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I. INTRODUCTION

In a parameter-sensitivity study, hydrologic-property uncertainty is found to insignificantly influence the range of TH conditions; therefore, it is unnecessary to propagate the influence of that uncertainty through the MSTHM. The influence of low-probability seismic-induced drift collapse on TH conditions is also addressed. The MSTHM is validated against field thermal tests and against an alternative numerical model [1, 2].

The MSTHM is an efficient alternative to nested or “telescoping” models as it breaks the problem into more

1-D SOT
(# N locations & M AMLs)

2-D LDTH
(# N locations & M AMLs)

3-D SMT

3-D LMTH

3-D DMTH

Sub-model output

- MTHAC variable
- MTHAC Calculation
- MTHAC Interpolation
- Real source geometry

Note:
 N = number of locations
 M = number of AMLs
 H = hydrologic variables

Fig. 1. This schematic shows the relationship of the four families of submodels used in the MSTHM. The LMTH model is an intermediate MSTHM result. The DMTH model is the final MSTHM result. The four submodel types: SDT, SMT, LDTH, and DDT, and the LMTH and DMTH models, are described in Table I.

The conceptual model for nonequilibrium fracture-matrix flow is a dual-permeability representation of overlapping fracture and matrix continua, modified from the traditional approach such that only a portion of connected fractures actively conduct liquid water [5]. For a complete MSTHM realization, four families of NUFT-submodel calculations [1, 2], of varying detail and scale, are conducted (Fig. 1 and Table I). The final MSTHM output is obtained by superposition of 3-D mountain-scale and 3-D drift-scale thermal-conduction-submodel results onto those of 2-D drift-scale TH-submodel results. This process is described in detail elsewhere [1, 2].

TABLE I. Submodel and model types are described with respect to their role in the MSTHM methodology.

| Submodel/ Model Type | Description |
|-------------------------|---|
| MSTHM | MultiScale ThermoHydrologic Model |
| SMT | Smeared-heat-source, Mountain-scale , Thermal-conduction (3-D) submodel represents mountain-scale heat flow, quantifying the edge-cooling effect |
| SDT | Smeared-heat-source, Drift-scale , Thermal-conduction (1-D) submodel is used in conjunction with the SMT submodel to incorporate the influence of mountain-scale heat flow on drift-scale TH conditions |
| LDTH | Line-averaged-heat-source , Drift-scale , Thermal-Hydrologic (2-D) submodel represents coupled TH processes |
| DDT | Discrete-heat-source , Drift-scale , Thermal-conduction (3-D) submodel represents the geometry of the waste package and drip shield and distinguishes the heat output histories of various waste-package types |
| LMTH | Line-averaged-heat-source , Mountain-scale , Thermal-Hydrologic (3-D) model is an intermediate MSTHM result |
| DMTH | Discrete-heat-source , Mountain-scale , Thermal-Hydrologic (3-D) model is the final MSTHM result |
| D/LMTH | Discrete/Line-averaged-heat-source , Mountain-scale , Thermal-Hydrologic (3-D) model is an alternative model, with a nested mesh, supporting validation of the MSTHM |

The radioactive heat of decay from waste packages strongly influences TH conditions within emplacement drifts (Fig. 2) and in the adjoining host rock. Heating of the host rock above the boiling point of water leads to boiling, vapor transport, and condensation. The net result is a region of rock dryout, with liquid-phase saturation and relative humidity less than ambient in the host rock around the drifts. Rock dryout causes a reduction in the relative humidity within the emplacement drifts. Fig. 3 plots the

heat-generation history for the entire repository, which is distributed along ~57 km of emplacement drifts, resulting in an initial line-averaged thermal load of 1.45 kW/m. The first 50 years following emplacement is called the preclosure ventilation period, during which the drifts are cooled by forced convection. During the preclosure ventilation period about 80 to 90 percent of the heat generation shown in Fig. 3 is removed from the repository. The MSTHM calculations account for this heat removal, but do not account for any moisture removal that may result from drift ventilation. During the post-closure period ($t > 50$ yr) 100 percent of the heat output shown in Fig. 3 is available to heat the host rock.

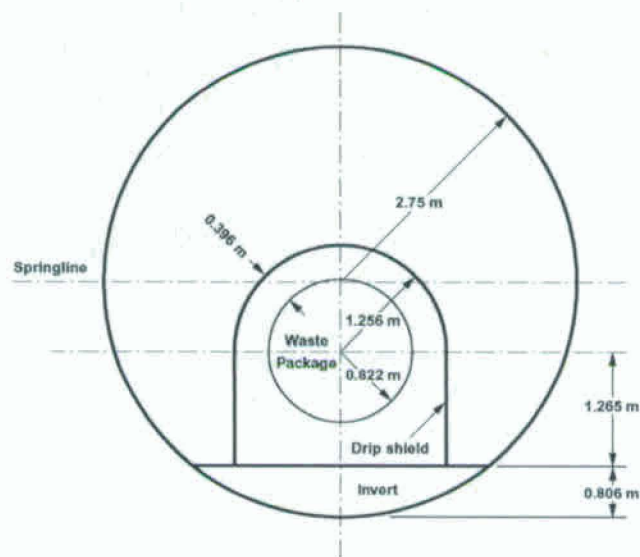


Fig. 2. A vertical cross-section shows the engineered components within an emplacement drift, including the invert (filled with crushed rock derived from the host rock), drip shield, and waste package.

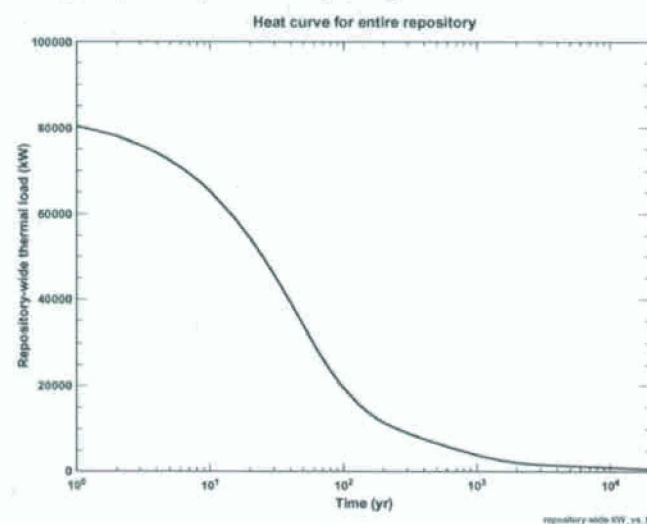


Fig. 3. The heat-generation history is plotted for the entire waste-package inventory in the repository.

The MSTHM predicts TH conditions within emplacement drifts, and in the adjoining host rock, for 2874 20-m-long segments lying along 95 emplacement drifts (Fig. 4). For each 20-m-long segment, TH conditions are predicted for 8 different waste packages, each with different heat-generation histories. One entire repository-wide MSTHM simulation results in 22,992 sets of TH histories.

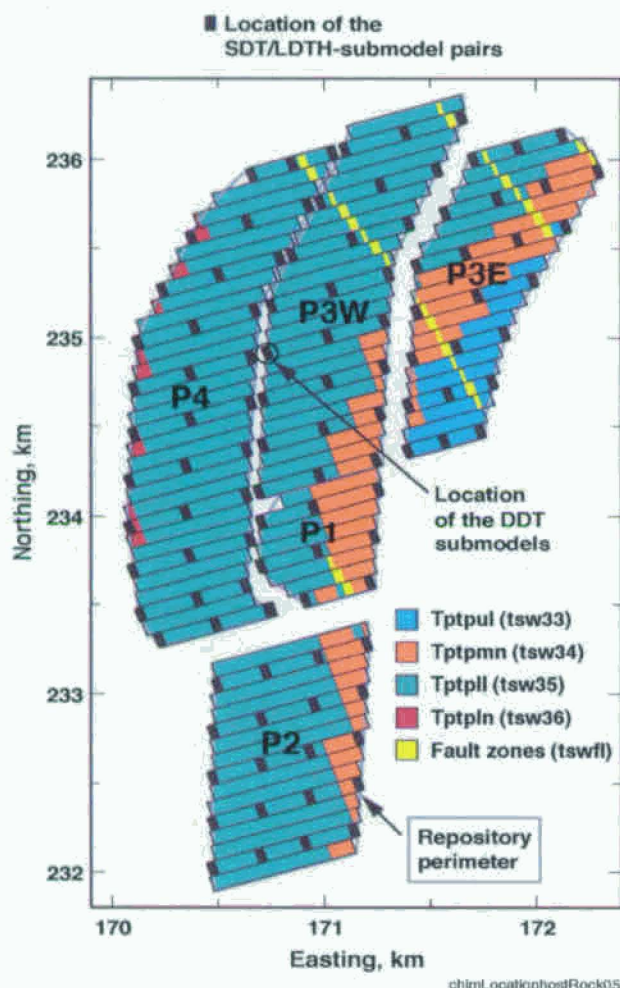


Fig. 4. Plan view of heated intervals of emplacement drifts shows the location of the LDTH and SDT submodels (black squares), and the DDT submodels (open circle).

Five repository-wide MSTHM calculations are made to address the influence of natural-system parametric uncertainty, including the following five cases:

- Lower-bound infiltration flux with low host-rock thermal conductivity
- Lower-bound infiltration flux with mean host-rock thermal conductivity
- Mean infiltration flux with mean host-rock thermal conductivity

- Upper-bound infiltration flux with mean host-rock thermal conductivity
- Upper-bound infiltration flux with high host-rock thermal conductivity

The low and high host-rock thermal-conductivity K_{th} cases have K_{th} values that are one standard deviation below and above the mean host-rock K_{th} values, respectively. These five cases, which are given appropriate probability weights as described in [2], result in 114,960 TH histories. These TH histories, along with their corresponding probability weights are used by downstream process models supporting the performance assessment of the proposed nuclear-waste repository at Yucca Mountain.

In addition to the repository-wide MSTHM calculations, various sensitivity analyses are conducted at selected locations in the repository to investigate the sensitivity of in-drift/near-field TH conditions to:

- Low-probability-seismic collapsed-drift scenarios
- Host-rock hydrologic-property variability and uncertainty
- Invert hydrologic-property variability and uncertainty
- Preclosure ventilation heat-removal efficiency uncertainty

The MSTHM is validated against temperature and liquid-phase saturation measurements from *in situ* thermal tests, including the Large Block Test and Drift Scale Test [2]. The MSTHM is also validated against an alternative conceptual model, which is described elsewhere [1, 2]. Those validation studies demonstrated that the influence of conceptual-model uncertainty is insignificant compared to the influence of parametric uncertainty, which is propagated through the repository-wide MSTHM results that are used in the performance assessment of the Yucca Mountain repository.

III. RESULTS

The MSTHM supports the performance assessment of the Yucca Mountain repository by predicting a reasonable range of TH conditions within emplacement drifts and in the adjoining host rock. Temperature and relative humidity on drip shields and waste packages is required to assess the degradation of those engineered components. Drift-wall temperature is required to assess the potential onset of drift seepage, which is based on analyses that show that seepage cannot occur during the above-boiling period [7]. Invert temperature, relative humidity, liquid-phase saturation and flux are required to assess radionuclide transport. Various parameter-sensitivity analyses [2, 6] have shown that the range of in-drift TH conditions across the repository are primarily affected by four factors ranked in Table II with respect to their importance.

TABLE II. The factors influencing waste-package (WP) temperature and relative humidity RH are ranked with respect to peak temperature, boiling duration, and the reduction of RH on WPs, compared to ambient conditions.

| Factor | Rank of relative importance for influencing waste-package temperature and relative humidity | | |
|--|---|------------------|---------------------|
| | $T_{wp, peak}$ | Boiling duration | RH_{wp} reduction |
| Edge-cooling effect | 2 | 1 | 1 |
| Host-rock K_{th} uncertainty | 1 | 2 | 2 |
| WP-to-WP heat output variability | 3 | 4 | 3 |
| Host-rock percolation-flux variability/uncertainty | 4 | 3 | 4 |

The influence of the edge-cooling effect is shown in Figs. 5 through 7 for the mean infiltration-flux, mean host-rock thermal-conductivity K_{th} case. Waste-package temperature and boiling duration, and the maximum lateral extent of boiling in the adjoining host rock, all increase with decreasing proximity to the repository edges. The edge-cooling effect has a more pronounced influence on boiling duration than on peak temperature and lateral extent of boiling. The maximum lateral extent of boiling is much less than the 81-m spacing between drift centerlines, allowing heat-generated condensation to shed around the boiling zones and drain below the repository horizon.

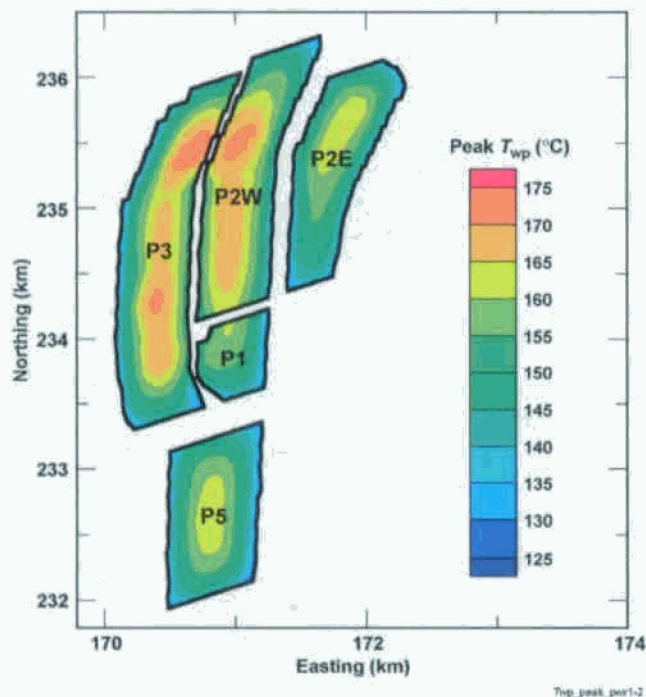


Fig. 5. Contour map of the distribution of peak temperature on 21-PWR AP CSNF waste packages for the mean infiltration-flux, mean host-rock K_{th} case.

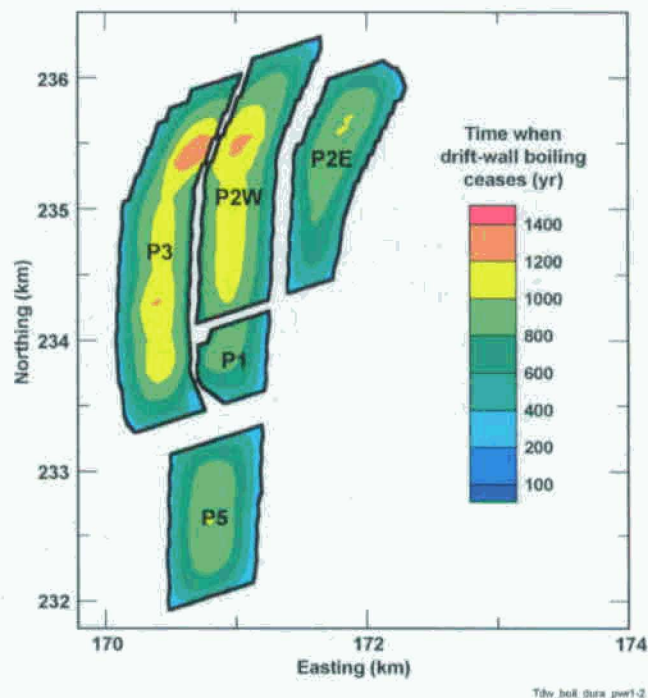


Fig. 6. Contour map of the distribution of boiling duration on 21-PWR AP CSNF waste packages for the mean infiltration-flux, mean host-rock K_{th} case.

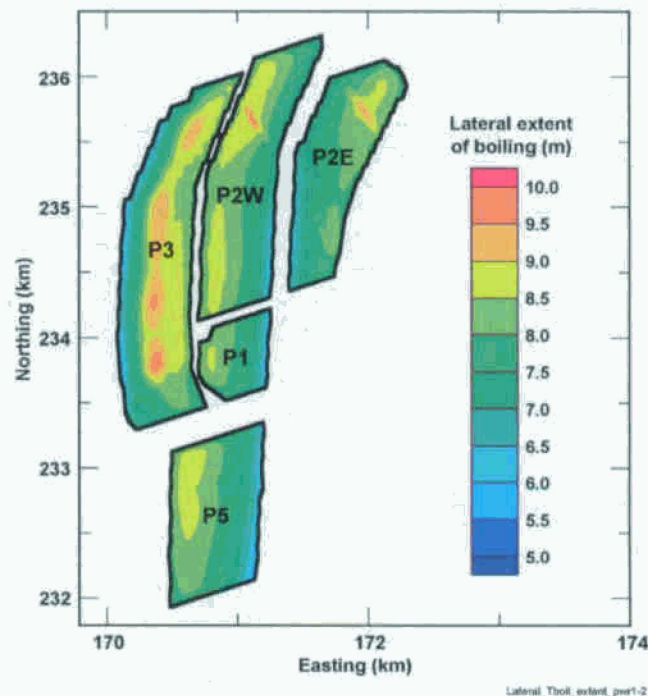


Fig. 7. Contour map of the distribution of maximum lateral extent of boiling for 21-PWR AP CSNF waste packages for the mean infiltration-flux, mean host-rock K_{th} case.

The range of MSTHM-predicted TH parameters across the repository, including the influences of engineered- and natural-system parametric variability and uncertainty, is

summarized in Fig. 8. Figs. 8a and 8b plot the range of waste-package temperature and relative humidity, which are TH parameters used in downstream process models supporting performance assessment of the Yucca Mountain repository. The complementary cumulative distribution function (CCDF) for peak drift-wall and waste-package temperature is plotted (Figs. 8c and 8d) for each of the five infiltration-flux/host-rock K_{th} cases. Peak drift-wall temperatures range from 92.3 to 175.2°C, with a median value of 133.0°C. Peak waste-package temperatures range from 102.0 to 203.1°C, with a median value of 152.9°C.

The CCDF of the time when the perimeter-averaged drift-wall temperature drops below boiling is plotted (Fig. 8e) for each of the five cases; this time ranges from 0 to 2176.5 yr, with a median value of 695.2 yr. For the few cases for which the perimeter-averaged drift-wall temperature never exceeds the boiling point, drift-wall temperatures located above the top of the invert always exceed boiling for a period of time. The CCDF of the maximum lateral extent of boiling is plotted (Fig. 8f) for each of the five cases. The lateral extent of boiling ranges from 4.1 to 27.9 m, with a median value of 7.9 m.

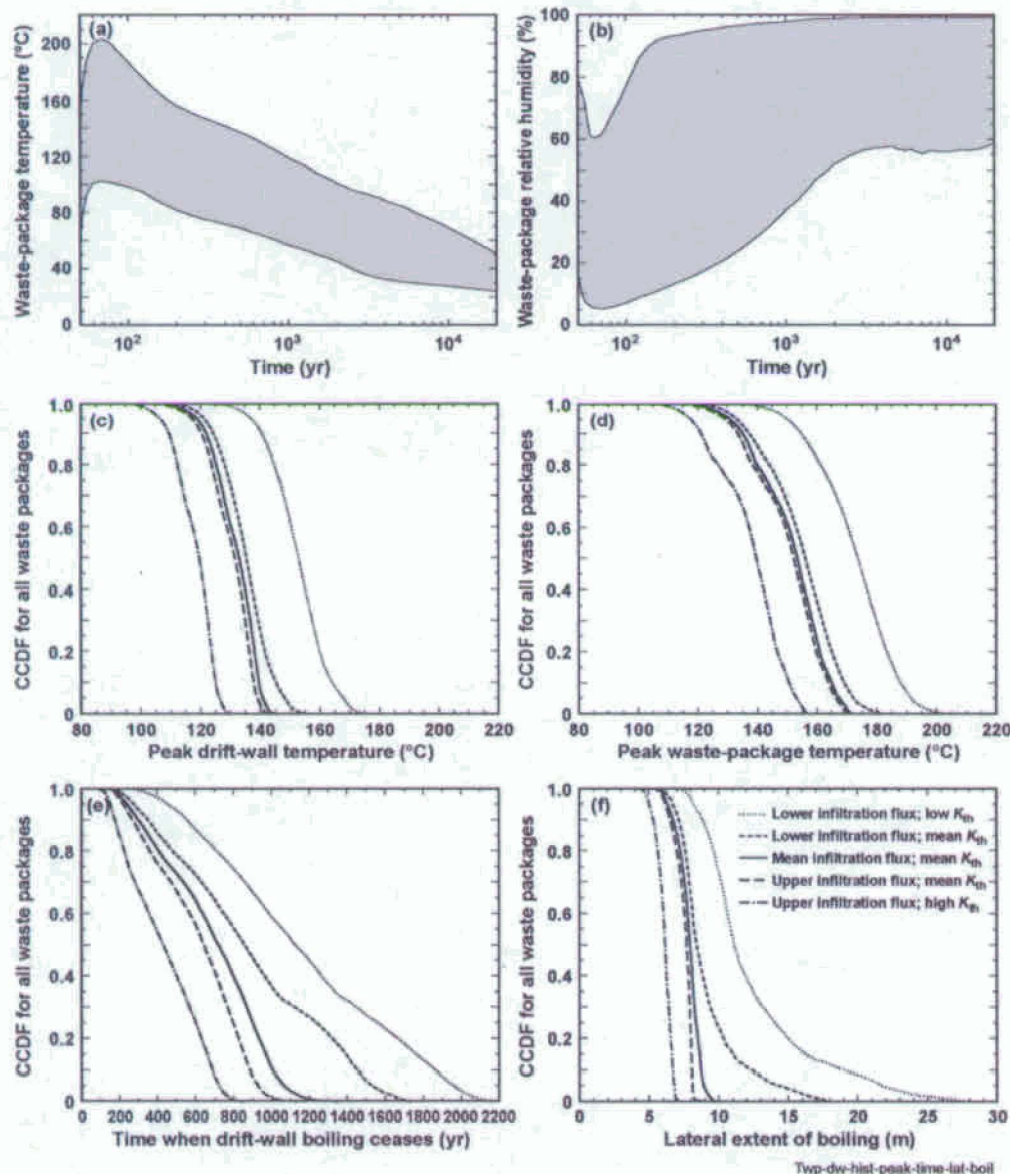


Fig. 8. The range in thermal-hydrologic (TH) conditions across the repository is plotted for 114,960 TH histories predicted by the MSTHM for the five infiltration-flux/host-rock thermal-conductivity K_{th} cases. The range in waste-package (a) temperature and (b) relative humidity is plotted as a function of time. The range in peak (c) drift-wall temperature and (d) waste-package temperature is plotted as a complementary distribution function (CCDF) for each of the five cases. Also plotted is the CCDF of the range in the (e) time when drift-wall boiling ceases and (f) the maximum lateral extent of boiling (96°C) for the five cases.

Fig. 8 pertains to the case where emplacement drifts in their original cylindrical shape. The influence of probability-seismic collapsed-drift scenario on initial TH conditions is analyzed for a location close to the repository center (Fig. 9). To address the uncertainty of thermal conductivity K_{th} of the collapsed host-rock, low and high K_{th} cases are considered. The collapse of the drift causes the original intact drift opening to be completely filled with rubble. Breakage of the host rock causes the rubble zone to extend into the region initially occupied by intact host rock. More details are available elsewhere [2]. Because heat flow through the rubble zone is less efficient than either thermal radiation within an intact drift opening, or heat conduction within original intact host rock, temperature on the waste

package and in the invert is greater than for the case with an intact drift (Figs. 9a and 9b). Higher temperatures reduce relative humidity (Fig. 9c) and liquid-phase saturation in the invert and rubble (Figs. 9d and 9e).

The MSTHM addresses repository-scale variability of hydrologic properties. As shown in Fig. 4, the MSTHM represents the four different hydrogeologic units (called host-rock units: Tptpul, Tptpmn, Tptpll, and Tptpln) that intersect the repository horizon. A parameter-sensitivity study of hydrologic properties [2] investigated whether drift-scale TH behavior is sensitive to differences in the hydrologic properties for the four host-rock units. LDTH-submodel calculations are made for a location close to the repository center (the open circle in Fig. 4). Note that the

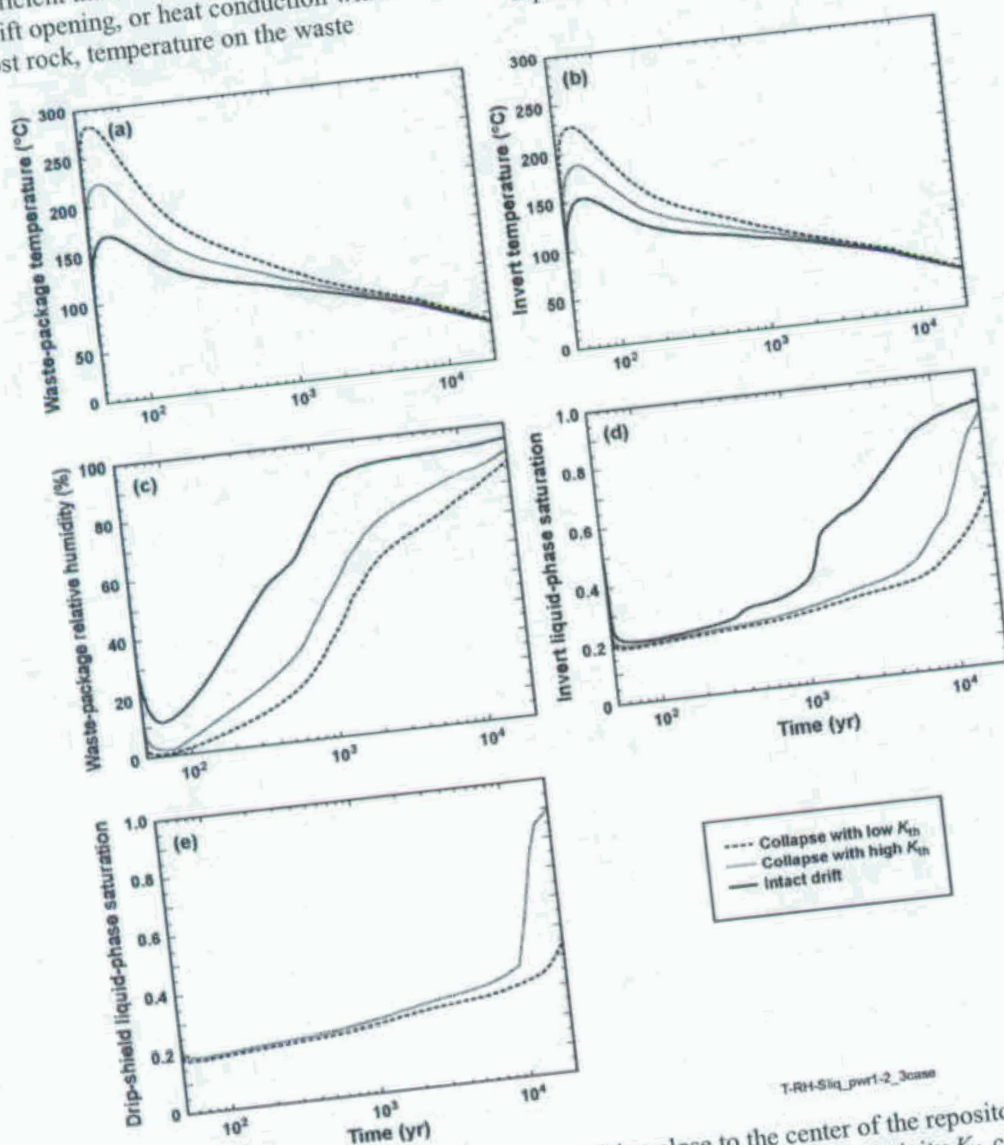


Fig. 9. Thermal-hydrologic (TH) conditions are plotted for a location close to the center of the repository for the low-probability-seismic drift-collapse scenario, and for the low and high rubble-thermal-conductivity K_{th} cases. The plotted TH parameters are (a) waste-package temperature, (b) invert temperature, (c) waste-package relative humidity, (d) invert liquid-phase saturation, and (e) drip-shield liquid-phase saturation.

local host-rock unit at this location is the Tptpl unit. For this parameter-sensitivity study, all LDTH-submodel calculations use the thermal properties applicable to the Tptpl unit for the mean host-rock K_{th} case. The LDTH-submodel calculations were repeated using the hydrologic properties of each of the four host-rock units. The LDTH-submodel calculations were also repeated for host-rock percolation flux values of 0.01, 0.1, 1.0, and 10.0 mm/yr, resulting in a total of 16 cases.

Fig. 10 plots the drip-shield temperature and relative humidity for those 16 cases. For a percolation flux greater than 0.1 mm/yr, temperature is insensitive to hydrologic properties (Figs. 10a, 10c and 10e). For a percolation flux

of 0.01 mm/yr, hydrologic properties exert a barely discernable influence on temperature (Fig. 10g). For a percolation flux of 1.0 mm/yr or greater, relative humidity is insensitive to hydrologic properties (Figs. 10b and 10d). For a percolation flux of 0.1 mm/yr or less, hydrologic properties exert a minor influence on relative humidity (Figs. 10f and 10h). The minor influence that hydrologic properties exert on temperature and relative humidity is found to be insignificant compared to the influence of host-rock K_{th} uncertainty and percolation-flux variability and uncertainty [2] that are propagated through the MSTHM. Therefore, hydrologic-property uncertainty does not need to be propagated through the repository-wide MSTHM results that support performance assessment [2].

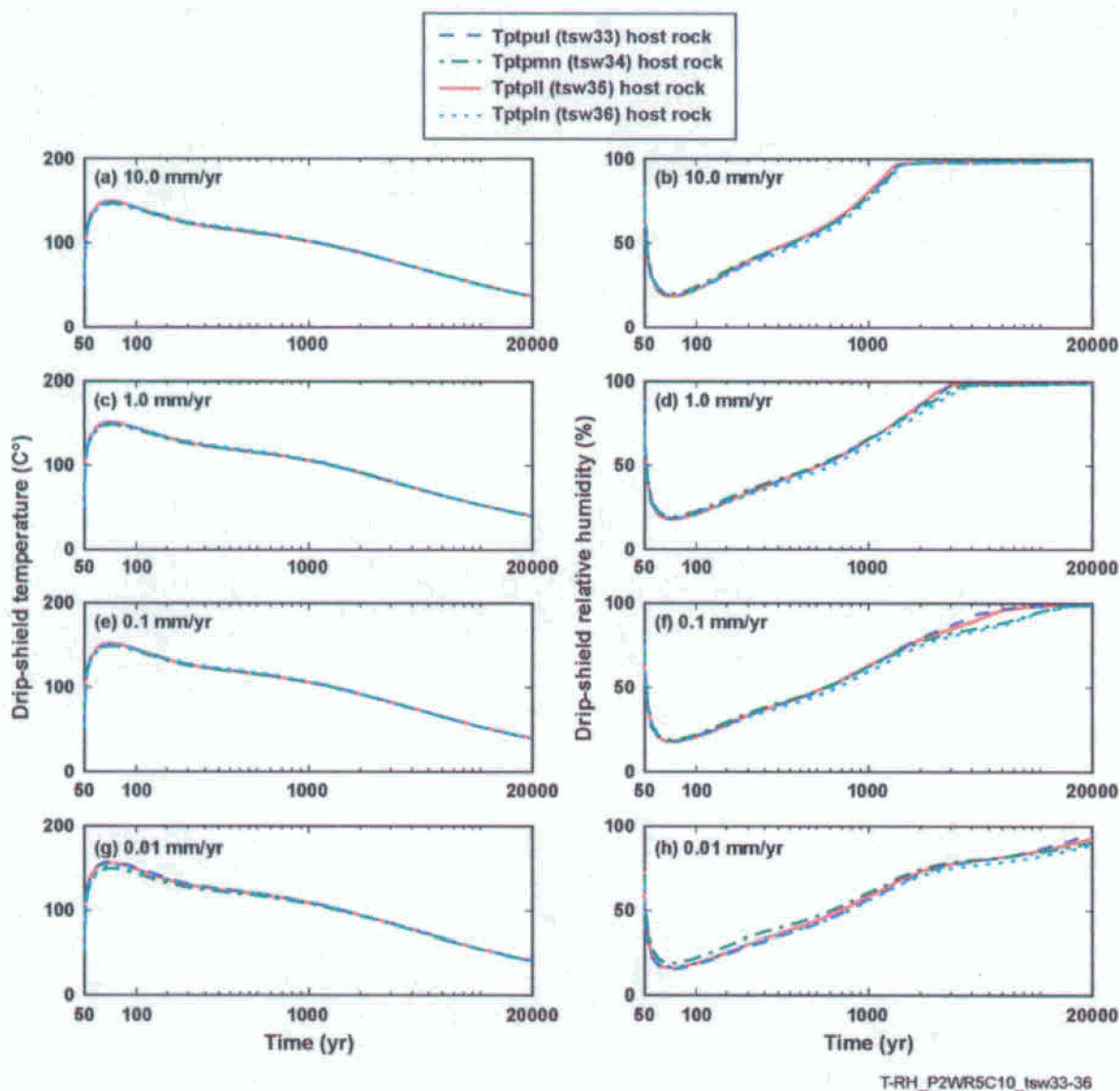


Fig. 10. Drip-shield temperature (a,c,e,g) and relative humidity (b,d,f,h) are plotted for a location close to the repository center for four values of percolation flux and for the hydrologic properties of each of the host-rock units. All cases use the thermal-property values, including thermal conductivity K_{th} for the Tptpl (tsw35) host-rock unit for the mean host-rock K_{th} case.

The lack of sensitivity of in-drift and near-field temperature and relative humidity to hydrologic properties can be understood by considering the key processes and factors governing thermal-hydrologic behavior in and around emplacement drifts. Thermal-hydrologic behavior in and around emplacement drifts can be understood by the considering the interaction of three fundamental processes:

1. **Heat Flow**—occurs in emplacement drifts, primarily by thermal radiation, and in the adjoining host-rock, primarily by thermal conduction. Consequently, host-rock K_{th} is the key natural-system parameter determining the magnitude of temperature buildup.
2. **Host-Rock Dryout**—is driven by temperature buildup, resulting in evaporation (boiling), which reduces the liquid-phase saturation and relative humidity in the host rock (resulting in the dryout zone), thereby reducing the relative humidity within the emplacement drifts.
3. **Host-Rock Rewetting**—is primarily driven by gravity-driven percolation in fractures, with capillary-driven imbibition in the adjoining matrix. The rate of rewetting (of the dryout zone) is controlled by the local percolation flux, except in regions of very low percolation flux (less than approximately 0.1 mm/yr), where it is controlled by capillary-driven imbibition in the matrix. The percolation-flux threshold of approximately 0.1 mm/yr is obtained by observing the sensitivity of temperature and relative humidity to percolation flux, described above.

For the range of hydrologic properties of the four host-rock units, vapor flow from the boiling zone to the condensation zone essentially occurs in an unthrottled (i.e., unrestricted) fashion [2]. Permeability in the fractures and matrix is sufficiently large, and fracture spacing is sufficiently small, to result in insignificant gas-phase pressure buildup with respect to boiling and vapor transport from the boiling zone to the condensation zone. The small gas-phase pressure buildup is indicative of unthrottled (i.e., unrestricted) boiling and vapor flux from the boiling zone to the condensation zone. The range in host-rock hydrologic properties causes insignificant differences in the rate at which boiling occurs in the host rock, as well as causing insignificant differences in the extent of host-rock dryout.

For the range of host-rock hydrologic properties of the four host-rock units, the contribution of buoyant gas-phase convection to overall heat flow is small compared to that of thermal conduction. Thus, the range in host-rock hydrologic properties of the four host-rock types results in insignificant differences in the temperature buildup in the host rock, as is evident in Figs. 10a, 10c, and 10e.

For the range of hydrologic properties of the four host-rock units, fracture permeability is sufficiently large and

fractures are sufficiently well connected to allow gravity-driven drainage of percolation to occur in an unrestricted fashion [8]. Percolation flux, not fracture permeability, is the rate-limiting quantity governing the magnitude of gravity-driven liquid-phase flow to the boiling/dryout zone. One caveat to this generalization relates to flow focusing, which arises due to heterogeneity in fracture permeability. The influence of flow focusing is addressed by including areal variability of percolation flux, which results in a broad range of percolation flux over the repository footprint, and by including uncertainty, as is addressed in the lower-bound, mean, and upper-bound infiltration-flux cases. Thus, the manner in which hydrologic properties primarily affect rewetting (and, thus, net dryout) behavior is related to the manner in which those properties affect capillary-driven flow, which primarily occurs as imbibition in the matrix.

For the range of hydrologic properties of the four host-rock units, capillary-driven imbibition always results in a rewetting magnitude that is effectively less than approximately 0.1 mm/yr. Accordingly, only in regions with very low percolation flux (less than 0.1 mm/yr) do the hydrologic properties exert a barely discernable influence on dryout and rewetting in the host rock, as seen in Fig. 10. However, this small influence is insignificant compared to that of parametric uncertainty of host-rock K_{th} and percolation flux [2]. For areas of the repository with a percolation flux greater than 0.1 mm/yr, which is the vast majority of the repository area for all three climate states [2], imbibition plays an indiscernible role in dryout and rewetting.

For the repository-wide MSTHM calculations of the five infiltration-flux/host-rock K_{th} cases, the crushed-tuff gravel invert is assumed to be derived from the Tptpl host-rock unit. This assumption is made because 75 percent of the emplacement drifts are in the Tptpl unit (Fig. 4). However, it is possible that the crushed-tuff gravel could be derived from the other three host-rock units. A parameter-sensitivity study of invert hydrologic properties was conducted to investigate the sensitivity of TH behavior to invert hydrologic properties. In this study, LDTH-submodel calculations are made for a location close to the repository center (the open circle in Fig. 4).

Fig. 11 shows the sensitivity of liquid-phase saturation and temperature to the hydrologic properties of the intragranular porosity. Note that the intragranular porosity is equivalent to the matrix continuum of fractured porous rock. Temperature is insensitive to the hydrologic properties of the intragranular porosity (Fig. 11b). With the exception of Tptpln-unit gravel, the dryout history is similar for these four gravels. Rewetting histories are similar for gravels derived from the lithophysal units (Tptpul and Tptpll). Rewetting is also similar for gravels from the two nonlithophysal units (Tptpmn and Tptpln).

Because matrix permeability is smaller in the nonlithophysal units, rewetting is slower than it is for the gravel from the lithophysal units. Differences in liquid-phase saturation histories are less than that arising from parametric uncertainty of infiltration flux and host-rock K_{th} that has been propagated through the repository-wide MSTHM results provided to TPSA-LA [2].

In addition to uncertainty about the hydrologic properties of the intragranular porosity, there is also uncertainty about the hydrologic properties of the intergranular porosity. A parameter-sensitivity study considered crushed tuff gravel with four grain sizes, including 0.317-, 3-, 10-, and 20-mm grains [2]. Fig. 12 shows that invert liquid-phase saturation and temperature are insensitive to the hydrologic properties of the intergranular porosity. These two studies show that invert hydrologic-property uncertainty does not need to be propagated through the repository-wide MSTHM results.

The MSTHM uses a time-dependent heat-removal-efficiency factor to account for the influence of convective cooling during the 50-yr preclosure ventilation period. To address the uncertainty of heat-removal efficiency, LDTH-submodel calculations were conducted for a location close to the repository center (the open circle in Fig. 4). These LDTH-submodel calculations were repeated for heat-removal efficiencies of 70, 80, 90, and 100 percent, as well as for the base case with time-dependent heat-removal efficiency. For this range in heat-removal efficiency, peak drip-shield temperatures range from about 9°C lower to 12°C higher than that of the base case (Fig. 13a), resulting in a relatively narrow range of relative-humidity histories (Fig. 13b). Compared to the influence of parametric uncertainty of host-rock K_{th} and percolation flux, the influence of heat-removal efficiency is insignificant.

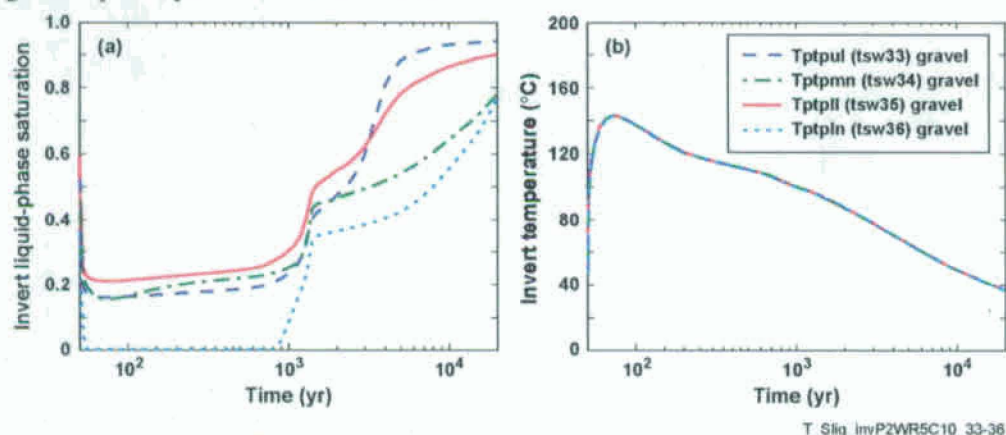


Fig. 11. Invert liquid-phase saturation (a) of the intragranular porosity and temperature (b) are plotted for a location close to the repository center for four invert-gravel cases. Each of the cases uses invert gravel derived from one of the four indicated host-rock units. The mean infiltration-flux, mean host-rock thermal-conductivity K_{th} case is applied to all four invert-gravel cases. Note that repository-wide MSTHM results supporting performance assessment assume the invert is filled with Tptpll gravel.

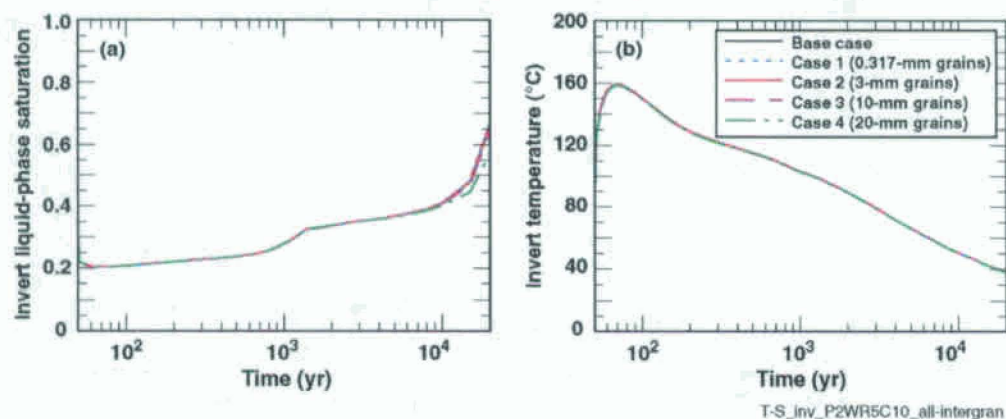


Fig. 12. Invert liquid-phase saturation (a) of the intragranular porosity and temperature (b) are plotted for a location close to the repository center for the four listed grain sizes. Each of the cases uses invert gravel derived from the Tptpll unit. The mean infiltration-flux, mean host-rock thermal-conductivity K_{th} case is applied to all four invert-gravel cases. Note that the repository-wide MSTHM results supporting performance assessment assume a modified case 2.

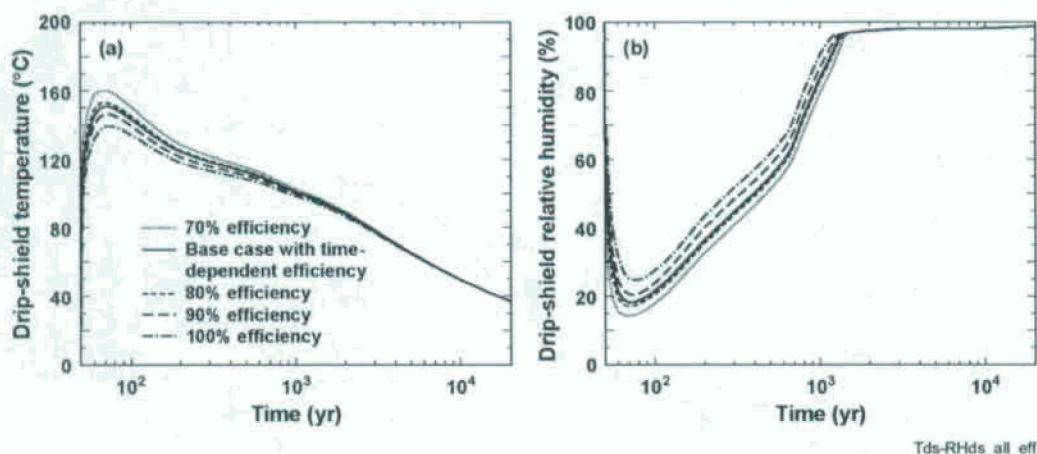


Fig. 13. Drip-shield (a) temperature and (b) relative humidity are plotted for a location close to the repository center for five listed heat-removal efficiencies. The mean infiltration-flux, mean host-rock thermal-conductivity K_{th} case is applied to all cases. Note that the MSTHM results supporting performance assessment used the base case with time-dependent efficiency.

IV. CONCLUSIONS AND DISCUSSION

The MultiScale ThermoHydrologic Model (MSTHM) is used to predict a reasonable range of thermal-hydrologic (TH) conditions within emplacement drifts, and in the adjoining host rock, across the entire repository, accounting for the variability and uncertainty of the engineered- and natural-system parameters that significantly influence those conditions. Parameter-sensitivity studies show that the significant natural-system parameters are host-rock thermal conductivity and percolation flux above the repository. These studies also show that the significant engineered-system parameter is the waste-package-to-waste-package variability in heat output. The edge-cooling effect, which increases with proximity to the repository edges, is found to be the most important factor causing variability in TH conditions across the repository. Parameter-sensitivity analyses demonstrate that variability and uncertainty in host-rock hydrologic properties, invert hydrologic properties, and in preclosure ventilation heat-removal efficiency do not need to be propagated through the MSTHM results supporting performance assessment of the Yucca Mountain repository. The influence of low-probability-seismic collapsed-drift scenarios on in-drift TH conditions is also addressed. The MSTHM is validated against measurements from *in situ* thermal tests as well as against an alternative conceptual model. The model-validation studies demonstrate that the influence of conceptual-model uncertainty is insignificant compared to the influence of parametric uncertainty that is propagated through the MSTHM.

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