INCREASED STORAGE CAPACITY AT YUCCA MOUNTAIN FAVORS THERMAL MANAGEMENT FOR A COLD REPOSITORY

RADIOACTIVE WASTE MANAGEMENT AND DISPOSAL

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The nuclear waste storage concept according to the baseline design of the proposed high-level nuclear waste repository at Yucca Mountain is analyzed. The high-temperature storage concept, in which the emplacement area is heated above the boiling temperature of water, is subject to criticism on the basis of uncertainties due to nonlinear multiphysics processes in the rock mass and in the storage airspace. The storage environment around the nuclear waste containers is reexamined using a new thermal-hydrologic airflow model. The complex nature of the thermal-hydraulic behavior in a superheated waste repository is described with fewer simplifying assumptions than those used in the baseline design. The emplacement area in the mountain is described as an open system, in which the air pressure is connected to the barometric pressure through fractures, faults, and partially sealed drifts. The cyclic variation of the atmospheric pressure that affects the heat and mass transport processes in the near-field rock mass is also modeled. The implications of evaporation into the drift airspace are discussed, and a hypothesis of salt accumulation in the near-field rock mass is established. Model calculation is also presented for a below–boiling temperature storage concept that is easier to predict and has fewer anomalies. The price for a below–boiling temperature storage is the extended preclosure ventilation time period. However, as demonstrated for a trade-off, it is possible to design a repository with below-boiling temperatures and doubled waste inventory at the same time.

I. INTRODUCTION

Using a new thermal-hydrologic, air and vapor flow model, the hot and cold storage concepts for the proposed nuclear waste repository at Yucca Mountain (YM) are reanalyzed, amid mounting pressure for increasing its storage capacity.[1–3] The first goal of the new model study is to critically examine the above–boiling temperature storage concept, known to be associated with a rapidly changing thermal-hydrologic storage environment involving complex, nonlinear, coupled, typically multiphysics processes.[4,5] The second goal is to provide an example of a cold conceptual repository with a doubled storage capacity and long-term ventilation as a trade-off, using the same repository footprint area of the current baseline design.

The high-temperature operation mode (HTOM) was selected in 2002 after careful evaluation of the scientific basis and the available simulation results.[6] HTOM was found to be best for meeting the safety and performance

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requirements of the proposed YM facility at its design capacity of 70 000 t U (tons of uranium). Since that time, more elaborate numerical simulation techniques have emerged, applying refined in-drift heat and moisture transport models.[7–10] These studies, using computational fluid dynamics (CFD) models for the in-drift domain, have discovered that airflow, driven by natural buoyancy effects in the emplacement drift, contribute to significant heat and moisture transports during the postclosure time period, when the drifts are sealed and no longer ventilated. Before the appearance of specific in-drift heat, moisture, and airflow CFD models,[7–10] the drift space was modeled as porous media with equivalent, effective properties to represent the air, waste package (WP), and drip shield.[5,11] In-drift vapor transport and condensation in the cold drift segments, called "cold trap," were studied with the porous media-equivalent model, and both were found insignificant,[5,11] supporting the conclusion that the multiscale thermal-hydraulic (MSTH) model (which, because of its construct, did not account for axial vapor transport) adequately described the relevant processes.[5,11] A quite different picture has emerged from a more advanced coupled rock mass and in-drift model[7] that included laminar or turbulent flow in the drift airspace.

One consequence of the air movement and convective moisture transport was the appearance of condensate water in the emplacement drift around some of the WPs. The highest amount of condensate water was found during the time period when both above-boiling and below-boiling temperatures coexisted within one drift, showing a strong and previously unquantified water-redistribution process associated also with a heat-load redistribution process along the length of the emplacement drift.[7] The convective heat and vapor transports along the drift axis during the thermally active time period were also analyzed with an independent CFD model, using FLUENT, uncoupled hydrologically from the rock mass. The model results[4,9] have shown strong in-drift convection transport, a mechanism that needs to be recognized during the thermally most active time period of a few thousand years, and especially during the period of above-boiling operation.

The allowable maximum temperature is also a key factor in analyzing a design concept, especially in the determination of the storage capacity of the proposed repository at YM. The emplacement density is limited by the permissible heat load generated by the nuclear waste. The heat load is responsible for developing a time-dependent temperature field around the emplacement area with characteristically two temperature peaks, one during the ventilated preclosure time period and one after the permanent closure of the repository.[5–7] The second temperature surge is the most important for three reasons: (a) it is spontaneous with no control left at hand for the operator to influence it; (b) it is higher in value than the preclosure peak, and thus it is the limiting factor in the WP as well as in the emplacement drift surface temperatures, both specified by design criteria, referenced in the MSTH model report[5]; and (c) it is protracted in time, causing long-term thermal-hydrologic effects and reaching the deepest penetrations into the rock mass from the emplacement drift surface. The current baseline design with HTOM and an emplacement density of 56 t U/acre draws its capacity limitation from the third effect, dictating the spacing of the emplacement drifts to be wide enough for keeping the water drainage pathway open from the ground surface to the water table. The coalescence of the above–boiling temperature regimes around the neighbor emplacement drifts is avoided in the baseline design by keeping part of the rock mass in the so-called pillar area between the drifts below the boiling temperature of water at all times. Wide drift spacing of 81 m was deemed necessary to designate drainage pathway in the pillar area in the current baseline design for HTOM. This design constraint imposes a serious geometry-driven limitation in the storage capacity of the proposed repository at YM.

Many design options have been considered for dealing with the thermal issues while increasing the storage capacity: heat-output–reducing aging of the nuclear waste, long-term preclosure ventilation, and multilevel emplacement-drift arrangement.[3] Alternative designs with reduced drift spacing that allows for a coalescent above–boiling temperature field between neighbor emplacement drifts have also been considered,[3] revisiting an old issue. In spite of early optimism for a supposedly dry storage solution[12,13] at YM, the superheated pillar area concept has been put to rest because of the complexity of the thermal-hydrologic problem to predict with confidence. Blocking the flow path of percolating water originated from annual precipitation and accumulating it above the repository horizon by a coalescent above–boiling temperature field carries the risk of collecting large amounts of water over long periods of time, e.g., thousands of years, above the repository horizon. Such accumulations have been considered and studied in view of thermally induced seepage. Water seepage into the emplacement drift during the above–boiling temperature operation has been the subject of numerical studies.[14–17] Considering a range of hydrologic property variations typical at YM and using Monte Carlo analysis, it was shown that water seepage into the emplacement drift through large rock fractures could not be ruled out during the above-boiling operation.[14,15] The key issues in deciding whether or not liquid water may penetrate through the superheated "thermal umbrella" and reach the crown of the drift are (a) the geometry, i.e., the aperture of the liquid finger; (b) the recharge rate of water to the penetrating finger; (c) the duration of the episodic event; and (d) the thickness of the superheated rock area above the drift. These studies, showing reasonably positive results for YM with the conclusion of unlikely seepage penetration,[15–17] are restricted to the current conceptual design with its typical thermal and hydrologic conditions and subboiling pillar areas. It must be recognized that model uncertainties and the statistical nature of the geologic formation limit the optimism established for short-term episodic water fingering that may not be able to break through the evaporation barrier.[16] The debate, however, is now reopened, suggesting a concept with large coalescent above-boiling rock areas.[3] Although higher temperatures increase, as a positive effect, the thickness of the superheated rock regime above the drift, the closure of the drainage pathways between the emplacement drifts fundamentally changes the entire water balance, a negative effect. Each thousand years of coalescent above-boiling operation adds 75 m to the thickness of fully saturated rock area above the repository horizon, assuming 15 mm/yr percolation and 0.2 rock-mass porosity. Currently available seepage studies all assume the current conceptual design with subboiling pillars. A continuous, large, saturated area that may form above the emplacement drifts if the pillars are superheated affects the recharge rate of potential water fingers and reopens the question of episodic or even continuous seepage into the relatively cold drift sections.

The evaluation of the hot or cold storage concepts are approached from a different perspective in this paper. Starting with the baseline design with the HTOM, the water redistribution phenomenon, via vapor transport through the drift airspace, and its consequence are revisited with more scrutiny using a new numerical model. Capacity limitation conditions dictated by a no coalescent temperature field requirement for open drainage pathways in the pillar area would no longer apply if the temperatures within the emplacement drift were kept always below boiling. From the geometrical layout of the available storage area at YM, at least three times more emplacement drifts can be constructed on the same repository footprint by decreasing the current drift spacing to one-third. A low-temperature operating mode (LTOM) with tight drift spacing for capacity increase offers an alternative solution to the current baseline design, provided that the increased amount of heat dissipation from the nuclear waste can be removed by ventilation. A close drift spacing of ~25 m is consistent with rock mechanics requirements for drift stability and used in previous design arrangements for YM. With always below-boiling temperatures in the drifts, neither the blockage of water drainage nor large-scale water redistribution around the emplacement area are expected.

Cross-flow ventilation for several hundred years for in-site cooling has been studied before and can be used for temperature reduction during the postclosure period.[18,19] The same principle may be used to design a cold, below-boiling facility in spite of increased storage capacity. The feasibility of the solution is investigated in the paper, keeping in sight that a long, monitored, open-system ventilation time period is also advantageous for accommodating possible new directions in nuclear waste management, such as waste reprocessing in the future.

II. A NEW, COUPLED, MULTISCALE, THERMAL-HYDROLOGIC MODEL

II.A. Review of Model Applications and Limitations

A specific aim of the model formulation is to accurately describe the physical processes that contribute to the formation of the near-field environment, the central driver for repository performance during the most critical first few thousand years. Issues with previous known models for YM are (a) multiscaling, that is, the incorporation of large mountain-scale heat and moisture transport effects in the fine-scale, near-field, and in-drift models; (b) the representation of the details of fine variations within the typically coarse meshing along the drift length; (c) modeling of the heat and moisture transport within the airspace, where transport is provided by air velocities; and (d) the closed, constant-volume, and constant-pressure boundary condition on the interface between the airspace and the rock. The composite MSTH model,[5,11,20] because of its construction, does not have any hydrologic model component to follow the moisture transport in the direction of the drift axis. The only submodel that incorporates coupled thermal-hydrologic processes in the MSTH model is the two-dimensional Line-average-heat-source Drift-scale Thermal-Hydrologic (LDTH), which is fine-discretized with centimeter-scale in radial direction normal to the drift axis but is isothermal, isobar, no heat flow, and no moisture flow in the axial direction. Two three-dimensional (3-D) model-elements are employed within the MSTH model: the Smeared-heat-source Mountain-scale Thermal (SMT) submodel, and the Discrete-heat-source Drift-scale Thermal-conduction (DDT), local temperature superposition submodel. Both SMT and DDT solve for thermal conditions but not for moisture flow, using heat conduction-only configuration in the NUFT code.[5,11,20] Longitudinal meshing along the drift length for moisture-vapor transport is not represented in the MSTH model, since the LDTH submodel is two-dimensional, i.e., a vertical slice that is separated with vertical no-flow boundary planes. The thermally driven hydrologic processes in axial direction along the continuous drift segments, filled with WPs of variable heat load, are not modeled in the MSTH model. When longitudinal heat and moisture flows are both important to model, such as in the verification exercise for the MSTH model technique,[5,11,20] a scaled-down monolithic block of rock is used. The 3-D rock-mass domain is represented by the monolith model, rather than by an assembly process of complementary submodels. Differences reported between the MSTH and the monolithic models are small at the center of the panel where the temperature change along the drift axis is low, but not quite negligible around the end of the drift.[5,11,20]

The issue taken with the MSTH model validation using a scaled test case is not the difference between the MSTH and the monolithic model results in temperature, humidity, and rock water content at the edge of the emplacement panel, although the difference is recognized.[5,11,20] The issue addressed here is that the monolithic model has several simplifying constraints and that its validity as a standard must be considered with skepticism.

First, the monolithic model[5,11,20] uses WP-scale longitudinal meshing along the drift length, for four detailed WP locations only in the middle and at the end of the drift. Between the fine-detailed sample locations, line-averaged heat load is used. However, no analysis is provided to prove that the replacement of individual meshing with line load representation is adequate for a validation standard solution.

Second, the monolithic model[5,11,20] applies an approximate porous-media representation of the drift airspace using the combination of an equivalent effective permeability of 10^{-8} m^2 and moisture dispersion coefficient ranging between 0.011 and 0.021 m^2/s. The question must be raised as to whether or not the 10^{-8} m^2 permeability is high enough for modeling the airway in an open drift. The permeability of an open airway with laminar flow is on the order of 10^{-1} m^2 in permeability. This is at least 10^7 times higher than the value used in the MSTH studies,[5,11,20] raising the potential of having 10^7 times lower pressure variation or 10^7 times lower axial gaseous flow along the axis of the drift for the same axial pressure difference or axial flow rate, respectively. What is expected in reality in a coupled in-drift and in-rock system is an enhanced vapor transport that originates in the drift airspace by strong convection and condensation in the near-field rock mass.[21] Will heat and moisture transport be significantly different from the monolithic model results because of strong axial connection within a real drift? This question cannot be answered by simply raising the permeability of 10^{-8} m^2 any higher in the monolithic model,[5,11,20] since the NUFT model solver would not converge. The addition of some axial vapor dispersion to convection in the monolithic model is an interesting solution to the problem caused by permeability limitations. However, the value selected is five to ten times lower than the dispersion coefficient of 0.1 m^2/s published for a case with axial temperature gradient by Webb and Itamura.[9]

Third, the monolithic model uses a scaled-down domain representing a drift length of only 243 m, approximately one-third of those in the proposed design for YM. However, no scaling has been applied in contemplating the error differences between the monolithic and the MSTH model results. Assuming linear scaling with the drift length raises the question of whether or not a threefold error difference between the monolithic and MSTH models is still acceptable. An independent model with uncompromised model conditions and input properties will be needed to verify the validity of the current monolithic model results and, if needed, revalidate the MSTH modeling method itself.

Several, previous models published for YM apply a simplified in-drift airspace model,[5,11,20,22,23] in which the airspace is modeled as an equivalent porous-media, integrated in the rock-mass model itself. The monolithic model of Birkholzer et al.[22,23] analyzes a full-scale emplacement drift, in which a few select WPs are effectively represented with their own grids, while most of the others are represented by averaged line heat load. The new element of this model[22,23] is the use of an increased, equivalent dispersion coefficient published by Webb and Itamura,[9] an improvement over previous models.[5,11,20] The advantage of this integrated approach is the automatic coupling between the rock-mass and in-drift model domains. The disadvantage is that only diffusive-dispersive and conductive transport mechanisms can be modeled in the airspace, being part of the porous-media model domain. The transports of heat and moisture by convection are only approximated with effective, bidirectional, diffusion-dispersion terms. Convective transport provided by laminar or turbulent natural air circulation is not correctly modeled, since the transport velocities in the drift cannot develop in the equivalent porous media model because of the high flow resistance, represented by the 10^7 times lower permeability than that in the open airspace of the drift. A previous study compared and found significant differences in the condensation patterns between two models, one using an equivalent dispersive transport model and the other using convective model elements with transport velocities.[10] The significance of the convective versus diffusive/dispersive transport will remain an issue for some time in the future for the equivalent porous-media models.

Connecting the drift airspace to the ambient pressure environment represents another modeling challenge. The YM facility is known to breathe, as if having a lung—the pores, fractures, faults, and lithophysae of the rock—and being on a respirator—the variable, outside, atmospheric pressure environment. The emplacement drifts are planned to be driven in fractured, porous, and lithophysal rock mass at YM, intersecting major fractures and interconnected lithophysae that do not hold pressure even if the drift ends are closed and pressure sealed. This fact is evidenced from barometric pressure measurement data[18] collected from sealed deep boreholes: The amplitude of the periodic variation of barometric pressure with time propagates along the depth of the boreholes without noticeable attenuation. The large-scale connectivity from the drift airspace to the atmospheric ambient pressure must take into consideration the manifold effect of the drift itself. Along its length, any emplacement drift will be connected to the outside atmosphere through various flow resistances, all in parallel connection. The resultant resistance of parallel branches in a manifold is lower than the lowest resistance, which means the connection along the lowest resistance, and not the average, will be dominant for the gaseous flow into or out of the closed drift airspace. Therefore, the drift airspace as a leaky manifold should be connected to the outside ambient pressure through the highest possible permeability connection in addition to its connection to the ambient atmosphere at the surface through the equivalent-continuum average permeability of the porous and fractured rock mass. Since no discharge of vapor along the drift axis is possible in the MSTH model, as discussed in the foregoing, the connection to the outside atmosphere is possible only through an average equivalent-continuum permeability through the rock mass. Therefore, the drift is a closed airspace in the porous-media in-drift models and communicates with the atmosphere exactly the same way as any in-rock volume does at the depth of the repository horizon.

The equivalent-porous media models for the drift naturally underpredict vapor or steam flow into the drift airspace, affecting temperature and humidity distributions. To provide pressure connection to the atmosphere, the technique of implanting a given pressure point into the drift airspace was used in the NUFT model evaluating the heated drift-scale test (DST) results[5] at YM. The same technique is employed for pressure connection in the postclosure studies using an integrated porous-media in-rock and in-drift model based on the TOUGH2 code.[22,23] Applying pressure as a boundary condition in the model at one point, however, requires full Dirichlet boundary conditions with the definition of other parameters (temperature and humidity) at the same point as well. In the DST evaluation exercise,[5] these were known from measurement. In a general case, no temperature and humidity can be a priori defined in the drift airspace without using iteration during postclosure, since both temperature and humidity vary everywhere because of in-rock and in-drift interactions.

Conventional CFD models can overcome difficulties with the porous-media in-drift models in the transport description and the open-volume airway assumption, but they require iteration on the air-rock interface with the rock-mass model. Such iteration, however, has not been implemented in any of the conventional CFD model applications[4,9,25] for YM. Neither Dirichlet nor Newman (flux) boundary conditions can be prescribed a priori for the solution without iteration for the interactions with the rock-mass model. The published CFD model results are, therefore, useful only for the limited purpose of evaluation of transport properties for the airspace model domain.[4,9]

II.B. The New Multiscale, Coupled, Thermal-Hydrologic Model

In the presented new model, the rock-mass domain around an emplacement drift is separated from the in-drift model that includes the open airspace (projecting a high equivalent permeability in the order of 10^{-1} m^2) and the WP. The rockmass is rigorously modeled as 3-D porous and fractured media (with a permeability range of 10^{-17} to 10^{-11} m^2) with mountain-scale connection between the heated and unheated drift sections, using the NUFT code.[24] The solvability of such a stiff thermal-hydrologic problem is the main underlying reason for separating the solution to two entirely distinct model domains in MULTIFLUX, one for the porous media with a permeability range of 10^{-17} to 10^{-8} and one for the airspace in the drift with any high permeability.

Figure 1 shows the rock-mass domain enclosing an emplacement drift in a slice of the mountain in the middle of an emplacement panel for the study. Sufficiently large, 80-m unheated areas at both ends of the emplacement drift are included in the model domain, a new element that has been found advantageous[21] and a deviation from previous configurations.[7,10,18] Other rock properties and boundary conditions on the ground surface and at the water table are essentially identical to those of previous studies.[7,10,18] The rock-mass model results from NUFT are checked against TOUGH2 results for a very similar model domain[21] and found to be in very good agreement.

The in-drift model is a 3-D lumped-parameter CFD model, fine-meshed to capture half WP-scale variations. The model configuration includes heat and mass transport connections in the airspace between the 80-m-long empty drift sections and the hot emplaced drift sections. Other data inputs for heat and moisture transport essentially agree with those of a previous study involving the conceptual baseline design for the YM facility.[18] The CFD model assumes an open boundary volume, allowing for change with atmospheric pressure variations and air and vapor expansion into the pores, fractures, and interconnected lithophysal cavities of the rock. The velocity field of the air and all relevant forms of heat and moisture transport are included in the airspace CFD model.[18,21,26] In the new model, the heat and moisture transport processes in the airspace of the drifts are first solved separately, and, second, numerically and iteratively coupled to the thermal-hydrologic processes in the rock mass. The coupled model is the first of its kind that produces convergent results on a small computational platform.

Key to the new solution is a novel numerical model coupling technique used in the MULTIFLUX code[27] for reconnecting the in-rock and in-drift model-elements. The iterative coupler enforces boundary coupling of the heat and moisture transport processes on the interface between the drift airspace and the rock mass surrounding the drift. A surrogate model-element, obtained from the Numerical Transport Code Functionalization (NTCF) procedure,[27] allows for rescaling the rock-mass results and reducing the number of NUFT runs during iteration. Support transport coefficient data for the in-drift lumped-parameter CFD model-element are imported from a CFD simulation from the literature.[4,9]

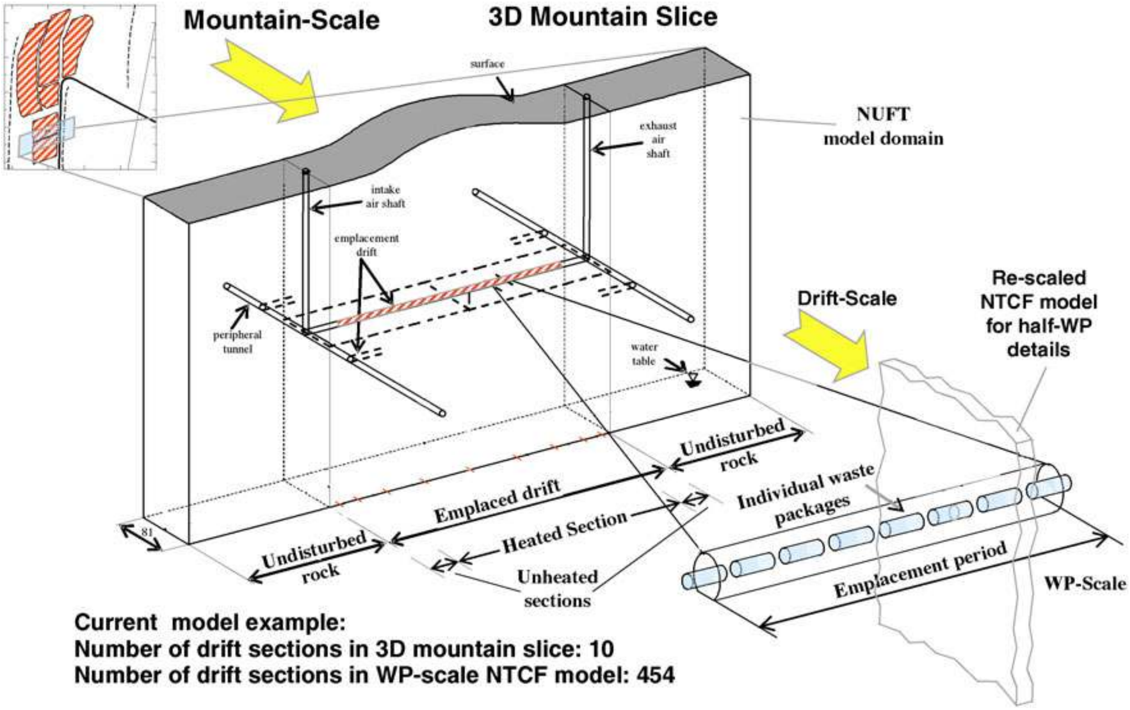

Fig. 1. The mountain-scale and in-drift model domains.

III. MODEL RESULTS

III.A. Thermal-Hydrologic Behavior of the Baseline Design

Results for the above–boiling temperature baseline design from the new model are shown in Figs. 2a and 2b for temperature and relative humidity distributions on the drift wall with time and along the length. Slight variations in the results with the drift length are caused by the heat dissipation variations between individual WPs.

Figure 3a shows spatial and temporal variations of condensation. The vapor inflow into the drift airspace is depicted in Fig. 3b in the form of the water attraction ratio, a nondimensional ratio between the spatial and temporal vapor flux into the drift and the percolation water flux calculated over the springline width D of the drift. The W in the W/D water attraction ratio may be pictured as an imaginary width over which the natural ambient water percolation flux is collected, and transported into the drift by evaporation or seepage. The $W/D = 1$ isoline is marked in Fig. 3b. In the domain where $W/D > 1$, the drift is effectively a water attractor. This domain approximately coincides with the spatial and temporal domain where the temperature is above boiling.

The result in Fig. 3b indicates that a significant amount of mountain-scale redistribution of percolation water is expected through evaporation and transport via the drift airspace during the above-boiling operation. The 3-D water redistribution mechanism through the highly permeable drift airspace was recently analyzed[18] in its full complexity using MULTIFLUX, the first model that provided a coupled, balanced solution to the conjugate three-dimensional thermal-hydrologic problem. A follow-up study[21] with the MULTIFLUX model analyzed the effect of the presence or absence of the unheated drift-end sections upon hydrologic and thermal conditions in the drift and credited the quite significant differences to the vapor transport via the drift airspace. The current results show once again in a robust way how important the moisture transport is along the direction of the drift axis between the hot superheat drift section and the long (80-m) unheated drift sections. Without such an axial moisture transport, the W/D water attraction ratio for the drift, shown in Fig. 3b, would never exceed unity. The results are consistent with what common sense suggests. As water evaporates in the rock mass, it follows the path of least resistance, entering the drift airspace and migrating to cold drift sections where it is trapped as condensates. Vapor, flowing along the drift from the hot middle section to the cold ends gradually condenses, effectively draining the incoming water and keeping the pressure at ambient level in the drift airspace. The new modeling result for YM is consistent with other published results.[22,23] Specifically, excellent agreement is found for both temperature and relative humidity at the center area of the emplacement drift, while somewhat higher

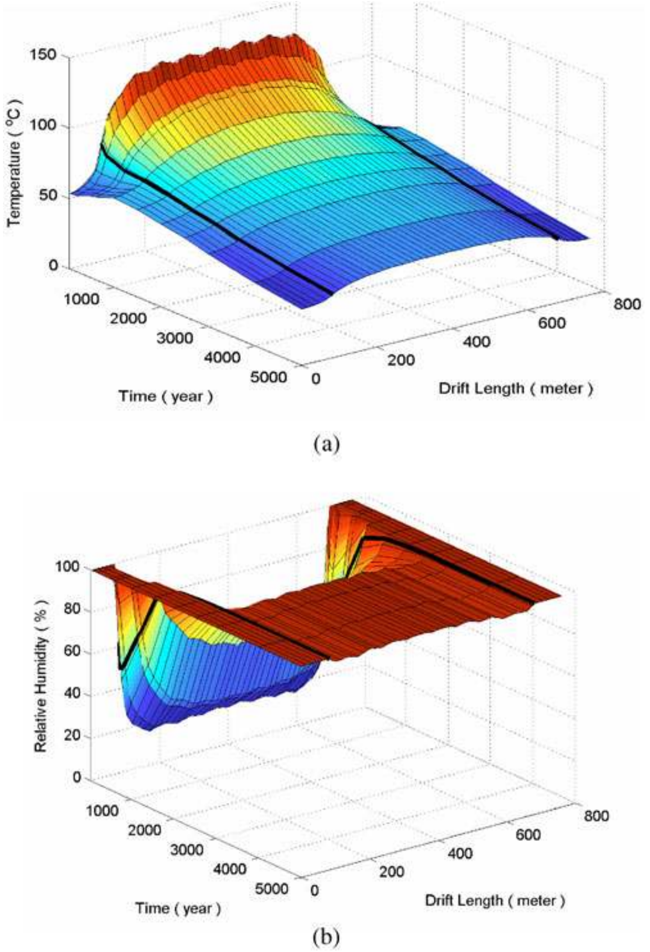

Fig. 2. Spatial and temporal variations of (a) the drift wall temperature and (b) the relative humidity in a hot emplacement drift for the U.S. Department of Energy's baseline design, according to a new, coupled thermal-hydrologic model.

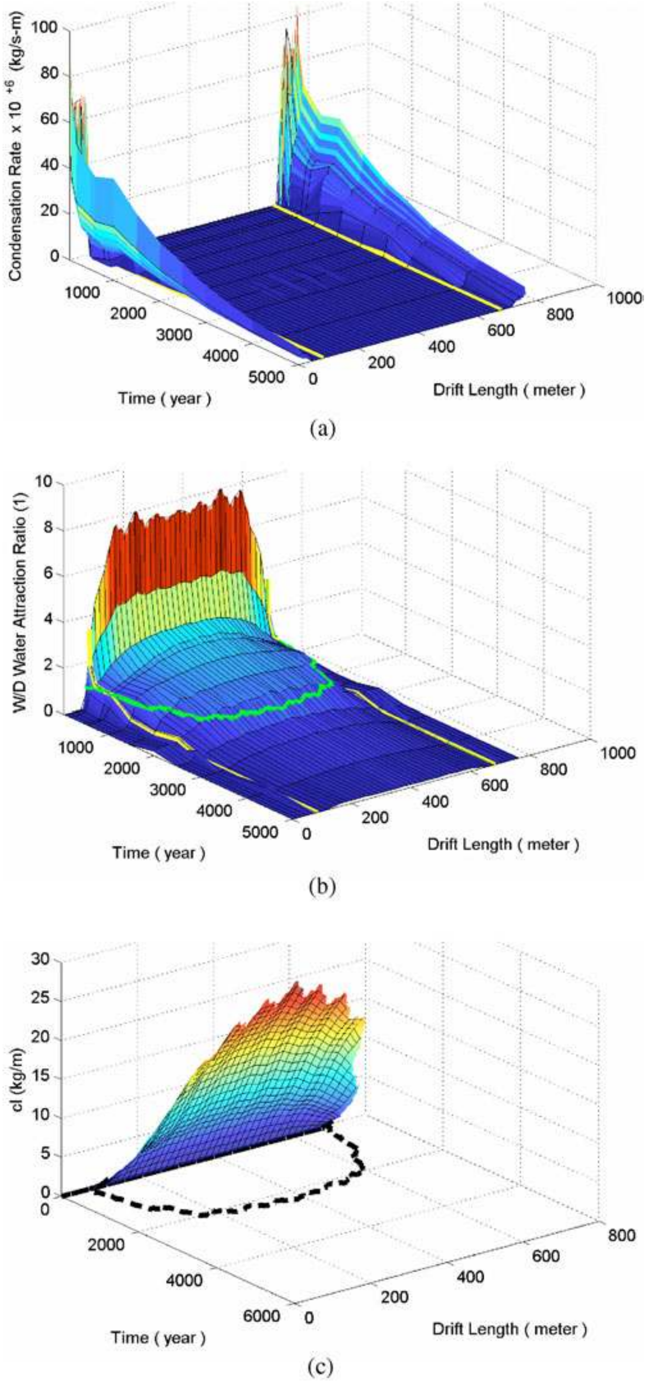

Fig. 3. Spatial and temporal variations of (a) water condensation rate at the emplacement drift wall, (b) the W/D water attraction ratio, and (c) chloride accumulation over the drift width D from mass balance during total evaporation; all for the baseline HTOM case.

temperature and lower humidity are obtained from the MULTIFLUX model when compared to the results from the monolithic porous-media model.[22,23]

Evaporation in the rock mass around the drift naturally means that dissolved ions from the source water will precipitate and accumulate as solids. Total evaporation of the percolation water flow as well as the pore water initially present in the rock matrix represents a source of solid species that must precipitate according to mass conservation. It is possible to estimate the accumulation over the drift crown numerically using the percolation flux toward the drift footprint for the time period over which the evaporation is complete, evidenced by dead-end percolation flow patterns. Figure 3c is an upper estimate of chloride ion (Cl^-) accumulation, associated with the total evaporation of water over the drift width D as a function of the axial position along drift length and time. The chloride accumulation at this point is a hypothesis based on the assumption that the concentration of chloride in pore water is 117 mg/ℓ at YM (Ref. 28), and that the total amount of chloride is deposited in the rock wall during complete evaporation. The numerical model results are used only within the boundaries of total evaporation with no dissolution due to lack of percolating liquid water leaving a control volume of the rock mass. Further trends are indicated in Fig. 3c as possible continuations with and without salt discharge. Two processes are in competition in the rock mass at the front of evaporation: (a) salt thickening (by liquid water evaporation) and (b) discharge (by water flow transport). The rate of deposition or dissolution is a complex phenomenon that can be modeled with the TOUGHREACT code.[29] However, during total evaporation and no liquid water discharge from a rock-mass volume, a simple estimation of salt accumulation is possible without using a kinetic model.

Examination of the water and flow directions in the rock mass provides evidence for total evaporation and reinforces the dissolved ion accumulation hypothesis with the new model results. Figure 4 shows water and vapor flow patterns from the NUFT model-element in the fractured and porous rock mass surrounding the emplacement drift in its middle section at three different time instants. Until year 1500 of postclosure, at which time the drift is already slightly below boiling, all percolating water disappears and turns into vapor form. The liquid water flow above the drift will dead-end in the rock mass and become a vapor source, as shown in the diverging vapor flow fields in Figs. 4b and 4d. Therefore, all salts in the percolating water must be deposited in the near-field rock mass, above the crown of the emplacement drift. A minute diversion of the percolation water flow at the drift crown is seen at year 2000 in Fig. 4e, indicating the onset of potential solute discharge and the effect of drift shadow. From this time on, vapor flow is still active all around the perimeter including the drift crown and the floor, as depicted in Fig. 4f, showing that accumulation and discharge may coexist for some time.

Different results are expected from the current design basis model,[5,11,20] lacking thermal-hydrologic water redistribution. An add-on in-drift condensation model[4] shows condensate at cold drift sections as a result of axial vapor transport, driven by 100% relative humidity at the drift wall, as a Dirichlet boundary condition. The vigorous evaporation from inside the rock wall and steam flowing into the drift airspace during the boiling regime is simply replaced with a passive transport driven by saturated humidity condition at the drift wall. No superheated steam flow into the drift has been shown in the baseline analysis used for YM because of applying a closed, pressure-holding hydrothermal system model to YM, instead of using an open system model with connection to the ambient atmosphere.

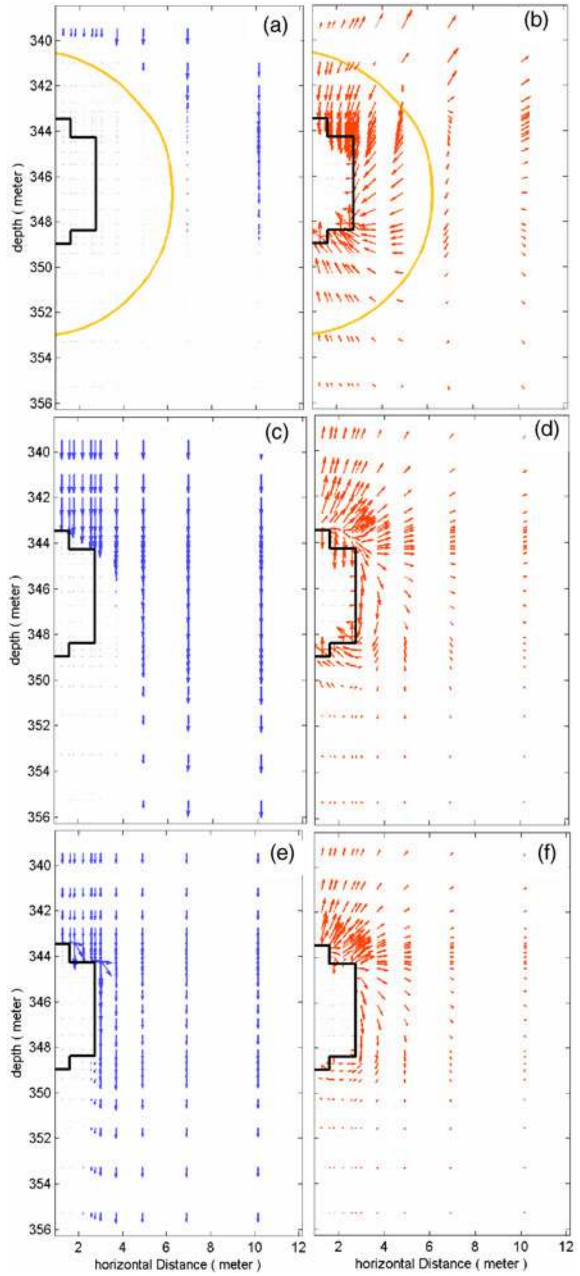

Fig. 4. Water pore velocity in the rock mass surrounding the emplacement drift in liquid phase (a, c, and e) and gas phase (b, d, and f) at year 600 (a and b), year 1500 (c and d), and year 2000 (e and f); solid line indicates 96°C contour, the boiling temperature at YM.

III.B. Implications of Potential Salt Accumulation in the Drift Wall

The study of the deposition of significant quantities of potentially corrosive salts in the rock at the crown of the drift is of great importance. Transport from the crown is naturally possible via roof degradation, such as spalling and rock fall, deliquescence, and/or dust formation. Therefore, the accumulation of salts in the rock above the emplacement drift may be critical to the corrosiveness of the storage environment during the time period of relatively high temperatures.[30] The simple salt accumulation model result in Fig. 3c covers just that time period. Salt will likely accumulate further for some time and later dissolve with percolation water flowing in the rock around the drift; the hypothesis of these processes needs further model investigations with an explicit salt transport model-element, such as provided in the TOUGHREACT code.[29]

Sufficient for further discussion is to observe the high rate of potential chloride accumulation and the predicted total salt deposits exceeding 20 kg per linear meter of drift length during the first 2000 yr of repository operation. The result represents a paradigm shift in our understanding of the effect of temperature upon the near-field

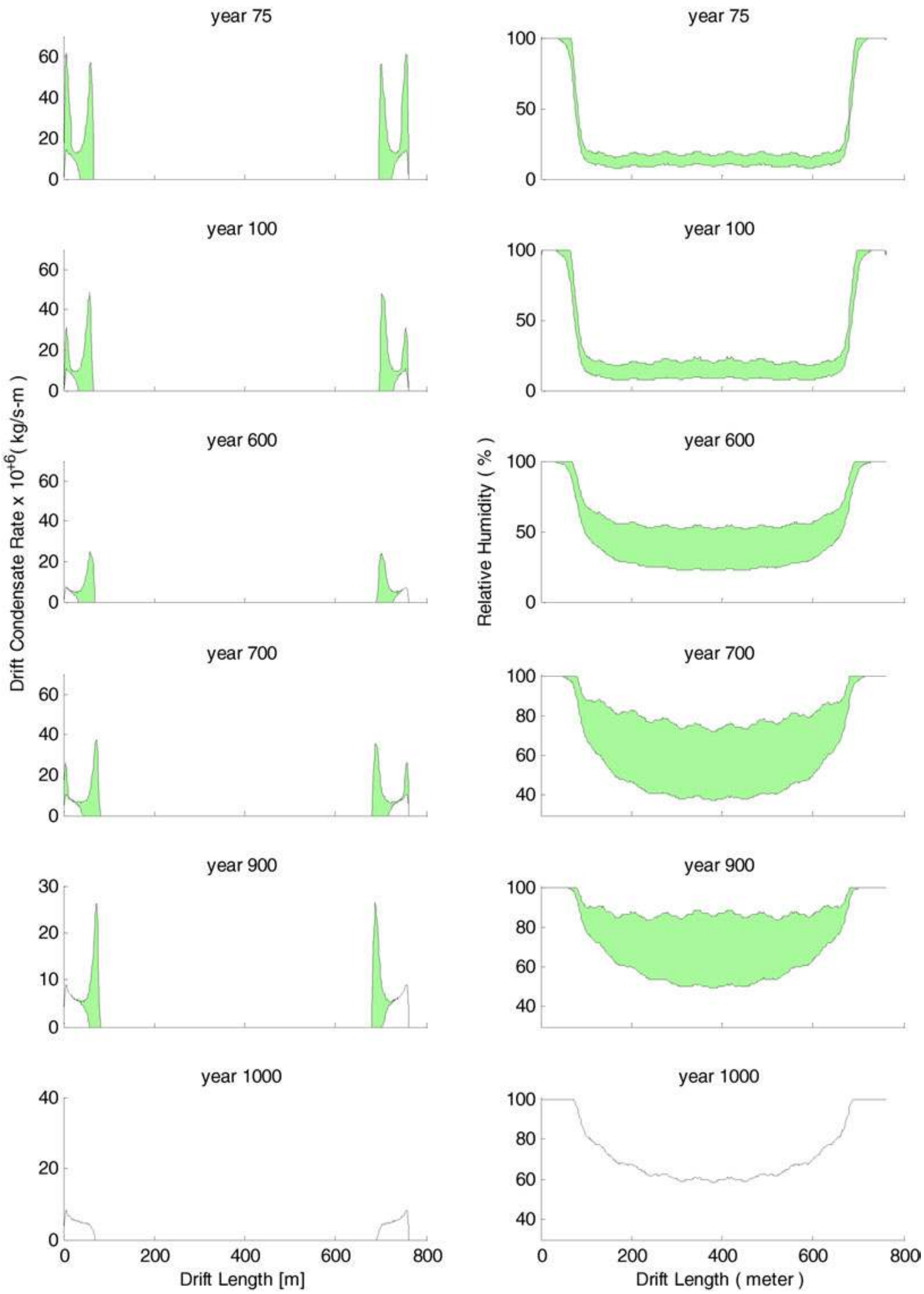

Fig. 5. Barometric pressure fluctuation effects on relative humidity and condensation rate, at the roof segment of the drift wall.

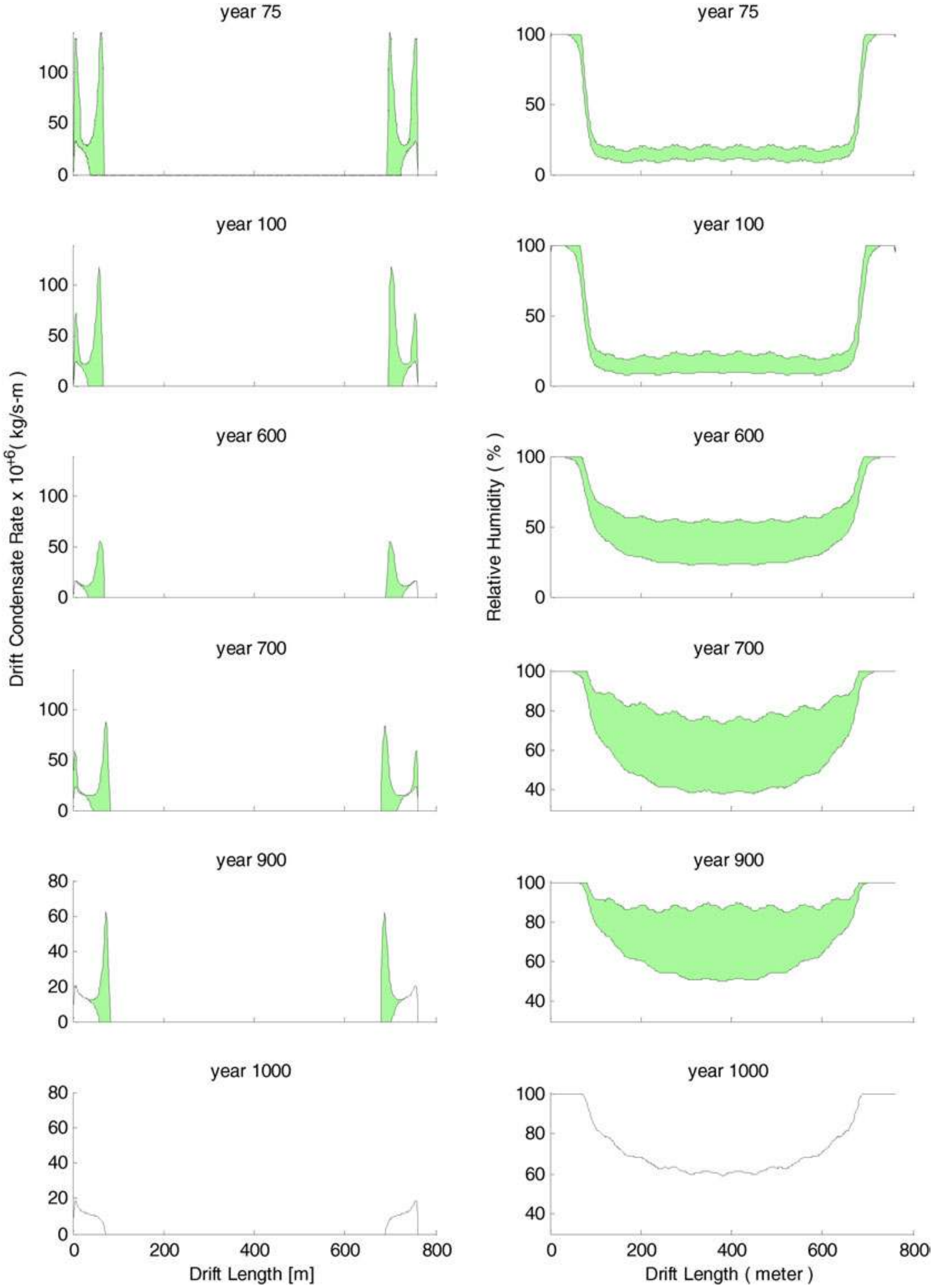

Fig. 6. Barometric pressure fluctuation effects on relative humidity and condensation rate, at the sidewalls segment of the drift wall.

environment. When vapor transport is predominantly into the rock, the current assumption at YM, condensation at a larger radial distance in the rock leads to the prediction of lateral flow (shedding) of water and dissolved salts around the drifts. Reversing the modeled direction of vapor flow during the thermal surge changes the system without soluble salt accumulation to one with potentially large accumulations of soluble salts in the near-field rock mass.

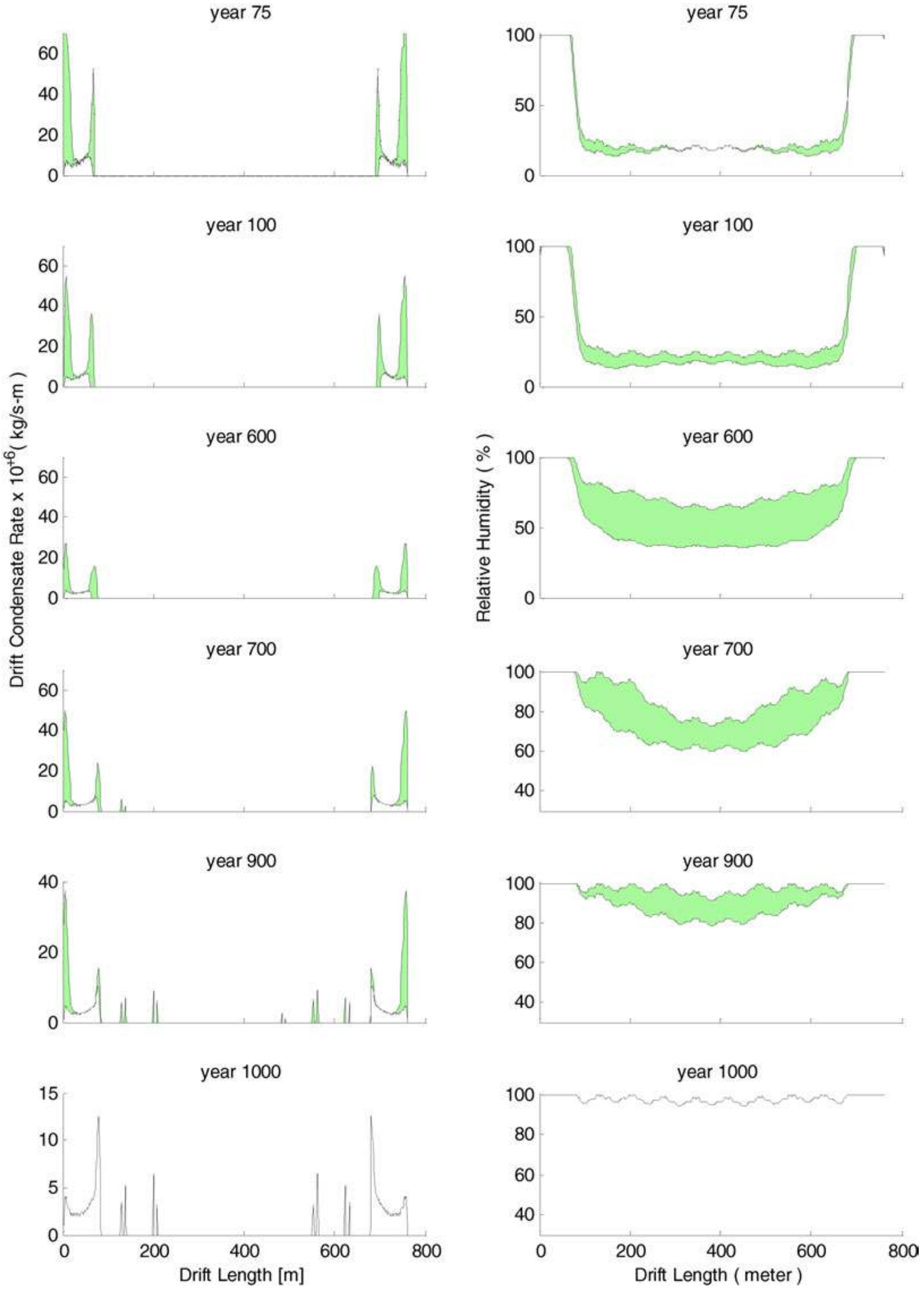

Fig. 7. Barometric pressure fluctuation effects on relative humidity and condensation rate, at the floor segment of the drift wall, over the invert.

III.C. The Effect of Barometric Pressure Variation on Evaporation in an Above-Boiling Repository

Barometric pressure fluctuates at YM with a time period of ~10 days and 1160 Pa amplitude, a change of ~1% in the average value.[18] The variation impacts the heat and moisture transport in the near-field and in-drift environment. The variations in moisture flux have shown to cause periodic fluctuations in relative humidity along the drifts.[18] The new model results are shown in Figs. 5, 6, and 7 for three different segments on the drift wall circumference: the roof, the sidewall, and the floor over the invert. The low pressure cycle (at 87 560 Pa) in Figs. 5, 6, and 7 corresponds to the upper bounds of the shaded areas of both condensate rate and relative humidity, while the high pressure cycle (at 89 880 Pa) corresponds to the lower bounds of the shaded areas. The relative humidity as well as the condensate rate will both swing between the upper and lower bounding curves as the barometric pressure cycles between the upper and lower average bounds. The primary importance of the variations in relative humidity is that some of the accumulated salts resulting from evaporation into the drifts are hygroscopic and will deliquesce. Deliquescence can lead to dripping of concentrated solutions from the roof of the drifts. Imagine, for example, a salt deposit in the rock wall. The anticipated response of the deposit to fluctuation in relative humidity is dependent upon temperature, relative humidity, and salt composition. As relative humidity rises, dry salts may deliquesce while existing aqueous solutions will become more dilute and potentially dissolve different salts. As solutions increase in volume, they may become mobile, potentially leading to flow separation of anions.[31] Drippage of the solution to the drip shield and seepage to the WP is a quite plausible scenario, in the case of increased water above the drift crown, e.g., if a hot repository is designed with increased storage capacity and with no pillar drainage. As relative humidity declines, the solutions will become more concentrated and may dry out completely (effloresce). The implication of fluctuating relative humidity is periodic concentration and dilution of salt solutions and the potential segregation of anions,[31] leading to a more aggressive chemical environment for WP corrosion. Contact of Alloy-22, the currently preferred outer material for the WP, with chloride solutions in the absence of nitrate at high temperatures experiencing periodic wetting and drying, can potentially lead to localized corrosion of the WPs with associated early penetration.

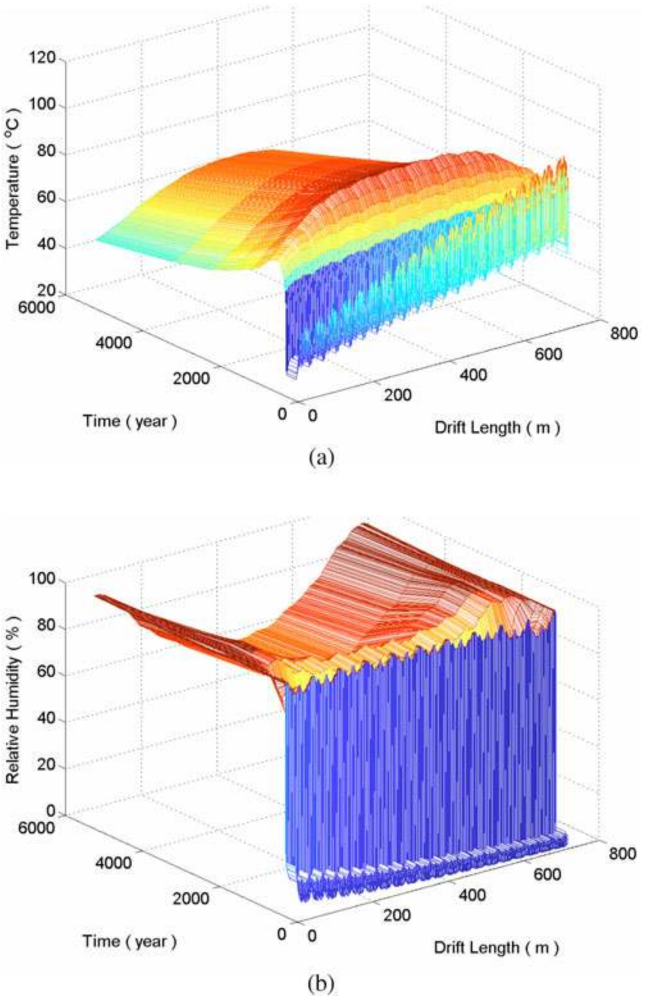

Fig. 8. Spatial and temporal variations of the drift wall (a) temperature and (b) relative humidity, both for the U.S. Department of Energy's baseline design with 300 yr of preclosure ventilation.

III.D. A Below-Boiling, LTOM Design Direction

The volatile processes associated with the above–boiling temperature design can be mitigated by reducing temperatures. Relative humidity variation with time reduces to insignificant levels at below-boiling temperatures. Repository performance at below-boiling temperatures can be predicted with greater confidence.[30] A series of studies for open-system repository ventilation[18,19] is available to support a conceptual solution to temperature reduction. Three hundred years of ventilation may bring the current baseline design below boiling. Figure 8 shows the temperature and relative humidity variations along the drift length for the preclosure and 5000 yr of postclosure time periods. As shown, the maximum temperatures are about the same, and close to boiling limit during (a) the 50-yr preclosure time period with cross-ventilation and (b) the postclosure time period with no powered ventilations.

III.E. LTOM with Storage Density and Capacity Increase

Capacity increase with doubling the storage density in the same, prime repository area requires a longer preclosure time period of ~600 yr. The baseline WP emplacement sequence is slightly rearranged by increasing the average line heat load close to the ends of the drift and decreasing it in the middle section, while keeping the average WP inventory doubled relative to the baseline design for the entire emplacement drift. The denser arrangement of the WPs close to the drift ends provides a flatter and lower temperature field in the middle of the emplacement drift. The WP heat generation along the drift length and with time is shown in Fig. 9a for the

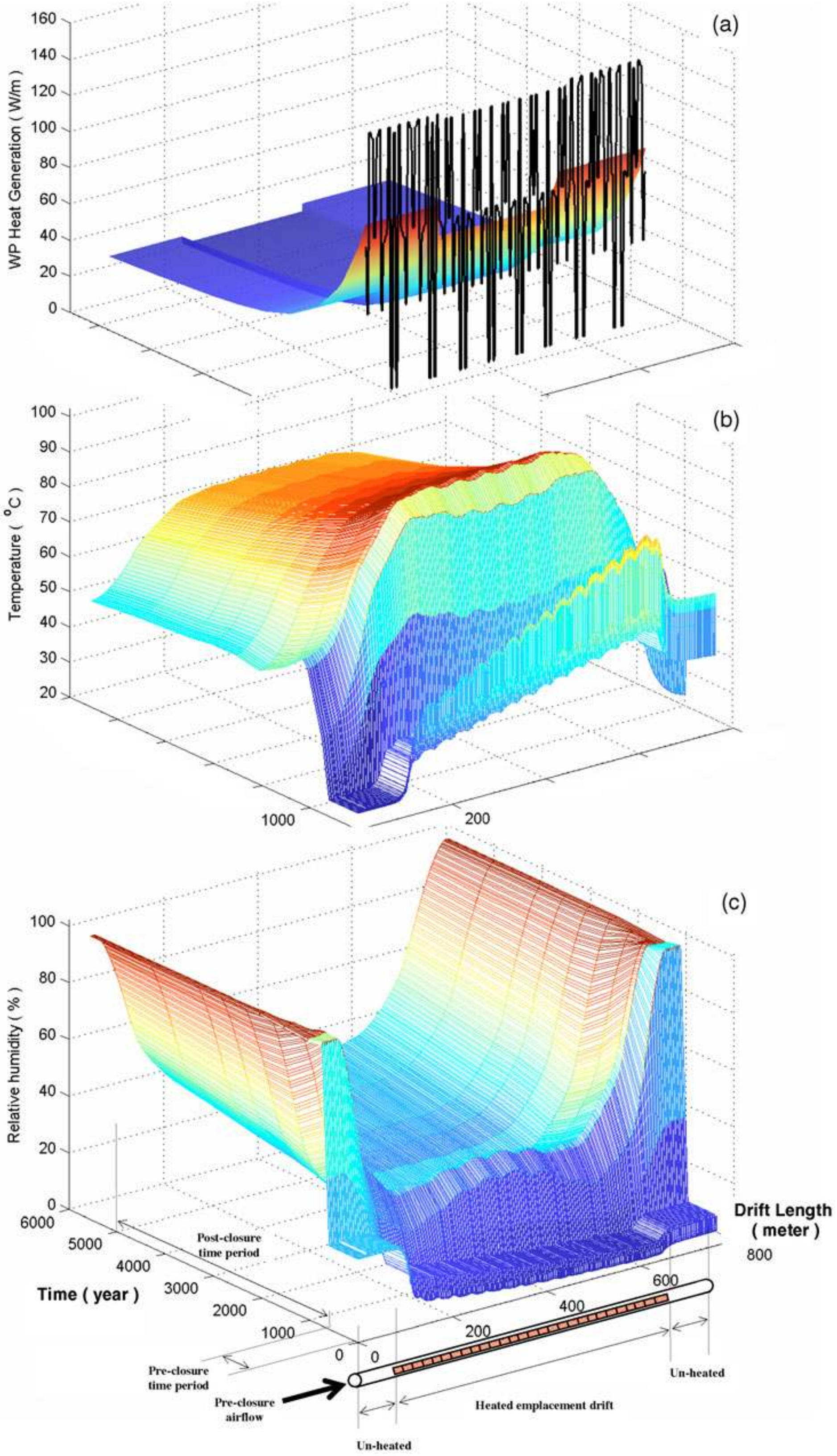

Fig. 9. (a) Variable, optimized postclosure heat load per unit length for individual WPs at year 600 (solid line), and line-averaged load equivalent (smooth surface); (b) temperature variation of a double-capacity low-temperature conceptual repository; and (c) relative humidity; all with 600 yr of preclosure ventilation, assuming no waste reprocessing.

rearranged emplacement representing double storage capacity. In Fig. 9a, the variable WP heat load is shown in thick line only at year 600, while for the rest of the time periods, only the line-averaged equivalent heat load is shown as a smooth surface for graphical presentation. However, the thermal-hydrologic model applied variable heat load all along time up to 5000 yr. The postclosure temperature and relative humidity variations with time and space of the double-capacity, low-temperature conceptual repository are shown in Figs. 9b and 9c.

Capacity increase for the proposed facility is made by reducing the drift spacing to 40.5 m from 81 m in the example. The modified conceptual design with double capacity is below boiling at all times, making it impossible to form a coalescent temperature field over neighbor emplacement drifts. Therefore, no unfavorable changes in the water pathways are expected. Less salt accumulation above the drift crown is anticipated for the below-boiling design, lacking saturated or superheated steam generation by boiling out pore and percolation water. However, more studies will be needed with the MULTIFLUX numerical model to verify this expectation if the high-capacity, below-boiling design receives further attention for application.

IV. CONCLUSIONS

Rethinking of the design direction for YM is suggested, supported by the results of a new, improved numerical model. The model results favor a below–boiling temperature design and show a feasible solution for doubling the current baseline storage capacity.

New model results are provided for the baseline conceptual design for YM with previously unquantified vapor flow phenomena that include two components: (a) significant vapor flow into the drift and (b) barometric pressure variation–driven vapor flow fluctuations, both during the above-boiling time period.

One consequence of the HTOM is that the vapor flow into the drift gives rise to salt accumulation in the rock wall, especially in the crown of the drift, during the above-boiling time period. This conclusion is supported by the analysis of total evaporation, and water mass balance in the rock above and around the emplacement drift, evidenced by vapor and water flow fields calculated by NUFT. In future studies, it is recommended that the salts precipitation be analyzed with direct simulation, using TOUGHREACT.

Another consequence of the HTOM is that the variable vapor flow, as a modulation due to barometric pressure variation, creates fluctuating relative humidity in the emplacement drift. The drift wall at certain locations may vary between dry and wet conditions periodically over time.

Salt accumulations in conditions conducive to flow separation of anions, combined with relative humidity cycling, may create a potentially more aggressive corrosion environment than that currently being considered for the above-boiling design.

Change to a below-boiling repository would reduce the potential for localized corrosion during the thermal period since (a) Alloy-22 is more resistant to localized corrosion at lower temperatures, (b) at below-boiling temperatures the accumulation of salts will be less, and (c) at below-boiling temperatures the barometric pressure changes will no longer lead to cycles of variations in relative humidity.

A below–boiling temperature design with doubled storage capacity may be achieved with 600 yr of preclosure ventilation, assuming no waste reprocessing. With waste reprocessing, the necessary preclosure ventilation cooling time period may be greatly reduced, or even eliminated.

The below–boiling temperature design with doubled storage capacity shows low relative humidity in most parts of the emplacement drift at extended periods of time, staying as low as 30% at the center of the drift in year 5000, an advantageous feature for the storage environment.

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