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Abstraction of Thermal Hydrology and Coupled Processes for TSPA

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Introduction

The thermal-hydrologic (TH) and coupled process models describe the evolution of a potential geologic repository as heat is released from emplaced waste. The evolution (thermal, hydrologic, chemical, and mechanical) of the engineered barrier and geologic systems is heavily dependent on the heat released by the waste packages and how the heat is transferred from the emplaced wastes through the drifts and through the repository host rock. The essential elements of this process are extracted (or abstracted) from the process-level models that incorporate the basic energy and mass conservation principles and applied to the total system models used to describe the overall performance of the potential repository. The process of total system performance assessment (TSPA) abstraction is the following. First is a description of the parameter inputs used in the process-level models. A brief description is given here of past inputs for the viability assessment (e.g., for TSPA-VA) and current inputs for the site recommendation (TSPA-SR). This is followed by a highlight of the process-level models from which the abstractions are made. These include descriptions of TH, thermal-hydrologic-chemical (THC), and thermal-mechanical (TM) processes used to describe the performance of individual waste packages and waste emplacement drifts as well as the repository as a whole. Next is a description of what (and how) information is abstracted from the process-level models. This also includes an accounting of the features, events, and processes (FEPs) that are important to both the regulators and the international repository community in general. Finally, an identification of the TSPA model components that utilize the abstracted information to characterize the overall performance of a potential geologic repository is given.

DISCLAIMER

Inputs used in the Process Models

The primary inputs incorporated into the thermal-hydrologic and coupled process models used to predict heat driven performance of the potential geologic repository are associated with the repository design and the natural system itself. The design inputs specify the layout of the repository such as the drift spacing, number of drifts, area of the repository footprint, waste package spacing, heat loading, etc., while the natural system specifies the hydrologeologic unit layering, hydrologic and thermal properties, and variability in ground surface infiltration rates among others.

Repository Design Inputs. Repository design criteria for TSPA-SR have been summarized in the reports by Francis et al.[1,2] and have been consistently implemented in the TH and THC models. A list of these features is: waste package types and numbers, waste package heat decay curves, waste package physical dimensions, spacings, and material properties, emplacement drift geometry, areal mass loading, repository footprint area and layout, and preclosure ventilation.

Many of these quantities have changed from previous TSPAs. Some of the more important of the changes are listed in Table 1 below.

Table 1. Design Feature Changes.

Parameter	TSPA-VA[3]	TSPA-SR[1,2]
Initial waste package heat output (commercial)	3 – 18 kW (approx)	7 – 11 kW (approx)
Drip shield physical dimensions and material properties	None	0.02 meter thick titanuim
Emplacement drift geometry (diameter)	5.5 meter including a 0.2 meter concrete liner	5.5 meter, no concrete liner
Waste package spacing	9 meters (approx)	0.1 meter
Emplacement drift spacing	28 meters	81 meters
Nominal areal mass loading	85 MTU[a]/acre	60 MTU[a]/acre
Preclosure ventilation	N/A	70% energy removed for 50 year period

[a]- MTU stands for metric tons of uranium

Each of the changes described in Table 1 are designed to redistribute moisture away from the waste packages by densely packing the waste packages in widely spaced drifts so that heat transfer processes serve to shed infiltrating and heat mobilized waters through the below-boiling portions of the emplacement drift pillars. For moisture that may enter the drift through the boiling zone (TSPA assumes that it can), the drip shield is available as a potential barrier.

Natural System Inputs. Descriptions of the natural system have also been consistently implemented in TSPA-SR models used for abstraction. These include: hydrogeologic layering of Yucca Mountain, hydrologic and thermal properties of different geologic layers, dual permeability conceptual flow model (active fracture model), infiltration rate and upper surface temperature variability, water table conditions, future climate states, geochemical systems (mineral assemblages), and initial water chemistry and gas composition.

Some of these quantities have changed from previous TSPAs. The most important changes are listed in Table 2 below.

Table 2. Natural System Input Changes.

Parameter/Model	TSPA-VA[3]	TSPA-SR[4,5,6,7]
Hydrologic properties for different geologic layers (shown here are repository host unit values)	Fracture porosity ~ 0.01%	Fracture porosity ~ 1%
Dual permeability conceptual flow model	Constant fracture-matrix contact area reduction factor	Calibrated active fracture parameter determines fraction of fractures hydraulically active
Future climate states	Mean infiltration flux case: Dry (average= 7.7 mm/yr), long-term-average (average= 42 mm/yr)	Medium infiltration flux case: Present day (average= 6 mm/yr), monsoonal (average= 16 mm/yr), glacial-transition (average= 25 mm/yr)
Geochemical systems (mineral assemblages)	N/A	2 different geochemical systems used to describe the potential repository host unit

The natural system inputs inherently contain uncertainty due to the complexity of the system being described. In the case of infiltration rate and hydrologic property (e.g., fracture permeability and characteristic curve parameters) specifications, a number of (different) representations can be used to describe the current ambient state of Yucca Mountain. Consequently, three infiltration flux cases (and associated hydrologic property sets) were developed: low, medium, and high infiltration flux fields and hydrologic property sets. In the present day climate, each representation reproduces the ambient state of the mountain through property calibration. The infiltration flux cases provide a representation of the uncertainty in infiltration rate at Yucca Mountain. Each of the three infiltration flux cases is applied in the thermal hydrology and coupled process models. Some uncertainties are not as well constrained. These include the reaction-rate parameters associated with the coupled reactive transport models (e.g., reactive surface areas for mineral assemblages). Another issue to be included in the models is an assessment of differences in processes associated with differences in scale of the properties. For the process-level models at the scale of the emplacement drift (e.g., one to a few meters), smaller scale (drift-scale) fracture permeability measurements are applied (e.g., on the order of 10^{-13} m^2). These include the air-permeability measurements made in the thermal test and experimental alcoves at the exploratory studies facility. For the process models at the scale of the mountain (tens to hundred meters), larger scale pneumatic permeability measurements are applied (on the order of 10^{-11} m^2).

Process-Level Model Descriptions

A brief discussion is given for each of the process-level models used in TH abstractions. The models described below use a variety of combinations of inputs previously described. The choice of input is largely dependent on the process being described.

Multiscale TH Model. The multiscale TH model described in Buscheck et al.[6] characterizes an assemblage of submodels that describe a number of different processes associated with repository heating. It is a hybrid drift-mountain scale TH model that includes repository edge effects associated with cooling processes that occur around the unheated rock mass surrounding the repository footprint. It includes the variability of waste disposal in different geologic host units as well as differences in layer thicknesses. Furthermore, it includes the variability (e.g., various repository locations) and uncertainty (e.g., three infiltration flux cases) in infiltration rate at the ground surface. Finally, the multiscale model includes waste package variability and heat transfer processes in-drift associated with different waste package types. The conceptual flow model and property set used in this process-level model was validated against experimental data gathered from three different field thermal tests.

Drift-Scale THC Model. The drift-scale THC model described in Sonnenthal et al.[7] is used to describe the chemical evolution of the host rock surrounding the emplacement drifts during repository heating. It is a coupled thermal hydrology model including the processes of reactive transport. It includes the mineral assemblages of two different geochemical systems. Both of the systems are validated and tested against drift-scale heater test (DST) results. The model also assesses infiltration rate uncertainty on chemical processes by including the three infiltration flux cases described above. This model also assesses changes in fracture porosity and permeability (by assuming plane parallel plate relationship between properties) due to mineral precipitation and dissolution processes described for these geochemical systems. The conceptual flow model applied in the TH submodel is the dual permeability active fracture flow model that applies the drift-scale hydrologic properties in the host units. This model characterizes THC processes within the near-field host rock by computing the water and gas composition as well as changes in the fracture properties by reactive transport processes. It too is validated against experimental data gathered from the field thermal tests.

Abstraction of the Process Models

Abstraction of the process models described above produces the in-drift thermodynamic environment (drip shield temperature, invert liquid saturation, etc.), percolation flux above the crown of the emplacement drift (used as an input in the TSPA seepage model), and the water and gas composition at the emplacement drift wall.

Abstraction of the Multiscale TH Model. Because it would be impossible to calculate the time of failure for each of the over 10,000 individual waste packages, a method to simplify the system was developed in order to reduce the computational burden. It is described by Itamura et al.[8] in the detailed description of abstraction methods. The abstraction of the multiscale TH model required a definition for a division of the repository footprint. Any division of the repository footprint should preserve and highlight the variability and uncertainty in the TH system supplied to the total system model. In the viability assessment, this was done by subdividing the repository area into six spatial regions based roughly on areas that contain similar infiltration rates. Since the quantity of seepage into the drift is expected to be the dominant mechanism for radionuclide dissolution and mobilization from the drift, the local infiltration rate during the glacial-transition climate was selected as the best variable to serve as a basis for subdivision in TSPA-SR. In this abstraction, the following infiltration ranges were specified for TSPA-SR: 0 – 3 mm/yr, 3 – 10, 10 – 20, 20 – 60, and > 60 mm/yr. The infiltration rate ranges (or "bins") provide the basis for abstraction such that each of the variables used to describe the thermal hydrologic performance of a potential geologic repository is grouped and averaged based on the infiltration rate ranges and areal weights.

Table 3 provides a description of the TH variables abstracted for the total system model component indicated in the table. Each of the 610 location-dependent results is sorted into five bins based on the location infiltration rate (glacial-transition climate). Each location represents the environmental conditions of a specified fraction of the repository area based on the multiscale TH process model from which it is abstracted.

Table 3. Abstraction Quantities.

Abstracted TH Variable	Total System Model Component Used In
Time (year)	All models
Waste package surface temperature[a,b] (°C)	Waste package degradation model Waste form degradation model
Bin maximum waste package surface temperature (°C)	Cladding degradation model
Drip shield temperature (°C)	Drip shield degradation model
Drift wall temperature[c] (°C)	In-Drift Microbial Communities
Invert temperature[c] (°C)	In-drift geochemical model
Waste package relative humidity	Waste package degradation model
Drip shield relative humidity	Drip shield degradation model
Drift wall relative humidity[c]	In-Drift Microbial Communities
Invert relative humidity[c]	In-drift geochemical model
Invert liquid saturation[c]	EBS[h] transport model
Top of drip shield evaporation rate[d] (m^3/yr)	In-drift geochemical model
Invert evaporation rate[c,e] (m^3/yr/ m-drift)	In-drift geochemical model
Percolation flux at 5 m above drift crown (mm/yr)	Abstracted seepage model
Volume flow rate at top of drip shield[f] (m^3/yr)	In-drift geochemical model
Volume flow rate at invert[c,g] (m^3/yr/m-drift)	In-drift geochemical model

NOTES:
[a]- Waste package degradation model uses location dependent results.
[b]- Waste form degradation model uses bin average computed based on area fraction.
[c]- Bin average computed based on area fraction.
[d]- Computed by energy balance.
[e]- Converted from kg/yr by dividing by 1000 kg/m^3.
[f]- Computed from abstracted seepage model.
[g]- Converted from mm/yr by (0.92m^2/1000mm).
[h]- EBS (Engineered Barrier System)
Quantities without superscripts use location dependent results.

Abstraction of the Drift-Scale THC Model. The abstraction of the drift-scale THC seepage model is given in detail in Francis et al.[9] The abstraction of the process model provides simplified results of the water and gas composition at the emplacement drift wall. It is this water chemistry or gas composition that may enter the drifts during repository heating. The process model results are simplified into four time periods spanning 10^5 years: preclosure, boiling, transitional cool-down, and extended cool-down. The abstracted water and gas compositions are constant in each time period. The abstraction is for five cations, six anions, and pH. In addition, this abstraction includes the partial pressure of carbon dioxide in the gas phase in fractures adjacent to the drift wall. In addition to providing an abstraction for water chemistry and gas-phase composition in the near-field host rock, it also illustrates the potential differences in the

TH response of a potential repository obtained from process models that either do or do not include reactive transport processes coupled with the thermal-hydrologic processes that occur in response to repository heat addition. It was shown that THC processes do not greatly influence TH response of the system (e.g., drift wall temperature, liquid flux in fractures, etc.).

Each of the process-level models described above provides input to the FEPs analyses as well as the abstractions for TSPA. This is described in the next section.

Features, Events and Processes

The intent of the FEPs process is to ensure that all of the important features, events, and processes that impact dose are included in the TSPA. If a FEP is excluded, then a justification for why the FEP was not included in the TSPA must be given; exclusion arguments can be for regulatory basis, based on a low consequence to dose argument, or based on a low probability (less than 10^{-4} chance in 10^{4} years) argument. A series of reports have been written within each of the various technical areas to address how FEPs have been included or excluded from TSPA.

The Yucca Mountain Project FEPs database contains approximately 1800 entries. These FEPs originate from the Canadian, Swiss, Swedish, United Kingdom (UK), and Waste Isolation Pilot Plant (WIPP) programs, as well as from Yucca Mountain Project (YMP) sources. They have been broken down into primary FEPs and secondary FEPs. Primary FEPs are those FEPs for which the project proposes to develop detailed screening arguments. The classification and description of Primary FEPs strives to capture the essence of all the Secondary FEPs that map to the primary. For example, the Primary FEP "Two-phase buoyant flow/heat pipes" can be used appropriately to resolve multiple and redundant Secondary FEPs that address the evolution and continuation of a heat pipe. By working to the Primary FEP description, the subject matter experts assigned to the Primary FEP address all relevant Secondary FEPs, and arguments for

Secondary FEPs can be rolled into the Primary FEP analysis. Secondary FEPs are either FEPs that are completely redundant or that can be aggregated into a single Primary FEP.

There are 26 primary and 112 secondary FEPs related to thermal hydrology and coupled processes. The subject of the thermal-hydrology and coupled process FEPs range from effects of the excavation of the tunnels, to specific chemical reactions, to basic heat transfer properties like evaporation and condensation.

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