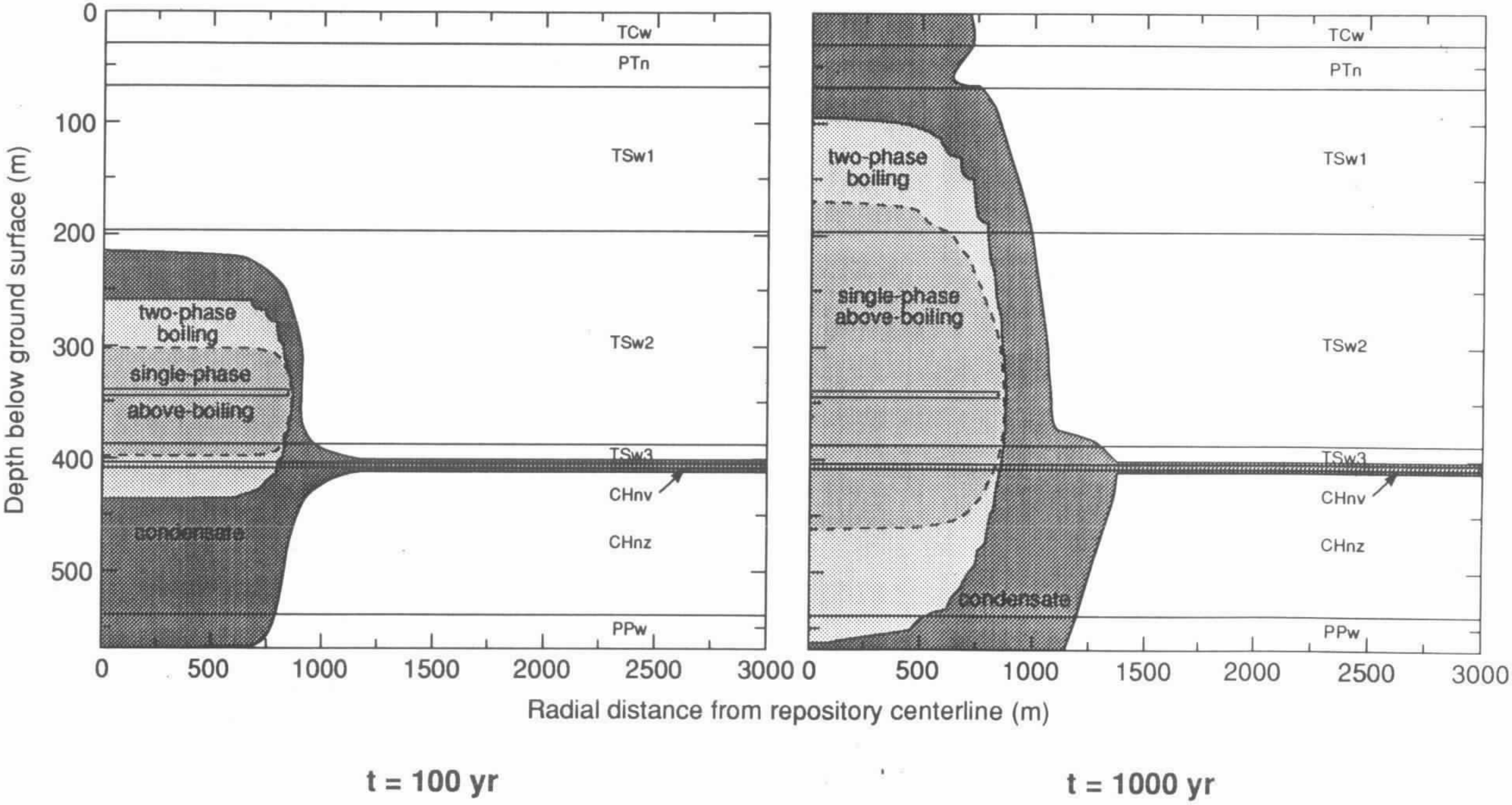


t = 100 yr

t = 1000 yr

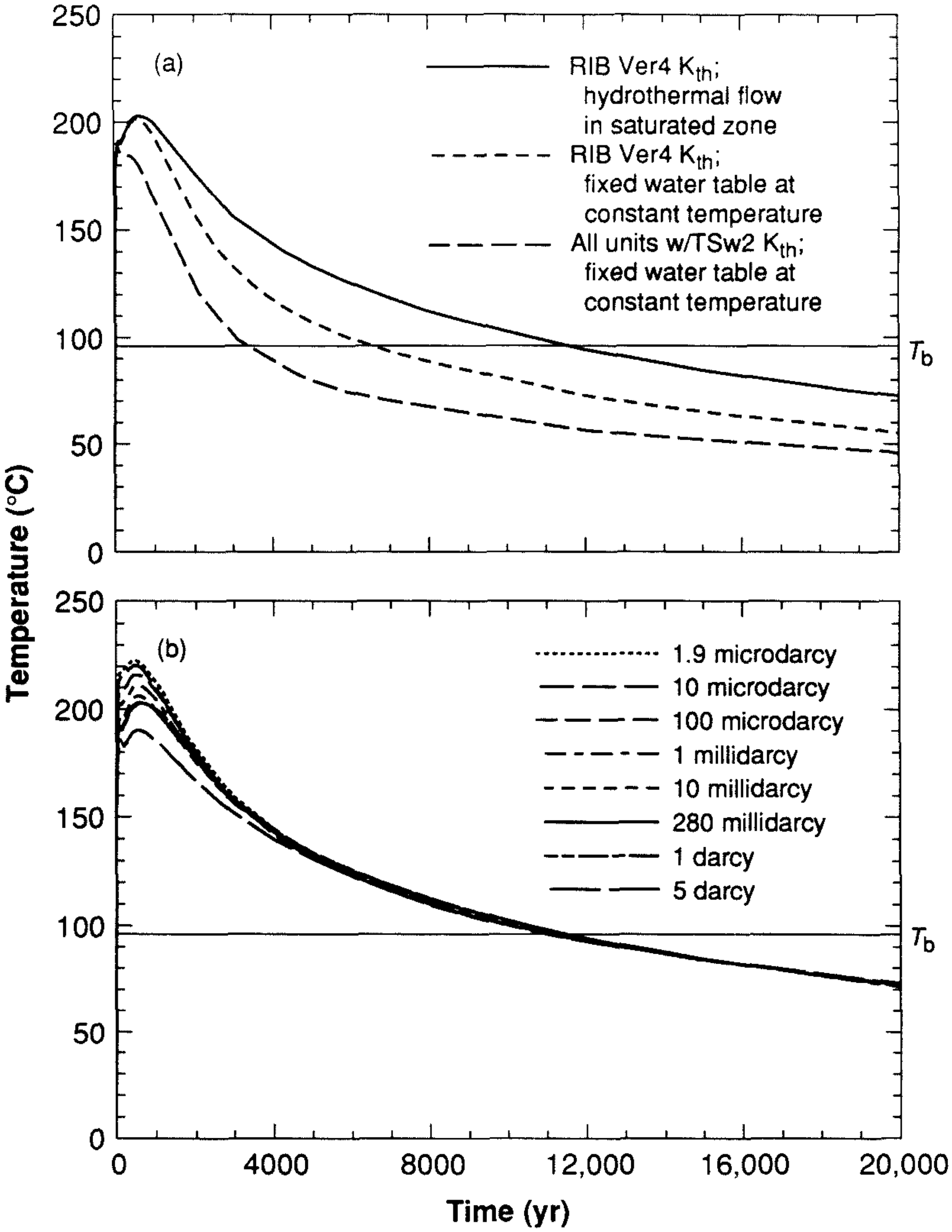
Repository heating can result in a single-phase above-boiling zone, a two-phase boiling zone, and a condensate zone

Dimensionless Liquid Saturation Contours for 30-year-old SNF,
an APD of 114 kW/acre, and an AML of 154.7 MTU/acre



Repository temperatures depend on thermal properties and boundary conditions; insensitive to a wide range in k_b

Temperature History at Repository Center for 30-yr-old SNF, an APD of 114 kW/acre, and an AML of 154.7 MTU/acre



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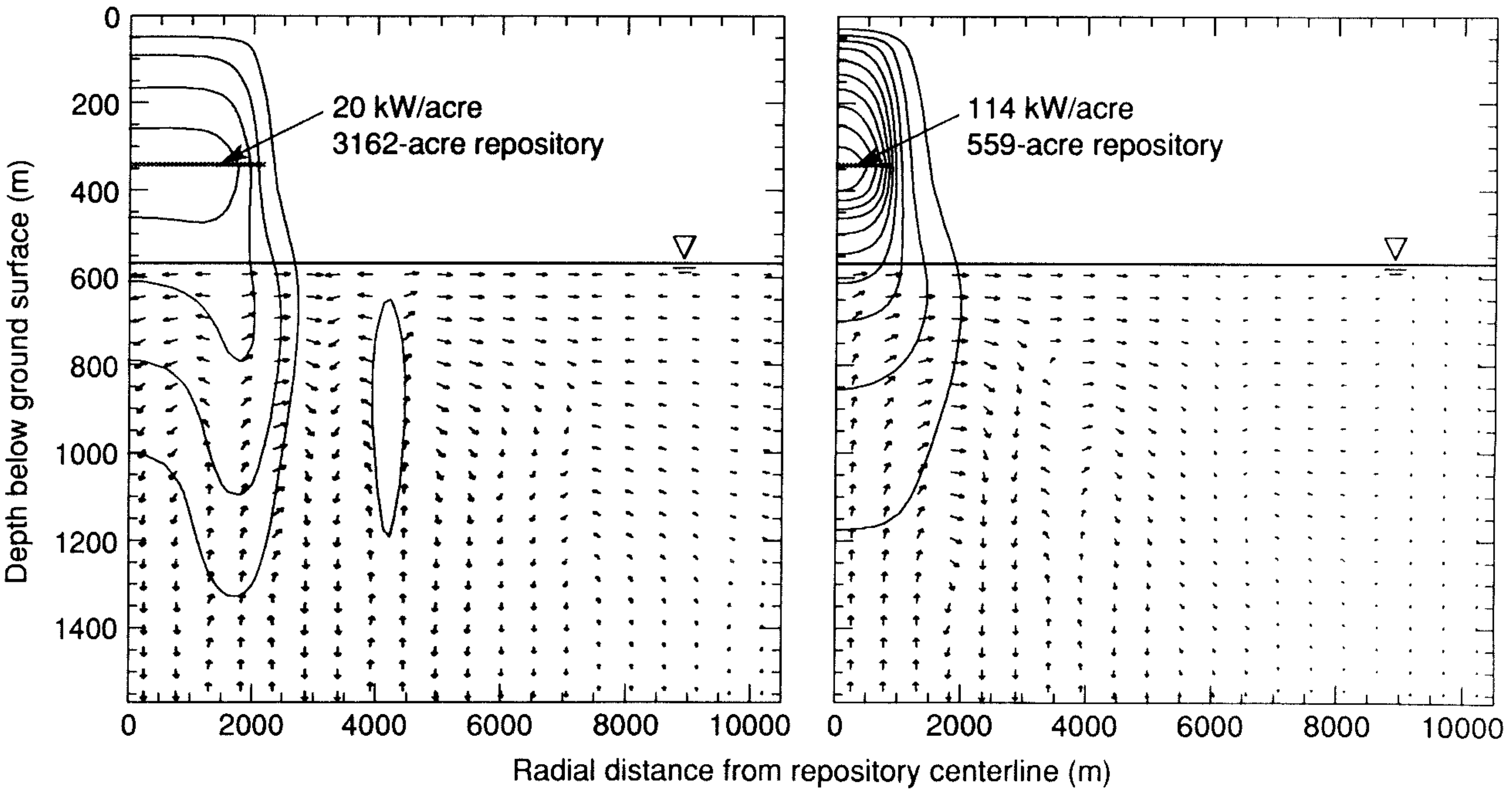
Convection in the Saturated Zone (SZ)

Temperature Buildup Contours and Liquid-Phase Velocity Vectors at t = 5000yr



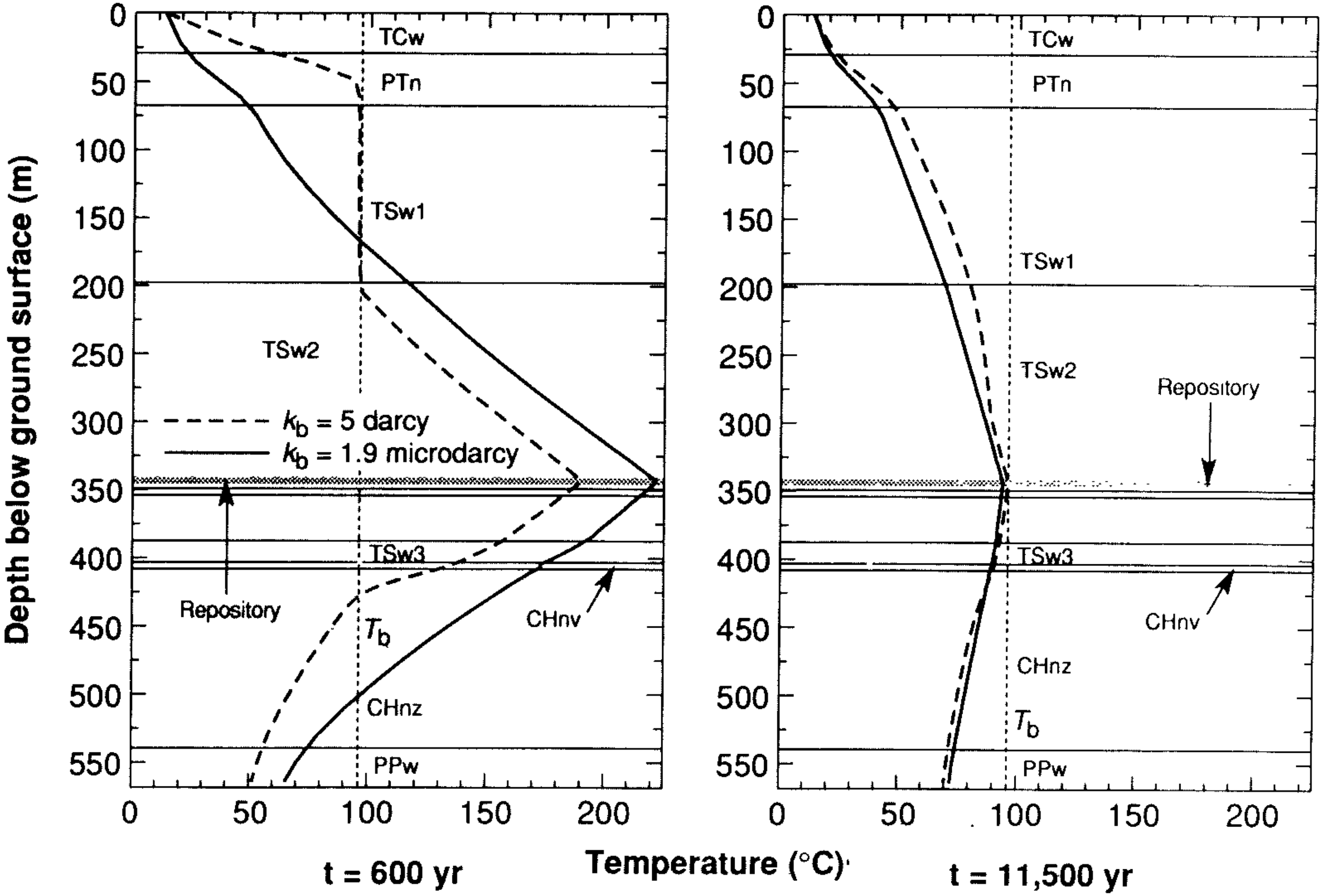
Convection in the Saturated Zone (SZ)

(Continued)

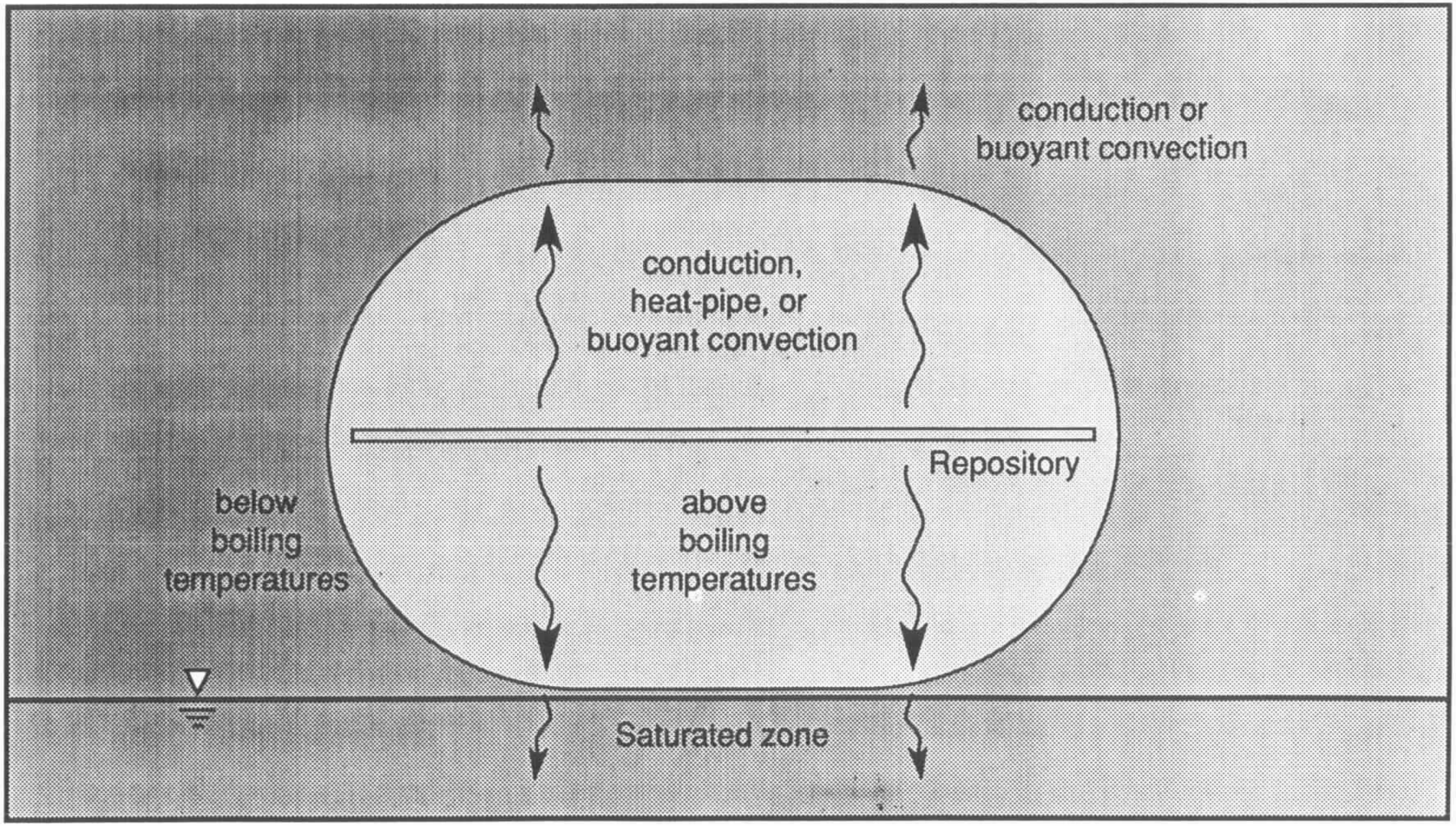
- The magnitude of buoyant convection in the SZ depends on the total mass (MTU) of SNF, but is insensitive to the Areal Mass Loading (MTU/acre) or Areal Power Density (kW/acre)
- Over a wide range of conditions, SZ heat flow is conduction-dominated

The duration of the repository boiling period largely depends on heat flow outside of the above-boiling region; convective processes that occur within the above-boiling region (heat pipes and buoyant vapor flow) affect the above-boiling temperature profile

Vertical Temperature profile along the Repository Centerline for 30-yr-old SNF, and APD of 114 kW/acre, and an AML of 154.7 MTU/acre

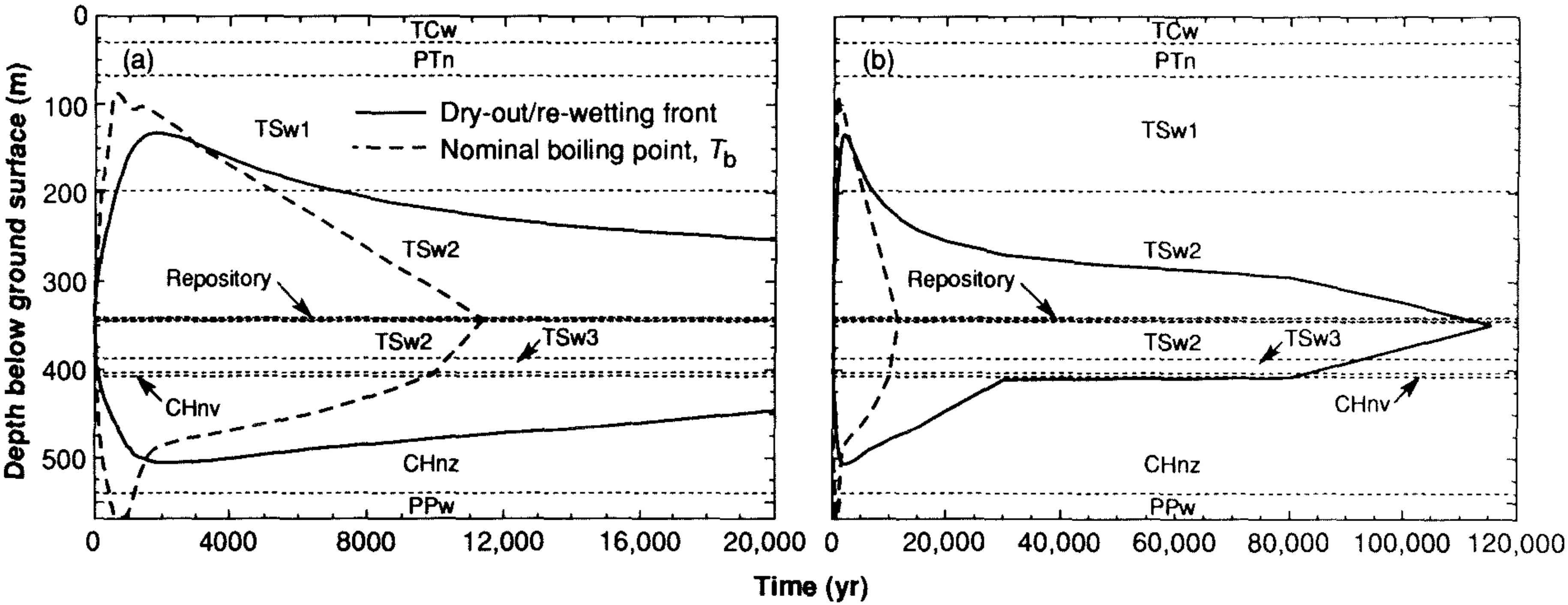


Conservation of heat within the above-boiling region largely depends on the influence of mountain-scale, buoyant, gas-phase convection; the effectiveness of heat pipes determines the temperature profile within the above-boiling region



Re-wetting of the dry-out zone lags behind the end of the boiling period; re-wetting of the repository horizon may take more than 100,000 yr

Vertical Location of the Nominal Boiling Point, Tb, and the Dry-Out/Re-Wetting Front
Along the Repository Centerline for 30-yr-old SNF, and APD of
114 kW/acre, and an AML of 154.7 MTU/acre



The use of Hypothesis Testing in Model Validation

The process of model validation must involve

- Using models to obtain a better physical understanding of the system
- Asking what it is about the system that needs to be predicted
- Utilizing this understanding to formulate fundamental hypotheses, which are the basis of the conceptual model and performance attributes of the system
- Perform analyses and experiments in an attempt to test, or to invalidate, the conceptual model (or hypotheses)
- Modifying the models on the basis of the test results

Hypothesis Testing can Help Focus Characterization, Analysis, and Testing Activities Required to Support Model Validation

Fundamental thermo-hydrological performance issues are addressed with the following hypothesis tests:

(1) Whether heat conduction dominates heat flow,

(2) Whether a region of above-boiling temperatures surrounding the repository corresponds to the absence of mobile liquid water at the WP environment,

(3) Whether fracture density and connectivity are sufficient to promote rock dry-out due to boiling and condensate shedding,

(4) Whether re-wetting of the dry-out zone back to ambient saturation significantly lags behind the end of the boiling period, and

(5) Whether mountain-scale, buoyant, gas-phase convection may eventually dominate moisture movement in the UZ

In situ heater tests at multiple locations are needed to test these hypotheses

Conclusions

Mountain-scale, repository-heat-driven, buoyant vapor flow may substantially alter the flux and saturation distribution in the unsaturated zone (UZ) for tens of thousands of years, affecting

- Saturation conditions in the vicinity of waste packages
- Episodic infiltration from meteoric sources

Given sufficiently large connected bulk permeability in the UZ, buoyant vapor flow can cause the saturation in the upper half of the UZ, including the repository horizon, to approach 100% for

- The reference SCP-CDR thermal load
- "Cool" repository thermal loads such as an APD of 20 kW/acre and 30-yr-old SNF

Conclusions

(Continued)

Large-scale *in situ* heater tests conducted under both sub-boiling and boiling conditions are critically important to any thermal-loading strategy, including

- "Cool" thermal loading conditions intended to minimize the hydrological impact of repository heat
- The reference SCP-CDR thermal load
- Higher thermal loads that have the potential of generating extended-dry conditions

The size and duration of *in situ* heater tests are independent of thermal loading strategy

The parallel use of heater tests conducted under sub-boiling, marginal-boiling, and above-boiling conditions is required to understand how repository heat influences the three major potential sources of fracture flow

Natural infiltration

Affected by repository-heat-driven changes to the

- moisture distribution
- intrinsic hydrological, geochemical, and geomechanical properties

Buoyant, gas-phase convection and condensate drainage		**Boiling and condensate drainage**	
Small-scale	Mountain-scale	Small-scale	Mountain-scale
Local heating conditions WP/EBS/repository design	Global heating conditions Areal Mass Loading AML (MTU/acre)	Local heating conditions WP/EBS/repository design	Global heating conditions Areal Mass Loading AML (MTU/acre)
Near-field hydrological properties	UZ-scale hydrological properties	Near-field hydrological properties	UZ-scale hydrological properties
Sub-boiling heater tests	Above-boiling heater tests	Marginal-boiling heater tests	Above-boiling heater tests

Conclusions

(Continued)

- Hydrostratigraphic units (such as the PTn unit) found to have substantially smaller bulk permeability can act as “vapor caps” limiting the vertical extent and magnitude of repository-heat-driven saturation alteration
- The role that the PTn may play in limiting these repository-heat-driven effects may prove to be more significant than its impact on limiting the infiltration of meteoric water

Conclusions

(Continued)

- The development of a large, persistent region of above-boiling conditions can suppress mountain-scale, buoyant vapor-flow for thousands of years
- A large, persistent, dry-out zone substantially reduces the potential for buoyant vapor-flow generating condensate flow at the repository horizon

Appendix

Conditions for Convection-influenced Moisture Movement

- **When large-scale, thermal-buoyancy-driven gas flow affects moisture movement**
- **Steam is carried from the boiling zone below the repository to the condensate zone above**

Occurs when buoyancy driven gas flow velocity becomes comparable or larger than velocity of generated steam

$$K_g \frac{\Delta T_{av}}{L_b T_0} > \frac{q_H}{h_{fg}\rho_s}$$

Therefore, convection influenced gas flow occurs at sufficiently high bulk pneumatic conductivities

$$K_g > \frac{q_H}{h_g \rho_s} \frac{L_b T_0}{L \, \Delta T_{av}}$$

K_g	bulk pneumatic conductivity (m/s)
q_H	areal heat load (W/m^2)
h_{fg}	latent heat of vaporization (J/kg)
ρ_s	steam density (kg/m^3)
ΔT_{av}	mean vertical change in temperature from ambient (°K)
L_b	thickness of boiling zone (m)
L	thickness of thermally perturbed zone
T_o	mean ambient temperature (°K)

Conditions for Convection-influenced Thermal Field

- **When large scale, thermal-buoyancy-driven gas flow affects temperature field**
- **Repository temperature is lowered due to upward, natural convection of relatively cooler gas phase**

Occurs when heat carried by buoyancy driven gas flow velocities becomes comparable or larger than repository areal heat load

$$\rho_g H_g K_g \frac{\Delta T_{av}}{T_0} > q_H$$

Therefore, convection influenced heat flow occurs at sum sufficiently high bulk pneumatic conductivities

$$K_g > \frac{q_H}{h_g \rho_g} \frac{T_0}{\Delta T_{av}}$$

K_g	bulk pneumatic conductivity (m/s)
q_H	areal heat load (W/M^2)
h_g	specific enthalpy of gas (J/kg)
ρ_g	gas density (kg/M^3)
T_0	mean ambient temperature (°K)
ΔT_{av}	mean vertical change in temperature from ambient (°K)

Model Assumptions

V-TOUGH code (LLNL's version of LBL's TOUGH code)
Equivalent Continuum Model (ECM)

- **Assumes capillary pressure and thermal equilibrium between matrix and fractures**
- **Bulk porosity, ϕ_b, bulk saturation, S_b, and bulk conductivity, K_b (thermal or hydraulic) are given by:**

$$\phi_b = \phi_f + (1-\phi_f)o_m$$

$$S_b = \frac{S_f\phi_f + Sm(1-\phi_f)\phi_m}{\phi_f + (1-\phi_f)\phi_m}$$

$$K_b = K_m(1-\phi_f) + K_f\phi_f$$

where ϕ_m, S_m, ϕ_f, and S_f are porosity and saturation of matrix and fractures

Model Assumptions

(Continued)

Hydrostratigraphic units are horizontal and constant thickness

- Repository and groundwater table are 343 and 568 m below ground surface
- Each unit with homogeneous, isotropic matrix properties taken from Klavetter and Peters (1986)
- Thermal properties from the Reference Information Base (RIB)
- Homogeneous, isotropic fracture properties; considered range of bulk permeability, k_b, from 1.9 microdarcy to 840 darcy; also considered layered k_b distribution

Model Assumptions

(Continued)

Repository-scale R-Z model

- Uniformly distributed thermal load over a 4.6-m-thick disk
- Repository areas of 348 to 3162 acres

Drift-scale X-Z model

- Infinite array of uniformly-spaced emplacement drifts
- Applicable to areally infinite repository
- Represents a symmetry element from WP centerline to pillar centerline
- Thermal load averaged along drift axis
- WP cross-section of 1.6 x 1.6 m, centered in 4.8-m-high x 6.0-m-wide drift

Model Assumptions

(Continued)

Initial vertical temperature, saturation, and pressure profiles correspond to geothermal and pneumatistatic pressure gradients and assumed recharge flux

- Saturation profiles for recharge flux of 0, 0.045, and 0. 1 32 mm/yr
- Upper constant-property boundary represents atmosphere
- Different models with lower constant-property boundary located (1) at water table, (2) 1 km below water table, and (3) 7 km below water table

Thermal-loading history with all WPs emplaced at t = 0 yr

- 10-, 30- and 60-yr old PWR SNF (33 GWD/MTU); 21 yr-old YFF (43.6 GWD/MTU), and 26-yr-old OFF (39.6 GWD/MTU)
- APDs of 20 to 114 kill/acre; AMLs of 27 to 249 MTU/acre

Modeling Statistical Variability in Condensate Drainage

- Analytical models for Performance Assessment
- Condensate flow idealized as a log-normal random field
- Estimates variability about the mean of the condensate flux computed from numerical models
- Transient fracture flow
  - Models cyclic refluxing and boiling in fractures
  - Calculates distance that channelized flow travels down fracture before water in the fracture is boiled away
  - Calculates fluxes for those fractures with flows reaching repository
- Focusing of condensate
  - Models focusing of steady condensate flow concentrated over a localized region
  - Estimate probability, *P*, that mean flow averaged over area with correlation length, *l*, exceeds local average condensate flux
  - Correlation length, *l*, for focusing of fracture flow is related to the thickness of the refluxing zone
  - Calculates probability that WP is wet and the expected value of condensate flux on WP

Average Thermo-hydrological Behavior for a "Cool" Areal Mass Loading of 27.1 MTU/acre

For $k_b < 10$ darcy, negligible dry-out due to mountain-scale, buoyant vapor flow

For $k_b > 10$ darcy, partial repository dry-out and condensate buildup above repository

- Mountain-scale, buoyant vapor flow and condensate drainage increases with k_b, persisting for 10,000 to 100,000+ yr

For $k_b > 100$ darcy, convection-dominated heat flow

Average Thermo-hydrological Behavior of the Reference SCP-CDR Thermal Load

For k_b < 1 millidarcy, negligible dry-out due to boiling
For k_b > 10 millidarcy and < 1 darcy, partial repository dry-out

- Boiling period duration, t_{bp}, of 600 to 2600 yr at repository center, negligible boiling at edge
- Substantial condensate drainage for 1000 yr
- Negligible mountain-scale, buoyant vapor flow and condensate drainage

For k_b > 1 darcy, partial repository dry-out and condensate buildup above repository

- t_{bp} declines with k_b due to mountain-scale, buoyant vapor flow
- Mountain-scale, buoyant vapor flow and condensate drainage increases with k_b, persisting for 10,000 to 100,000+ yr

For k_b > 40 darcy, convection-dominated heat flow