CNWRA *A center of excellence in earth sciences and engineering*

A Division of Southwest Research Institute™
6220 Culebra Road • San Antonio, Texas, U.S.A. 78228-5166
(210) 522-5160 • Fax (210) 522-5155

July 27, 2000
Contract No. NRC-02-97-009
Account No. 20.01402.661

U.S. Nuclear Regulatory Commission
ATTN: Mr. Jeffrey Pohle
Division of Waste Management
TWFN, Mail Stop 7-D13
Washington, DC 20555

SUBJECT: Thermal Effects on Flow KTI Intermediate Milestone 01402.661.040: Process-Level Sensitivity Analysis-Status Report

Dear Mr. Pohle:

Enclosed please find the report titled "Thermal Effects on Flow Process-Level Sensitivity Analysis Status Report." This technical document fulfills the requirements for the subject milestone, which is due July 30, 2000.

The work documented in this report was performed under the Thermal Effects on Flow Key Technical Issue to evaluate the sensitivity of repository performance to thermal perturbations in unsaturated zone flow near the proposed waste emplacement drifts at Yucca Mountain, Nevada. In this report, the effects on thermal hydrology of repository design changes are evaluated and compared to the design utilized for the viability assessment. Parameter distributions for use in the REFLUX3 module of the Total-System Performance Assessment Version 4.0 code, representing the repository design modifications, are estimated from process-level thermal hydrology modeling results. Analyses using the TPA Version 4.0 code are presented to assess the sensitivity of both performance of the repository and performance of the geological barrier to parameters describing thermal hydrology.

Washington Office • Twinbrook Metro Plaza #210
12300 Twinbrook Parkway • Rockville, Maryland 20852-1606

Analyses and conclusions of this report can be used to assess effects of the repository design changes on thermal mobilization of water, repository performance, and evaluation of assumptions in the U.S. Department of Energy approach.

If you have any questions, please contact Dr. Debra Hughson at 210.522.3805 or me at 210.522.5151.

Sincerely yours,

Asadul H. Chowdhury, Manager
Mining, Geotechnical, and
Facility Engineering

AHC/ph
Enclosure

cc:	J. Linehan (w/o enclosure)	K. Stablein	B. Leslie	CNWRA Directors	G. Ofoegbu
	D. DeMarco	D. Brooks	M. Nataraja	CNWRA Element Mgrs.	S. Hsiung
	B. Meehan	T. McCartin	J. Trapp	T. Nagy (SwRI Contracts)	
	E. Whitt	P. Justus	T. Essig	P. Maldonado	
	J. Holonich	J. Greeves		R. Green	
	W. Reamer	R. Codell		S. Mohanty	

THERMAL EFFECTS ON FLOW PROCESS-LEVEL SENSITIVITY ANALYSIS STATUS REPORT

Prepared for

Nuclear Regulatory Commission
Contract NRC–02–97–009

Prepared by

Debra L. Hughson

Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

July 2000

ABSTRACT

Thermal perturbations to unsaturated flow in the vicinity of waste emplacement drifts at the proposed repository at Yucca Mountain, Nevada, are evaluated and compared for areal mass loadings (AML) of 85 metric tons of uranium (MTU)/acre specified in the design used for the Viability Assessment (U.S. Department of Energy, 1998) and 60 MTU/acre specified for one of the enhanced design alternatives. The lower thermal loading corresponding to the smaller AML, along with forced ventilation for a period of 50 yr, has the effect of reducing the time of above-boiling temperatures in the drifts to about 10^3 yr and maintaining the pillars between drifts at below boiling. The consequences to repository performance of water entering the drifts during the thermal period are evaluated using the Total-System Performance Assessment (TPA) Version 4.0 code (Mohanty et al. 2000). Performance assessments conducted including Alloy 22 overpack waste package material and a Ti dripshield show thermal perturbations in unsaturated flow have negligible consequences to performance. Presuming a premature failure of the engineered materials, water entering drifts during the thermal period would result in radionuclides arriving at the compliance boundary approximately 10^3 yr earlier than if water were excluded from the drifts during the same period. Adjustments to distributions of parameters characterizing disposition of thermally mobilized water above drifts in the TPA Version 4.0 code REFLUX3 module are recommended to better align the abstraction of thermal hydrology to repository design changes.

CONTENTS

Section Page

FIGURES iv
TABLES v
ACKNOWLEDGMENTS vi

1 INTRODUCITON 1-1

2 THERMAL HYDROLOGY OF VIABILITY ASSESSMENT AND ENHANCED DESIGN ALTERNATIVE II DESIGNS 2-1
2.1 MODEL DESCRIPTION 2-1
2.2 MODEL RESULTS 2-4

3 REFLUX3 MODULE IN TOTAL-SYSTEM PERFORMANCE ASSESSMENT VERSION 4.0 CODE 3-1

4 REFLUX3 PARAMETER SENSITIVITY 4-1

5 REFLUX3 PARAMETER DISTRIBUTIONS 5-1

6 DISCUSSION AND RECOMMENDATIONS 6-1

7 CONCLUSION 7-1

8 REFERENCES 8-1

APPENDIX

FIGURES

Figure Page

2-1 Structured grid and hydrostratigraphy used for MULTIFLO simulation of the Viability Assessment design 2-2
2-2 Structured grid and hydrostratigraphy used for MULTIFLO simulation of the Enhanced Design Alternative II design 2-3
2-3 Thermal loading scenarios used for MULTIFLO simulations of the Enhanced Design Alternative II design 2-5
2-4 Comparison of the extent of above-boiling temperatures in the fracture continuum of MULTIFLO simulations of the Viability Assessment (VA) and Enhanced Design Alternative II (EDA-II) designs 2-6
2-5 Vertical component of flux in the fracture continuum at 300, 500, and 1,000 yr of heating for the Enhanced Design Alternative II design with 50 percent reduction of heat 2-7
2-6 Comparison of two heat removal ventilation scenarios for the Enhanced Design Alternative II design 2-8

4-1 Comparison of groundwater dose for a scenario where no water enters drifts during the thermal period 4-2
4-2 Comparison of groundwater dose for the same simulations as shown in figure 4-1 except with the engineered barrier system removed 4-2
4-3 Comparison of the sensitivity of groundwater dose (without engineered barrier system) to the dryout zone thickness calculated by MULTIFLO for the Viability Assessment and Enhanced Design Alternative II designs 4-4
4-4 Comparison the sensitivity of groundwater dose (without engineered barrier system) to temperature gradient in the vicinity of the boiling isotherm 4-4

6-1 Comparison of groundwater dose from the Total-System Performance Assessment Version 4.0 code basecase results (without engineered barrier system) to dose computed using distributions for the REFLUX3 parameters 6-2

TABLES

Table Page

3-1 Dryout zone thickness as a function of time for the Enhanced Design Alternative II design . . 3-2
3-2 Factors controlling the distribution of thermally perched water in Total-System Performance Assessment Version 4.0 code 3-2

6-1 Suggested parameter distributions for REFLUX3 6-2

ACKNOWLEDGMENTS

This report was prepared to document work performed by the Center for Nuclear Waste Regulatory Analyses (CNWRA) for the U.S. Nuclear Regulatory Commission (NRC) under Contract No. NRC–02–97–009. The activities reported here were performed on behalf of the NRC Office of Nuclear Material Safety and Safeguards, Division of Waste Management. The report is an independent product of the CNWRA and does not necessarily reflect the views or regulatory position of the NRC.

Assistance from Melissa Hill in modification of input files and the numerical mesh incorporating repository design changes is greatly appreciated. The author wishes to thank Stefan Mayer for a thorough technical review and useful insights, Barbara Long and Alana Woods for their editorial expertise, Janie Gonzalez for format review, and Patrick Mackin for programmatic review. The administrative and format support provided by Paulette Houston is also appreciated.

QUALITY OF DATA AND CODE DEVELOPMENT

DATA: Some data used to support conclusions in this report are taken from documents published by U.S. Department of Energy contractors and supporting organizations who operate under the quality assurance (QA) program developed for the Yucca Mountain Project. The reader should refer to data source documents, referenced throughout this report, to determine data QA status.

CODE: Modeling of thermohydrological processes was performed using CNWRA-developed MULTIFLO code, Version 1.2, and performance assessments were conducted using the Total-System Performance Assessment code, Version 4.0, both of which were developed following the procedures described in the CNWRA Technical Operating Procedure, TOP-018, which implements the guidance contained in the CNWRA QA Manual.

1 INTRODUCTION

Design for the Viability Assessment (VA) of a Repository at Yucca Mountain (U.S. Department of Energy, 1998) specified that 85 metric tons of uranium (MTU) be placed per acre of repository area in drifts spaced 28 m apart. The resulting heat generated by radioactive decay would have thermally perturbed the mountain for thousands of years, drying out large regions of host rock in the vicinity of the waste emplacement drifts and mobilizing large quantities of water stored in the low permeability welded tuff matrix. Subsequently, after considering numerous alternatives, the U.S. Department of Energy (DOE) proposed the design designated as Enhanced Design Alternative II (EDA-II) (Civilian Radioactive Waste Management System Management and Operating Contractor, 1999a) that specified an areal mass loading (AML) of 60 MTU/acre in drifts spaced 81 m apart. This report summarizes independent analyses, using the two-phase fluid and heat flow module METRA of the MULTIFLO code Version 1.2 (Lichtner et al., 2000) and the Total-System Performance Assessment (TPA) Version 4.0 code (Mohanty et al., 2000), of the effect of this design change on thermal hydrology (TH) and consequent performance of the proposed high-level waste repository at Yucca Mountain, Nevada. Hereafter, MULTIFLO code Version 1.2 (Lichtner et al., 2000) and the Total-System Performance Assessment (TPA) Version 4.0 code (Mohanty et al., 2000) will be referred to as MULTIFLO and TPA Version 4.0 code, without references.

Comparative two-dimensional TH calculations, on a model domain extending from the ground surface to the water table, are presented showing the duration and intensity of the thermal perturbation to unsaturated flow in the vicinity of the waste emplacement drifts for the VA and EDA-II designs. Notable differences between these designs include the extent of rock dryout, volume of matrix pore water mobilized, liquid flux in the zone of refluxing, and the length of time the rock adjacent to the emplacement drifts is above boiling. Implementation of the REFLUX3 module of the TPA Version 4.0 code is described, and the physical processes intended to be represented by REFLUX3 are discussed. Sensitivity of groundwater dose summed over all radionuclides to important REFLUX3 parameters is presented followed by a discussion of reasonable ranges for the distribution of these parameters. This report concludes with recommendations for distributions of three REFLUX3 parameters controlling the allocation of thermally mobilized water toward and away from the repository.

The primary theme of this document is the difference between the effects of thermal loading in the VA and EDA-II designs and the potential impact on repository performance. With the current predictions for longevity of the waste packages (WPs) and the presence of the drip shield, the presence or absence of TH has no effect on the dose calculated by the TPA Version 4.0 code. From the perspective of risk-informed, performance-based regulation, this may be a satisfactory conclusion. From the perspective of defense in depth and multiple barriers, however, it may be useful to examine the performance of a single barrier. It is from this perspective that most of the sensitivity analyses in this report are presented. All of the sensitivity analyses, except those presented in figure 4-1, consider only the performance of the geological barrier. The results for total system performance, including the reliance on the longevity and durability of the WPs, are presented in figure 4-1. Analyses of repository performance, which include current projections for longevity of the WPs, show no sensitivity to TH parameters.

2 THERMAL HYDROLOGY OF VIABILITY ASSESSMENT AND ENHANCED DESIGN ALTERNATIVE II DESIGNS

A significant reduction in the thermal loading of the repository may result as a consequence of the change in repository design from that presented in the VA (U.S. Department of Energy, 1998) to the current design (EDA-II). This reduced thermal loading results, in part, from the increased spacing of the waste emplacement drifts from 28 m to 81 m on centerlines. Additionally, the EDA-II design specifies at least a 50-yr period of forced ventilation prior to closure of the repository. Comparative modeling results are presented here to illustrate the differing TH flow regimes that may occur in these two designs.

2.1 MODEL DESCRIPTION

Structured grids (i.e., constructed of rectangular, regularly spaced elements) were used to create model domains extending from the ground surface to the water table. Figure 2-1 shows the model grid representing the VA design, and figure 2-2 shows the model grid representing the EDA-II design. The horizontal dimension is exaggerated by a factor of 5 in figures 2-1 and 2-2. The left-hand boundary of these two-dimensional slices is the centerline of an emplacement drift, and the right-hand boundary is the centerline between emplacement drifts. These no-flow boundaries create periodic symmetry such that continuations beyond the boundaries to the left and right are mirror images of the modeled domain. Symmetric boundary conditions are applicable for horizontally layered, homogeneous formation properties in the central portion of the repository. Thus these model results do not account for heterogeneity, repository edge effects, or dipping contacts between layers. The top boundaries are prescribed infiltration flux of 5.5 mm/yr, and the bottom boundaries are prescribed pressure and saturation representing a water table. The water table boundary is at a depth of 726.9 m from ground surface. A linear, geothermal gradient is imposed on the ambient system from 20 °C at the ground surface to 30 °C at the water table.

Hydrostratigraphic units are indicated schematically alongside the model grids. This stratigraphy is approximately representative of a location around Northing 233750 m and Easting 559340 m in Nevada-State coordinates where the emplacement drifts are projected to be entirely within the Topopah Spring Lower Lithophysal unit (Tptpll or TSw35). Hydrological and thermophysical properties for these hydrostratigraphic units were taken from the Total System Performance Assessment—Viability Assessment (TRW Environmental Safety Systems Inc., 1998) and are included in the appendix. These properties are also available on the Internet at Universal Resource Locator http://domino.ymp.gov/va/support/tspa-vatbr/chap3.nsf by following the links to tables 3-18, 3-30, 3-31, and 3-32.

A heat source, representing the thermal loading resulting from decay of radioactive waste, was placed in the model element at a depth of 386.25 m from the ground surface and adjacent to the left hand boundary. The model element containing the heat source had horizontal and vertical dimensions of 0.5 m and a thickness of 1.0 m. A portion of the TSw35 unit, 5 m vertically and 2.5 m horizontally, was given a thermal conductivity of 20 W/(mK) to simulate the radiant heat transfer from WP to drift wall. Otherwise, the material surrounding the heat source had the properties of the TSw35 model unit. Relatively uniform drift wall temperatures in the Drift-Scale Heater Test (DST) and simulations of radiative heat transfer in open drifts (Hardin, 1998) indicate that 80–90 percent of the heat transfer within open drifts is by radiation (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000a). Simulation of heat transfer in open drifts through effective porous medium properties (conduction and convection alone) results

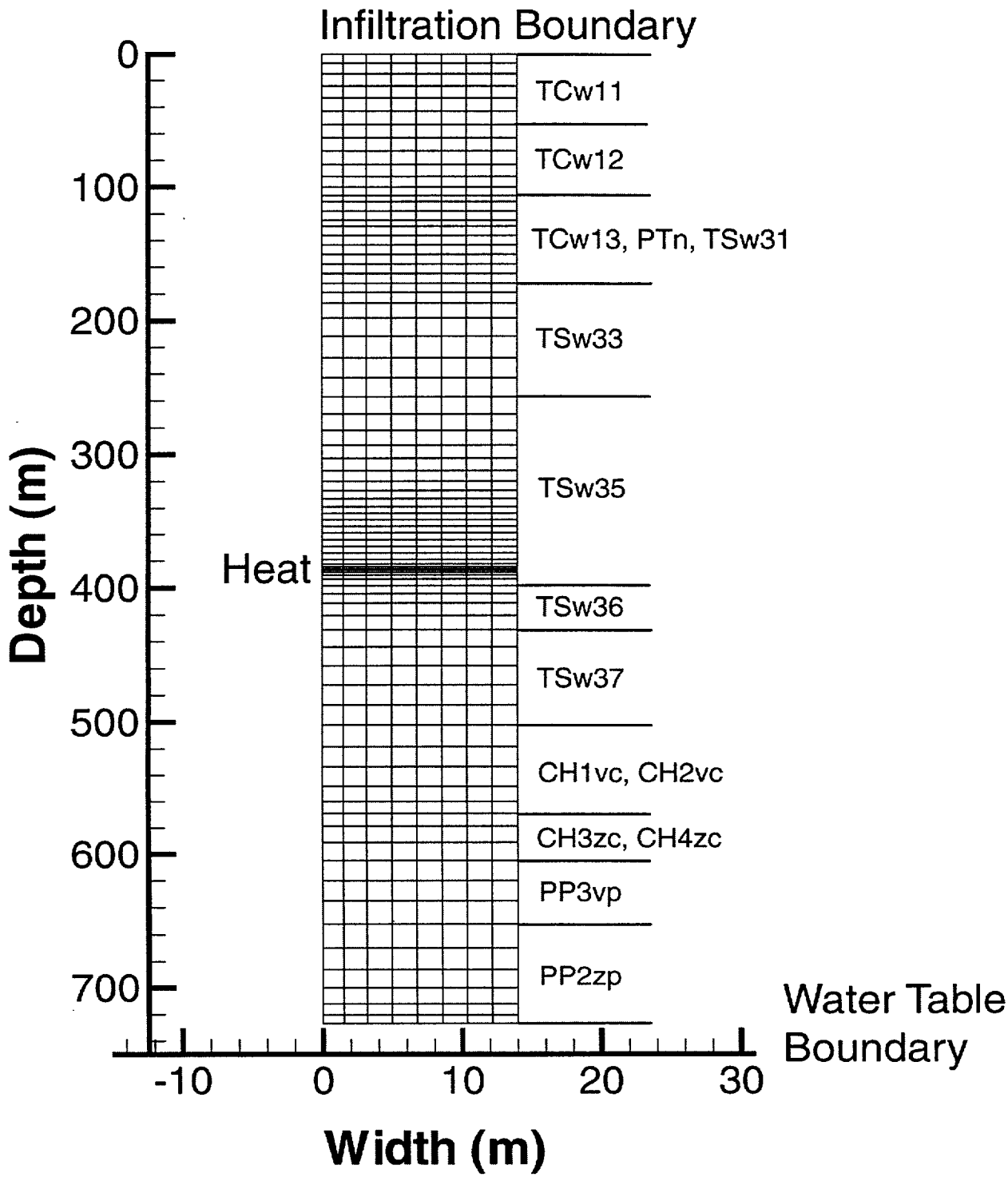

Figure 2-1. Structured grid and hydrostratigraphy used for MULTIFLO simulations of the Viability Assessment design

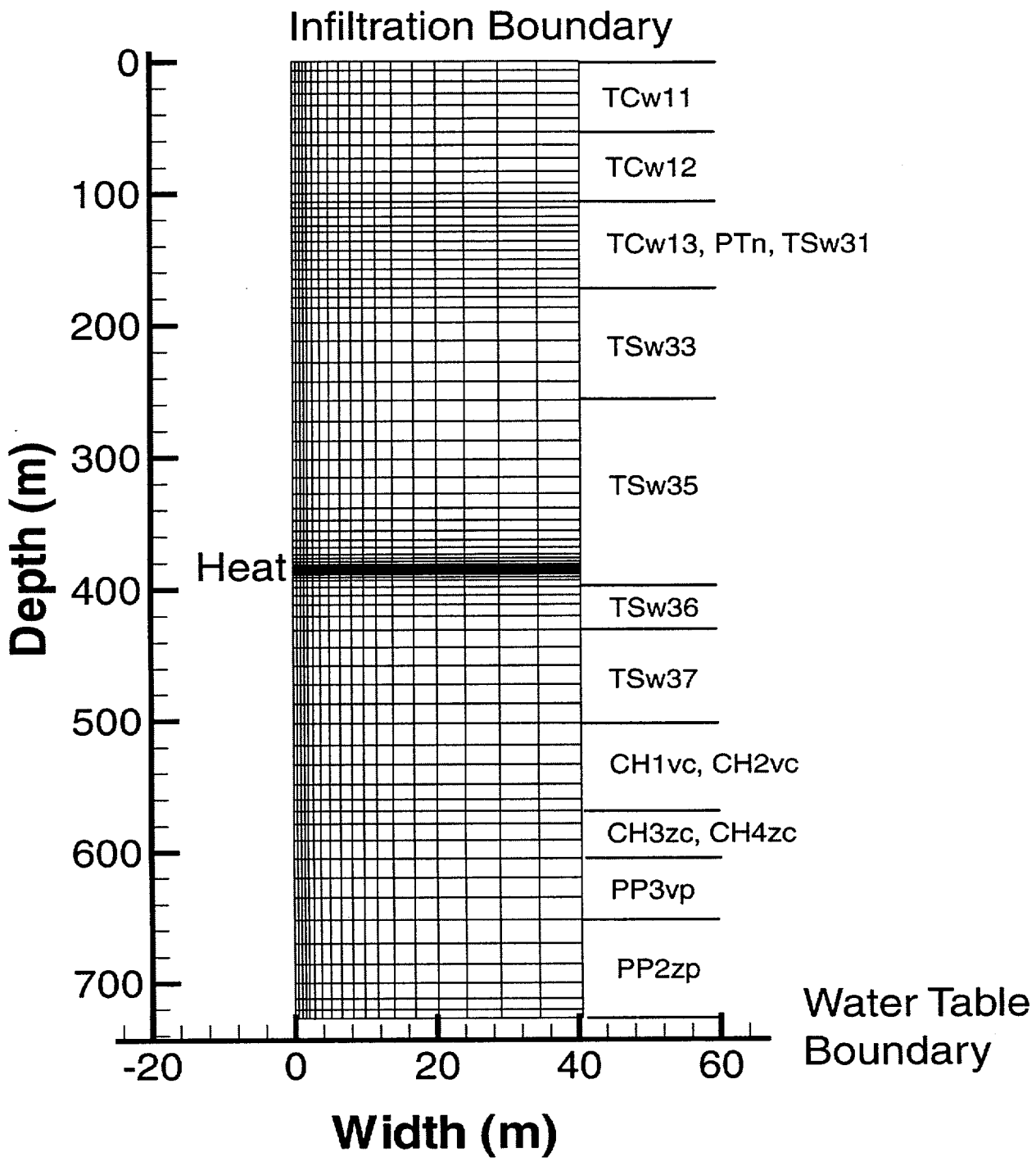

Figure 2-2. Structured grid and hydrostratigraphy used for MULTIFLO simulations of the Enhanced Design Alternative II design

in significant temperature errors along the drift walls. The overall temperature and saturation distributions, however, are not significantly affected by this assumption if the heat load is accurately represented (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000a). The choice of 20 W/(mK) as an effective thermal conductivity for open drifts was based on comparative modeling of the DST (comparing model simulated to measured drift wall temperatures) where heater power and drift wall temperature data are available. The modeling results presented here do not attempt to represent details of the drift, and temperatures close to the heat source should be considered approximate. The dark band extending across the model grids in figures 2-1 and 2-2 next to the label "Heat" results because the very fine model grid discretization cannot be resolved by the graphics at this scale. The thermal energy source in the heated element was calculated as follows. Thermal output data for Pressurized Water Reactor (PWR) and Boiling Water Reactor (BWR) fuel assemblies used in TPA Version 4.0 code were combined as 35 percent BWR and 65 percent PWR. From this data the thermal output of 26-yr-old commercial spent nuclear fuel was estimated to be 920 W/MTU. For an AML of 60 MTU/acre, this results in an initial smeared heat loading of 13.6 W/m^2 over the repository footprint. A drift spacing of 81 m yields 1.1 kW/m of initial heat load along the length of the emplacement drifts. Since the model domains shown in figures 2-1 and 2-2 have a symmetry boundary condition through the centerline of the drifts, this initial heat load was halved to get the value used in the model. Figure 2-3 shows the power output of PWR/BWR spent fuel as a function of age used in the TPA 4.0 code and the thermal loading used for modeling the EDA-II design in W/m of emplacement drift. The effects of ventilation were simulated by reducing the thermal loading by 30 percent and 50 percent for a period of 50 yr. These percentage reductions are not based on process-level models but are from sensitivity analyses. The heat reduction of 30 percent by loss to ventilation is currently used in TPA Version 4.0 code, and the 50 percent reduction estimate is based on DOE contractor calculations. For 50 yr of ventilation at a rate of 10 m^3/s, estimates by DOE contractors suggest 68 percent of the heat is removed. This estimate is increased to 78 percent removal by ventilation at a rate of 15 m^3/s (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000b).

2.2 MODEL RESULTS

The 60-MTU/acre AML, 81-m drift spacing, and 50 yr of forced ventilation specified in the EDA-II design result in a significantly cooler repository than the design used in the VA (U.S. Department of Energy, 1998). This difference is illustrated in figure 2-4, which shows the boiling isotherm (97 °C contour) at 300, 500, and 1,000 yr for the VA design compared to the EDA-II design, where ventilation has been simulated by removal of 50 percent of the heat generated for the first 50 yr. In the VA design, the boiling isotherm has coalesced between emplacement drifts, and a thickness of the formation in excess of 200 m is above boiling 1,000 yr after waste emplacement. In contrast, the boiling isotherm never coalesces between drifts in the EDA II design. The pillars between emplacement drifts are always below boiling. At 1,000 yr after waste emplacement in the EDA II design, only the interior of the emplacement drifts remains above boiling.

One purpose of the cooler EDA-II design is to maintain the pillars between emplacement drifts at below boiling temperatures to allow deep percolation flux and condensate to drain between drifts (Civilian Radioactive Waste Management System Management and Operating Contractor, 1999b). The vertical component of fluxes in the fracture continuum is shown in figure 2-5 for the 50-percent heat reduction by ventilation scenario of the EDA-II design in the right-hand column of figure 2-5. This figure shows condensate drainage above the heated repository migrating laterally and shedding through the cooler pillars between drifts. At 1,000 yr, the condensate zone above the repository is diminished but still evident.

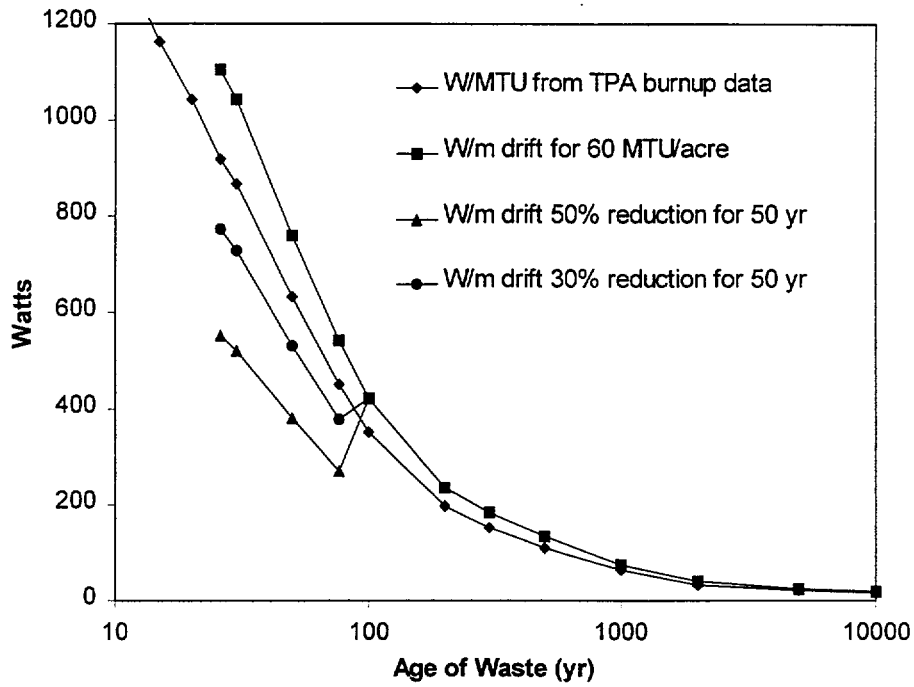

Figure 2-3. Thermal loading scenarios used for MULTIFLO simulations of the Enhanced Design Alternative II design (MTU = metric tons of uranium; TPA = Total-System Performance Assessment)

Note that capillary diversion will result in fluxes in excess of deep percolation along the drift walls under ambient conditions after the thermally mobilized condensate has drained away. Achievement of this goal of maintaining pillar temperatures below boiling, however, is subject to the efficacy of heat removal by forced ventilation as shown in figure 2-6 and, by extrapolation, to the age of the waste. As previously described, the heat loads used for this modeling study were derived from a 26-yr-old blend of PWR and BWR fuel assemblies. The column on the left in figure 2-6 shows the 97 °C contour at 300, 500, and 1,000 yr where 30 percent of the heat has been removed by ventilation during the first 50 yr. The column on the right shows the 97 °C contour for the same times where no heat has been removed by ventilation. These results indicate that the ventilation period of EDA-II is required to prevent coalescence of the boiling isotherm. The EDA-II design retains flexible options for thermal load management, including options for up to 300 yr of ventilation and aging or blending of waste, in order to achieve the design goal of maintaining pillars between drifts at below boiling temperatures (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000c). Thermal calculations performed in support of enhanced design alternatives (Civilian Radioactive Waste Management System Management and Operating Contractor, 1999c) show drift wall temperatures never rising above boiling for the 200-yr and 300-yr ventilation scenarios. In that scenario the thermal effects on flow may be negligible.

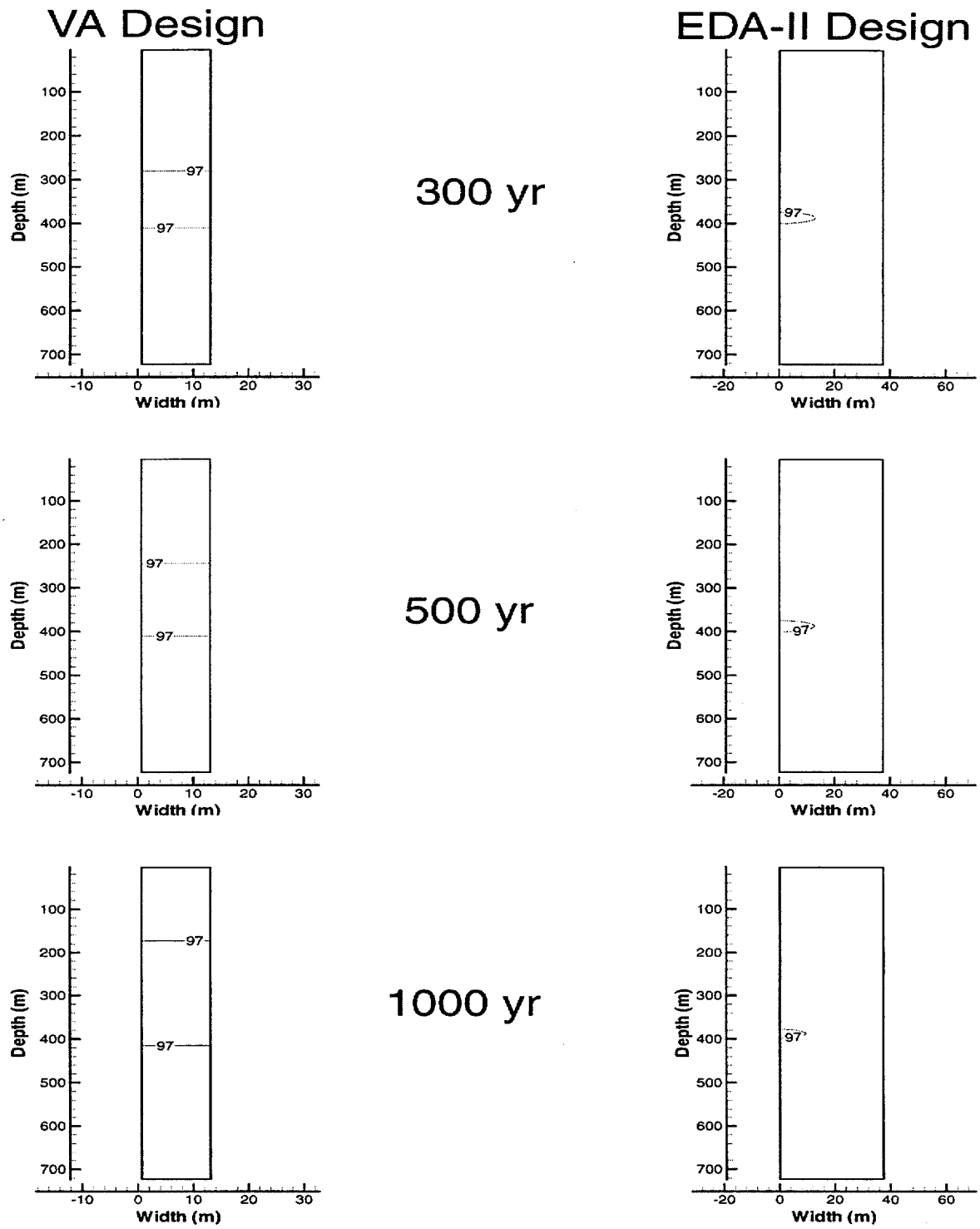

Figure 2-4. Comparison of the extent of above-boiling temperatures in the fracture continuum of MULTIFLO simulations for the Viability Assessment (VA) and Enhanced Design Alternative II (EDA-II) designs. The column on the left is the VA design, and the column on the right is the EDA-II design. The top row shows results at 300 yr, the middle row at 500 yr, and the bottom row at 1,000 yr. Only the 97 °C contour line is displayed.

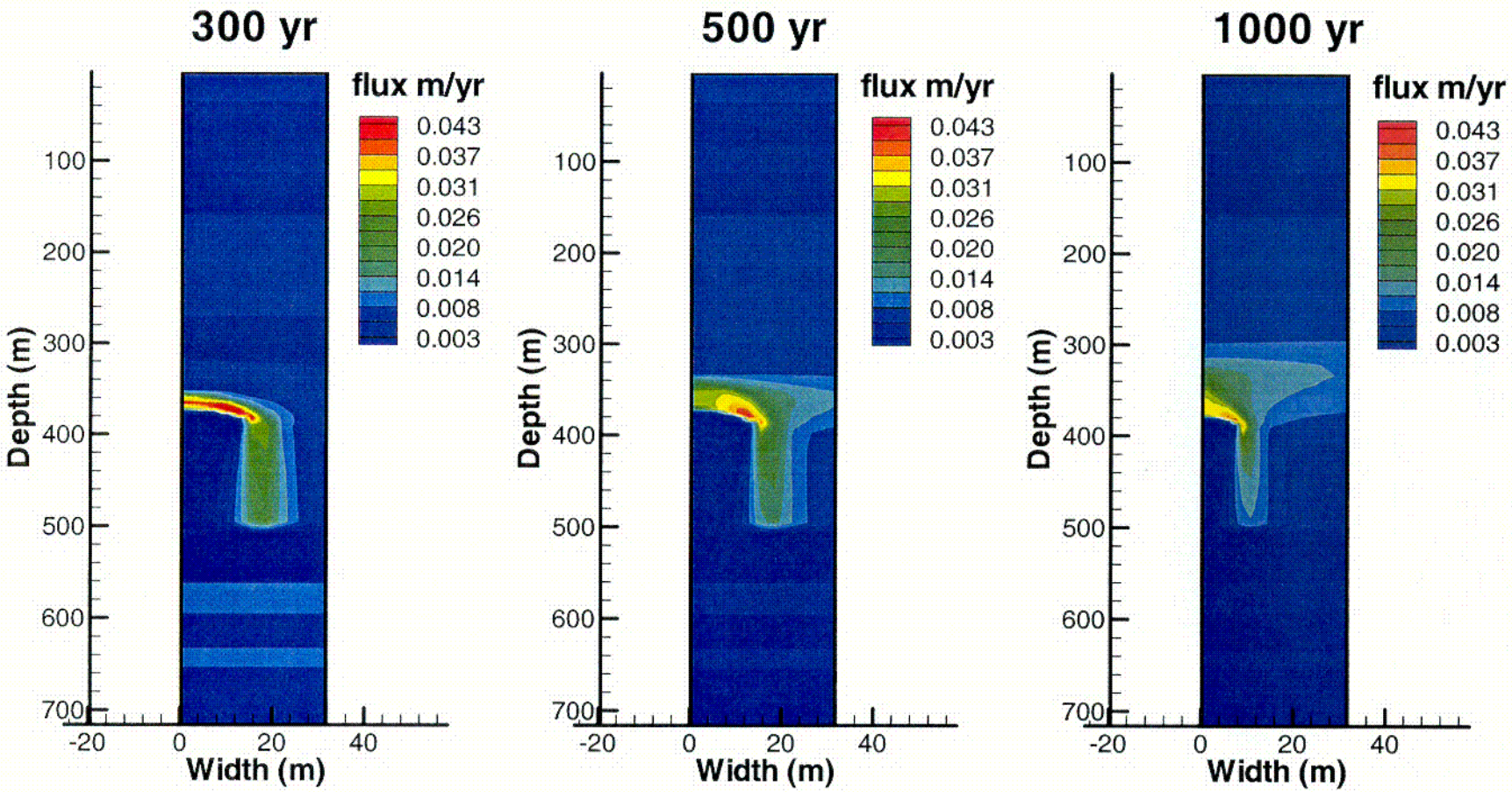

Figure 2-5. Vertical component of flux in the fracture continuum at 300, 500, and 1,000 yr of heating for the Enhanced Design Alternative II design with 50 percent reduction of heat during the first 50 yr, illustrating condensate drainage through subboiling pillars

C01

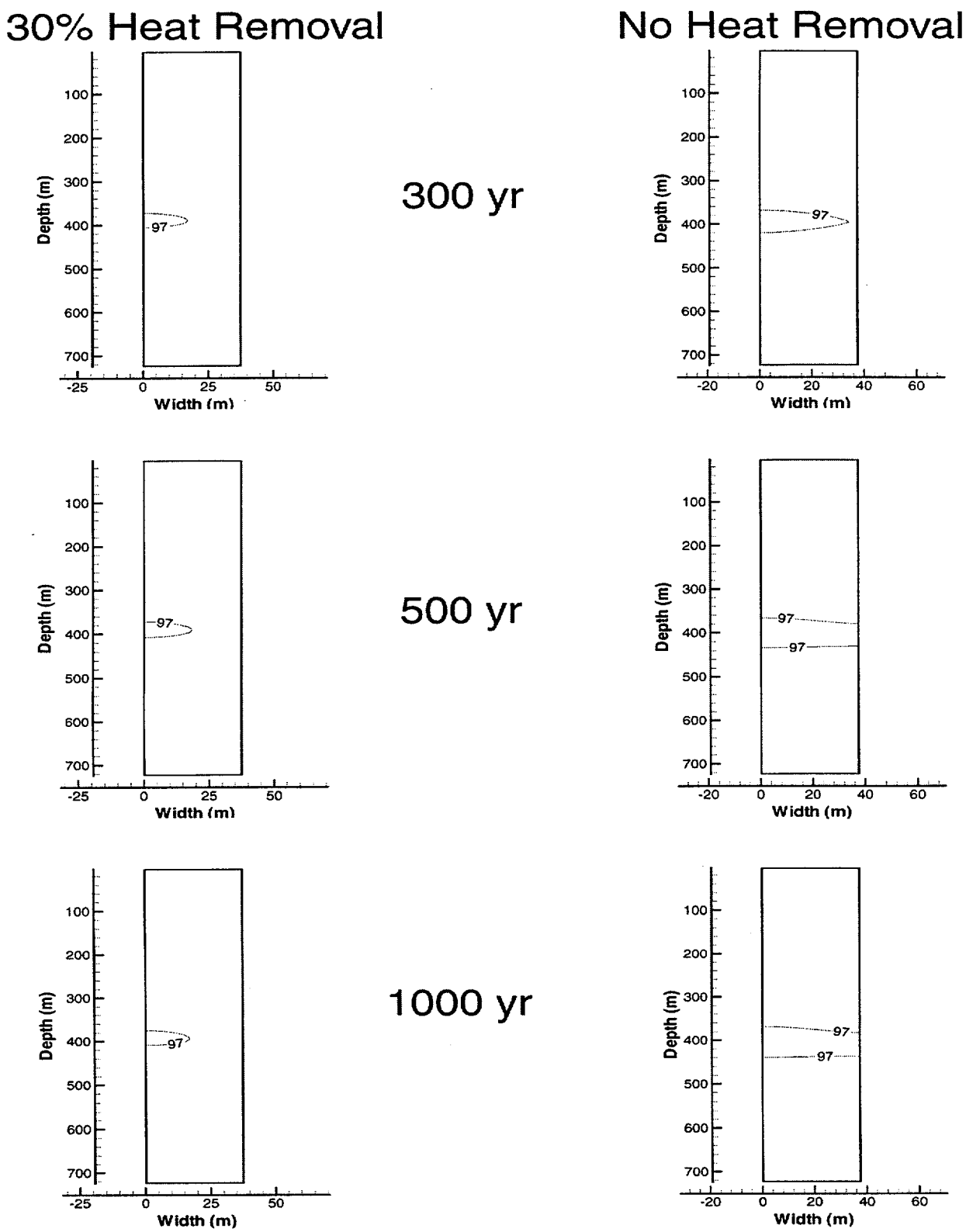

Figure 2-6. Comparison of two heat removal ventilation scenarios for the Enhanced Design Alternative II design. The column on the left shows MULTIFLO simulations with 30-percent heat reduction for 50 yr, and the column on the right shows results with no heat removal. The top row shows results at 300 yr, the middle row at 500 yr, and the bottom row at 1,000 yr. Compare these to the right-hand column of figure 2-4, which shows the effect of a 50-percent reduction in heat for 50 yr.

3 REFLUX3 MODULE IN TOTAL-SYSTEM PERFORMANCE ASSESSMENT VERSION 4.0 CODE

The TPA Version 4.0 code includes three modules, REFLUX1, REFLUX2, and REFLUX3, for evaluating the effect of thermally induced water refluxing on performance. The last one in this list, REFLUX3, has superceded the previous modules and should be used in preference to the others. Reflux of water, also referred to as a heat pipe, is a dynamic process of evaporation of deep percolation flux and vaporization of water stored in the rock matrix, buoyant convection of water vapor upwards through the permeable fracture network, condensation in the cooler region above the repository, and condensate drainage down through the fractures back toward the repository. Vaporization of water removes heat at the bottom of the reflux zone, and condensation deposits heat at the top of the reflux zone. This process maintains the entire zone of refluxing, which can be several to tens of meters thick, at a nearly uniform temperature. The TPA Version 4.0 code treats this dynamic reflux and condensate zone as a static reservoir of water available to potentially enter emplacement drifts. Water in this reservoir is derived from the condensation of vapor driven from the dryout zone and deep percolation. The thickness of the zone of dryout around emplacement drifts is calculated offline using the METRA module of the MULTIFLO code and is read into the TPA Version 4.0 code from the file *drythick.dat*. Users of the TPA Version 4.0 code should note that it reads in a default *drythick.dat*, which represents the TH expected in the VA design where the thickness of the dryout zone reaches a maximum of 80.7 m at 1,000 yr. Updated calculations for the EDA-II design were performed and are shown in table 3-1. Sensitivity of repository performance to this change in dryout thickness is discussed below.

Water is added to the perched zone above the repository by thermal effects each time step up to the maximum amount contributed from the dryout zone. The amount of water driven from the dryout zone and available to potentially drain toward the repository is calculated as

$$D = Tn(S - S_r) \tag{3-1}$$

where T is the dryout zone thickness, n is matrix porosity of the repository host formation, S is ambient saturation of the host formation matrix, and S_r is residual saturation of the matrix host rock. Once the maximum dryout thickness is reached, all water thus contributed is available for drainage toward the repository in subsequent years. The perched volume of water available to drain toward the repository during the thermal period is obtained by adding the quantity calculated in Eq. (3-1) to the deep percolation flux through the unsaturated zone (UZ). The REFLUX3 module allocates water in the perched volume above the repository according to three factors, summarized in table 3-2, which are input by the user of the TPA Version 4.0 code. The complete names of the parameters in REFLUX3 are given in table 3-2, along with the names of the parameters as used in the code. These parameters are subsequently referred to only by the shorter code names.

For each time step of the thermal period, a quantity (Shed1 × perched volume) is subtracted from the thermally perched volume of water above the repository and is removed from the system. For the VA design, the boiling isotherm extended a significant distance above repository horizon and coalesced between emplacement drifts (figure 2-4) creating a barrier for condensate drainage and potentially trapping the perched volume above the repository for the duration of the thermal period. The factor Shed1 was implemented in REFLUX3 to provide for possible lateral flow of the condensate and shedding around the edges of the repository. The EDA-II design specifies that temperatures in the pillars between emplacement

Table 3-1. Dryout zone thickness as a function of time for the Enhanced Design Alternative II design

Line Number	Time (yr)	Dryout Thickness (m)
1	1.0	0.0
2	10.0	0.1
3	20.0	1.0
4	30.0	1.5
5	40.0	1.7
6	50.0	1.6
7	60.0	1.5
8	70.0	1.8
9	80.0	2.9
10	100.0	4.6
11	200.0	7.3
12	300.0	7.4
13	500.0	6.6
14	600.0	5.6
15	700.0	4.7
16	800.0	3.8
17	900.0	2.7

Table 3-2. Factors controlling the distribution of thermally perched water in Total-System Performance Assessment Version 4.0 code

Factor	Code name	Distribution
FractionOfCondensateRemoved [yr^{-1}]	Shed1	loguniform (1.0E-8, 1.0)
FractionOfCondensateTowardRepository [yr^{-1}]	Qfact	uniform (0.0, 1.0)
FractionOfCondensateTowardRepositoryRemoved [yr^{-1}]	Shed2	loguniform (1.0E-8, 1.0)

drifts remain below boiling, which provides an avenue for condensate drainage between drifts. Thus the mechanism of lateral flow and shedding around the repository edges may be negligible in the new design. One of the suggestions of this report is that the Shed1 factor could be used to account for condensate drainage between drifts through the cool pillars.

Each time step a fraction of the remaining water in the perched volume above the repository flows toward the emplacement drifts. This fraction is computed by multiplying the perched volume remaining after the Shed1 fraction is removed by the factor Qfact. Water flowing toward the emplacement drifts will be vaporized in the zone of above-boiling temperatures unless condensate drainage is focused into flowing rivulets or fingers. Water flowing in a rivulet or finger will penetrate into the zone of above-boiling temperatures a distance of approximately (Phillips, 1996)

$$L = \sqrt{\frac{Q\rho h}{k_r \nabla T}} \tag{3-2}$$

where Q is the volumetric steady flow rate in the rivulet; ρ is density of liquid water at boiling (960.5 kg/m^3); h is enthalpy of phase change for water (2.4×10^6 J/kg); k_r is thermal conductivity of the dry rock, which is uniformly distributed on the interval from 1.8 to 2.2 W/(m-K) in the TPA Version 4.0 code basecase; and∇T is the temperature gradient in the surrounding rock. The process described by Eq. (3-2) (Phillips, 1996) is preferential flow of a finger or ribbon of liquid water in a fracture. Volumetric flow rate in Eq. (3-2) from water in the perched volume toward the repository is focused over an area defined by the spacing of the implacement drifts and the spacing of WPs along the length of a drift (503.4 m^2). This flow focusing is not a user-supplied parameter, but is implied in the code formulation. Focusing of condensate into preferential flow paths along subvertical, highly permeable fractures or fracture zones will occur as a consequence of gravitational instability and permeability heterogeneity. Focusing of flow over this area, currently implemented in TPA Version 4.0 code, into a single rivulet is likely conservative. Although a more accurate estimate of this flow-focusing factor could perhaps be obtained from models of the spacing of active or flowing fractures in the Topopah Spring formation, it would likely result in less flow reaching the repository during the thermal period.

Water at the repository horizon available to enter emplacement drifts is the portion of$Q$ from Eq. (3-2) that is not vaporized by superheated rock or removed by the Shed2 factor. Water is removed from the system in REFLUX3 by the Shed2 factor after it has contributed to penetration of the boiling isotherm as expressed in Eq. (3-1), but before flux through the superheated region arrives at the repository. The quantity removed by Shed2 is calculated as $Q \times$ Shed2, and the amount vaporized is calculated as $Q \times (1 -$ Shed2) times the ratio of the thickness of the dryout zone to the length calculated from Eq. (3-2). The quantity determined by Shed2 to bypass the drifts is removed from the system, and the quantity vaporized by superheated rock is returned to the reflux cycle in the perched volume. Water at the repository horizon available to enter emplacement drifts is multiplied by the factors, F_{ow} and F_{mult}, in the EBSREL module prior to actually contacting waste forms. The factors, F_{ow} and F_{mult}, in the EBSREL module are intended to account for flow focusing or diversion resulting from processes such as capillary diversion. The EBSREL module is sthe module of the TPA Version 4.0 code that models release of radionuclides from the engineered barrier system (EBS).

4 REFLUX3 PARAMETER SENSITIVITY

Thermal effects on factors that affect repository performance include changes in the WP environment, potential corrosion of engineered components, couplings with water and gas chemistry, and mechanical behavior of the rock mass— to name a few. The Thermal Effects on Flow (TEF) Key Technical Issue (KTI), however, has evaluated only the potential effects of water contacting waste forms, WPs, and components of the EBS during the period of thermal refluxing. Alloy 22 is predicted by DOE to give the WPs a lifetime on the order of 10^5 yr (Civilian Radioactive Waste Management System Management and Operating Contractor, 2000c), much longer than the compliance period of 10^4 yr. Such extremely long-term predictions are uncertain. Concerns regarding the technical bases for these assumptions and predictions are documented in the Container Life and Source Term Issue Resolution Status Report (U.S. Nuclear Regulatory Commission, 1999). Other design features of the EBS, such as the Ti drip shield, are expected to last for a significant portion of the compliance period. The period of thermal refluxing, on the other hand, will likely end within the first 10^3 yr with the EDA-II design (figure 2-4). Thus, since the EBS is expected to remain intact during the thermal period, the most significant thermal effects on performance may result from long-term or permanent changes to the near-field environment as a consequence of coupled thermal-hydrological-chemical and thermal-hydrological-mechanical processes and potential degradation of the EBS. These effects are addressed in the Evolution of the Near-Field Environment, Repository Design and Thermal-Mechanical Effects, and Container Life and Source Term KTIs and are not considered here.

The REFLUX3 module assesses the flux of water at the repository horizon during the period of thermal refluxing. The thermal period may have a positive influence on repository performance by forming a dryout zone that prevents water from contacting WPs. Alternatively, the thermal period may have an adverse influence on repository performance because water vaporized from the matrix rock of the dryout zone may come into contact with the WPs. Figure 4-1 shows a comparison of the time history of groundwater dose summed over all nuclides and averaged over all realizations resulting when no water enters the drifts during the thermal period and when water enters the drifts as if there were no thermal effects on flow. The first case is where no water enters the drift during the thermal period (dotted line with diamond symbols), and the second case is where water enters the drifts directly from deep percolation without refluxing. This second case is indicated as *no TH* (solid line) in figure 4-1. These results were obtained from 100 realizations. Unless otherwise noted, all results from TPA Version 4.0 code simulations presented here are groundwater dose summed over all nuclides averaged over 100 realizations initialized using the same random number seed with the volcanism scenario off and the faulting and seismic scenarios on. If the EBS functions as designed and remains intact for 10^5 yr, water entering emplacement drifts during the thermal period would only contact waste forms exposed by some juvenile failure mechanism. As shown in figure 4-1, the dose consequence from water entering drifts during the thermal period under these conditions would average approximately 2×10^{-9} rem/yr.

An important barrier component of the geological repository is the geology itself, consisting in part of a deep UZ in fractured volcanics. A valid question is: what effect might TH have on the efficacy of the geological barrier? Figure 4-2 shows the same simulations as presented in figure 4-1 with the EBS removed. These simulations indicate that the absence of water in the drifts during the thermal period would have the maximum effect of delaying the arrival of radionuclides to the consumer by a time period slightly less than the length of the thermal period. This shifting, or delay, of the radionuclide arrival also has the effect of reducing the maximum average dose that occurs at 10,000 yr. As discussed in section 6, increased maximum average dose at 10,000 yr would be expected if refluxing into drifts during the thermal period were increased.

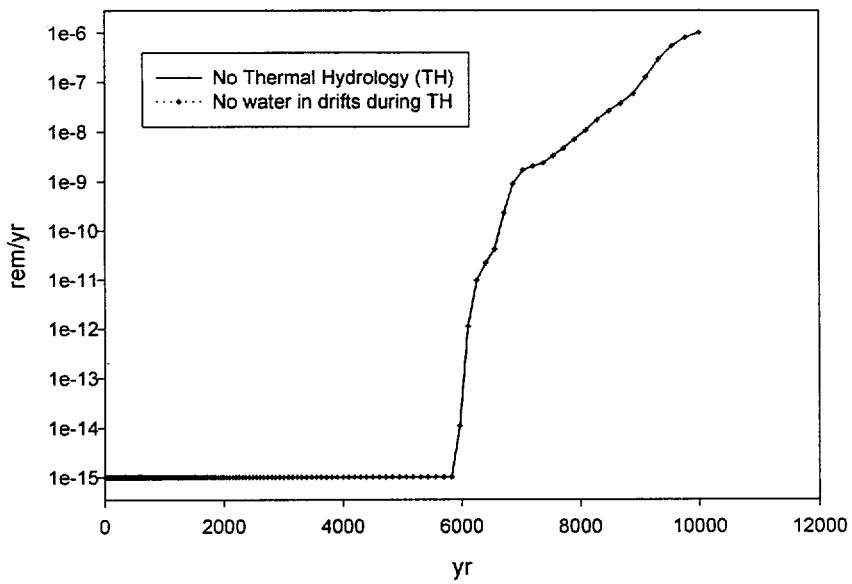

Figure 4-1. Comparison of groundwater dose for a scenario where no water enters drifts during the thermal period (dotted line with diamond symbols) to a scenario where water arrives at the repository level directly from deep percolation through the unsaturated zone without refluxing(solid line). With the engineered barrier system and waste package as represented in the Total-System Performance Assessment Version 4.0 code basecase, the only radionuclide releases are from juvenile failures.

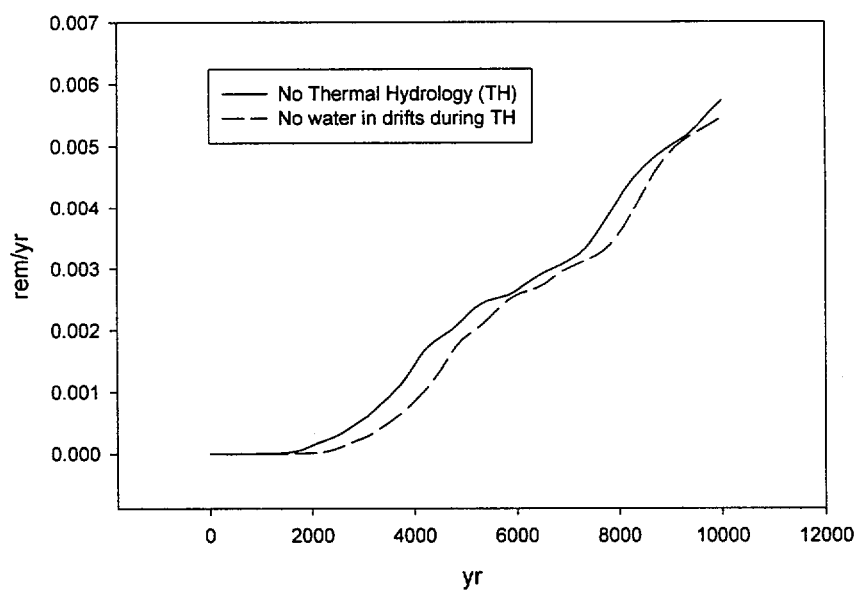

Figure 4-2. Comparison of groundwater dose for the same simulations as shown in figure 4-1 except with the engineered barrier system removed so that the results reflect only the geological barrier

Time dependant thickness of the dryout zone is calculated outside the TPA Version 4.0 code and is read in by the REFLUX3 module from the file *drythick.dat*. As previously mentioned, the *drythick.dat* file released with Version 4.0 of the TPA code represents dryout zone thickness expected around the repository for the VA design. Dryout zone thickness for the EDA-II design was calculated with MULTIFLO 1.2 using the grid shown in figure 2-2. Results of this calculation are presented in table 3-1. Note that the coarseness of the grid prohibits determination of the dryout zone thickness in detail since the vertical dimension of the grid blocks is on the same order as the thickness of the dryout zone. The grid used for this MULTIFLO simulation is being refined in the vicinity of the drifts to capture more detail in these calculations. Sensitivity of groundwater dose to dryout zone thickness is shown in figure 4-3. Again these sensitivities reflect the effects of the geological barrier alone. Otherwise, given the predicted lifetime of the EBS, all sensitivities to TH would appear identical to figure 4-1. The thickness of the dryout zone may have either a positive or a negative influence on repository performance. The potentially positive effect is that a thicker, more extensive dryout zone would tend to keep water away from drifts. The potentially negative effect is that a large volume of matrix pore water is vaporized and becomes condensate drainage that may focus into preferential flow paths and penetrate through the superheated zone, perhaps contacting the WPs. The situation is reversed with the EDA-II design. For the EDA-II design, the zone of superheated rock is small and provides scant insulation from seepage, but at the same time very little matrix pore water is mobilized. The results shown in figure 4-3 suggest that the thickness of the dryout zone has a relatively small effect on respository performance.

Some parameters used in the REFLUX3 calculations are sufficiently well known or naturally vary over a sufficiently small range so that extensive sensitivity analyses do not seem warranted. Parameters in this report that fall into this category include thermal conductivity of the rock, matrix porosity, and matrix saturations. A matrix saturation of 0.9 versus 0.99 may make a big difference when used for estimating UZ flow model parameters or calibrating seepage models but would not make a significant difference in the volume of water removed from the dryout zone in the EDA-II design. Other parameters used in REFLUX3 are specified by the design, such as drift spacing and WP spacing, while others are precisely known constants, such as the density of water at boiling or the enthalpy of phase change. Deep percolation flux and factors in EBSREL describing seepage into drifts, which have a significant impact on performance, are outside the scope of this analysis. Sensitivity of performance to the temperature gradient in the vicinity of the boiling isotherm, used in Eq. (3-2) to calculate the distance focused rivulet flow will penetrate into superheated rock, is depicted in figure 4-4. The distribution of this parameter assumed for TPA Version 4.0 code is uniform between 1 and 100 K/m. The solid line in figure 4-4 shows the groundwater dose summed over all radionuclides averaged over 100 realizations where temperature gradient in the vicinity of the boiling isotherm was set to a constant value of 1 K/m, and the dashed line is the same except with the temperature gradient set to 100 K/m. This range of temperature gradients bounds the results obtained from process models using MULTIFLO, and performance appears to be insensitive to this parameter. Results of the TPA Version 4.0 code sensitivity simulations in figure 4-4 are plotted on a log scale so that the solid and dashed lines can be distinguished graphically. The maximum difference of 8×10^{-5} rem/yr occurs at close to 8,000 yr.

In summary, there is very little sensitivity of groundwater dose to the parameters of REFLUX3 given the predicted lifetime of the EBS. The performance of the geological barrier, however, is affected by REFLUX3 parameters. Groundwater dose would be increased, and arrival time of radionuclides to the receptor population decreased, if water were to enter drifts during the thermal period.

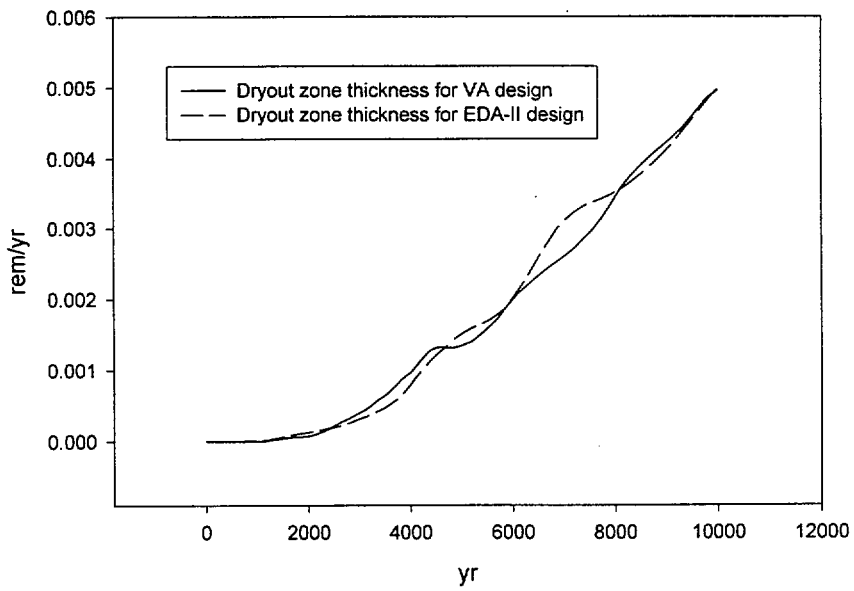

Figure 4-3. Comparison of the sensitivity of groundwater dose (without engineered barrier system) to the dryout zone thickness calculated by MULTIFLO for the Viability Assessment (VA) and Enhanced Design Alternative II (EDA-II) designs

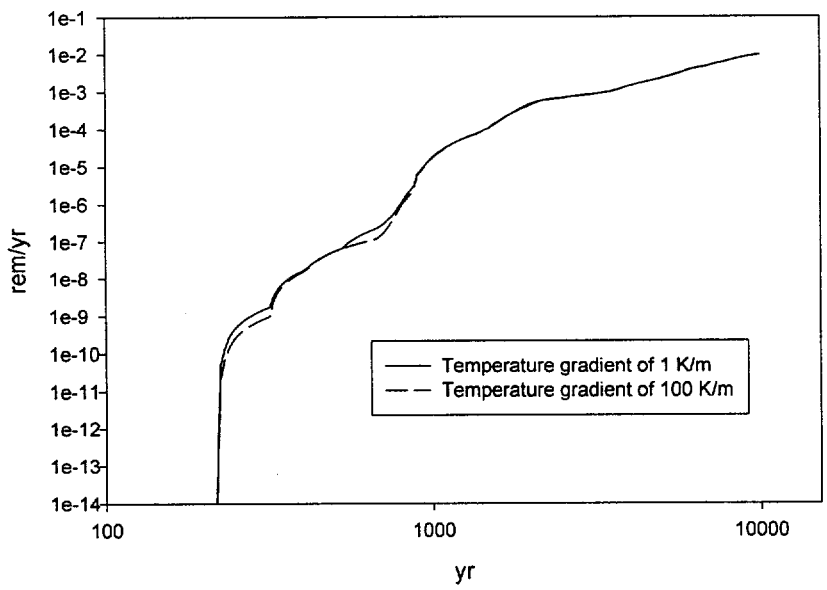

Figure 4-4. Comparison of the sensitivity of groundwater dose (without engineered barrier system) to the temperature gradient in the vicinity of the boiling isotherm

5 REFLUX3 PARAMETER DISTRIBUTIONS

The three parameters listed in table 3-2 control the flux of water at the repository during the thermal period and, as indicated in table 3-2, the statistical distributions for these parameters are set to reflect maximum uncertainty. As discussed briefly in section 4, the parameter Shed1 was intended to account for condensate shedding off the repository edges during that part of the thermal period when the boiling isotherm coalesced between drifts. Since EDA-II is designed to maintain pillar temperatures below boiling, the mechanism of shedding off repository edges may no longer need to be considered. Presently, the TPA Version 4.0 code specifies the distribution of this parameter to be loguniform on the range from 10^{-8} to 1.0. However, if this parameter takes on the value of 1.0, no water will reach the repository for the entire compliance period. This problem was observed when the extreme value of 1.0 was used for Shed1, 0.0 was used for Qfact, and 1.0 was used for Shed2. No water will reach the repository during the entire simulation if any of these extreme values are realized.

The parameter Qfact controls the volume of condensate that flows toward the repository each year as a function of the quantity of water stored in the perched volume. The MULTIFLO simulation results for the EDA-II design shown in figure 2-4 have an infiltration boundary condition at the surface of 5.5 mm/yr. The maximum flux of condensate drainage through the fractures above the repository from these simulations of 149 mm/yr occurs 80 yr after closure at a location approximately 7–8 m above the drift crown. However, the condensate drainage flux quickly drops to 46 mm/yr at 300 yr, then remains fairly steady at about 40 mm/yr until the reflux zone collapses at the end of the thermal period (figure 2-5). As this flux drains through the fractures into regions of higher temperature in the simulations, it evaporates, the flux rate decreases, and all of the water in the fractures evaporates as the flux reaches the boiling isotherm. The maximum dryout zone thickness of the matrix calculated by MULTIFLO simulations for the EDA-II design is approximately 7.4 m at 300 yr (table 3-1). Using the TPA Version 4.0 code parameters of 0.9 matrix saturation, 0.1 matrix residual saturation, and 0.14 matrix porosity, results in a maximum volume per unit area of 0.83 m^3/m^2 in the perched volume derived from matrix pore water. Neglecting the contribution from deep percolation, the value of Qfact, at 300 yr would be about 0.055 (46 mm/yr = 0.83 m × Qfact). As the thermal pulse recedes, water remaining in the perched volume is reimbibed into the matrix; and the rate of refluxing approaches the rate of deep percolation flux. As the perched volume becomes smaller and the matrix resaturates, Qfact should increase in order to maintain a non negligible flux toward the repository. For example, a Qfact of 1 would result in 5-mm/yr flow toward the repository with a perched volume reduced to 0.005 m^3/m^2. The parameter Qfact is a fixed constant for each realization, as implemented in the TPA Version 4.0 code. Presently, as indicated in table 3-2, the TPA Version 4.0 code uses a uniform distribution over the range of 0.0 to 1.0 to characterize this parameter. The 0.0 end-member of this distribution is nonphysical because the condensate in the perched volume is draining constantly by gravity. Given the uncertainty in process-level modeling of refluxing and model simplifications (e.g., neglecting heterogeneity), the range of this distribution should not be significantly reduced. A uniform distribution on the interval of approximately 0.05–1.0 for Qfact is recommended.

The final flux distribution factor in REFLUX3 applied to calculate the flow rate at the repository horizon is Shed2. As indicated in table 3-2, the distribution used in TPA Version 4.0 code for this parameter is loguniform on the range from 10^{-8} to 1.0, which gives a mean value of 10^{-4}. The quantity of water represented by Shed2 contributes to the volumetric flow rate that penetrates into the region of superheated rock but does not evaporate and does not reach the drifts. The physical mechanism by which this occurs is not well defined. In addition, focusing flow from an area of 503.4 m^2 into a single flow path by Qfact,

although conservative, may not be physically realistic. A possible approach for redefining the REFLUX3 parameters is suggested below as an interim measure while improvements to the reflux module of TPA Version 4.0 code are developed.

6 DISCUSSION AND RECOMMENDATIONS

An intent of the EDA-II design is to maintain pillar temperatures below boiling to allow condensate drainage between drifts. The zone of condensation above the repository will tend to diffuse laterally by vapor flow through fractures (figure 2-5). Condensate draining out of this zone will preferentially focus into fingers or rivulets as a consequence of gravity instability and heterogeneity. The spacing of these fingers will likely be dominated by heterogeneity so only a few of the fractures carry the bulk of the flux. Possible distributions of the spacing of flowing fractures are given in Hughson et al. (2000). Rivulets not flowing directly toward a drift may either pass harmlessly through the pillars and leave the system or evaporate and return to the zone of condensation. This process could be abstracted using the Shed1 parameter. The statistical distribution of this parameter would approximately represent the ratio of the area of below-boiling temperatures to the total area, reduced by some amount to account for evaporation in regions at elevated, but below-boiling temperatures.

Focusing the Qfact fraction over the area of the perched volume into a single flowing fracture is the bounding case. However, this process is currently the only mechanism incorporated into TPA Version 4.0 code by which water can reach the drifts during the thermal period and, without it, the drifts would remain dry as long as drift wall temperatures remain above boiling. The MULTIFLO process models of TH on the drift scale suggest that the rate of drainage from the condensate zone does not change significantly during the thermal period but stays at some fairly constant multiple of the deep percolation flux. However, the range of the distribution presently used in the TPA Version 4.0 code may bound possible effects of transient, episodic flux not included in the process-level model. At this time, no changes to the range of the distribution are recommended, except that the lower bound should be greater than zero. A value of 0.05 may be appropriate, as discussed in section 5.

Water flowing toward a drift in a rivulet penetrating the boiling isotherm should either vaporize and return to the condensate zone or arrive at the drift. The effects of capillary diversion at the drift wall boundary are already incorporated into the F_{ow} or F_{mult} parameters of the EBSREL module. In this suggested approach for abstracting TH in the EDA-II design, the factor Shed2 does not represent a well-defined physical process independent of the diversion parameters in EBSREL.

Figure 6-1 shows the groundwater dose averaged over 100 realizations for the basecase TPA Version 4.0 code input file (with WP thickness and drip shield life expectancy set to zero for geological barrier analyses) compared with proposed REFLUX3 parameter distribution ranges given in table 6-1. These simulations both use the dryout zone thickness file included as table 3-1. The net effect of increasing the mean Shed1 factor from 10^{-4} to 0.125, increasing mean Qfact from 0.5 to 0.525, and decreasing the mean Shed2 factor from 10^{-4} to 0 is to increase the average groundwater dose from 5.0×10^{-3} to 9.16×10^{-3} rem/yr.

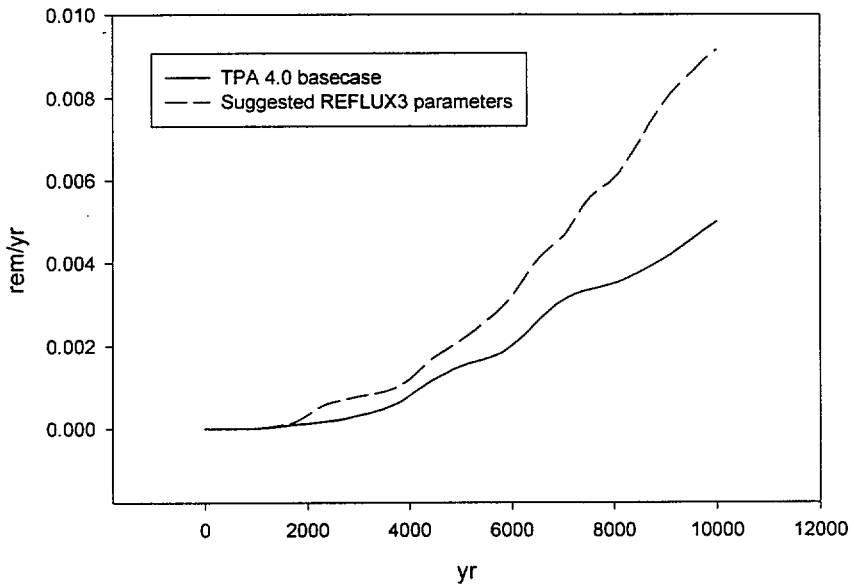

Figure 6-1. Comparison of groundwater dose from the Total-System Performance Assessment Version 4.0 code basecase results (without engineered barrier system) to dose computed using

Table 6-1. Suggested parameter distributions for REFLUX3

Factor	Code name	Distribution
FractionOfCondensateRemoved [yr^{-1}]	Shed1	uniform (0.0, 0.25)
FractionOfCondensateTowardRepository [yr^{-1}]	Qfact	uniform (0.05, 1.0)
FractionOfCondensateTowardRepositoryRemoved [yr^{-1}]	Shed2	constant (0.0)

These suggested modifications to the REFLUX3 parameters are intended to be more representative of the EDA-II repository design. For a more realistic representation of TH, however, improvements to the abstracted conceptual model could be made. These improvements should include well-defined mechanisms for focusing flow toward the repository into preferential flow paths for evaluation of the length scale of Eq. (3-2) and a process-model-based abstraction of water distribution in the condensation and refluxing zones. Distribution of condensate flow in preferential flow paths for estimation of thermal reflux and flow through superheated rock is a straight-forward extension of the conceptual model of Hughson et al. (2000).

7 CONCLUSION

An intent of the EDA-II repository design is to maintain temperatures in the pillars between drifts at below boiling throughout the duration of the thermal period. As indicated in figures 2-4 and 2-5, achieving this design goal depends on the efficacy of forced ventilation for removing heat generated by the waste. The cooler repository design of EDA-II results in a few meters of rock matrix dryout and thermally driven water refluxing lasting for about 10^3 yr. The EDA-II design also specifies WP fabrication from Alloy 22 and a Ti dripshield covering. With these enhancements of the engineered barriers, and the current estimates of their life expectancy, the TPA Version 4.0 code shows little or no sensitivity of dose to the thermal influences on UZ hydrology. An analysis of the geological barrier alone shows that the thermal period could have the effect of shifting the timing and increasing average radionuclide dose to the receptor population if water enters the drifts during the thermal period.

8 REFERENCES

Civilian Radioactive Waste Management System Management and Operating Contractor. *License Application Design Selection Report.* B00000000–01717–4600–00123. Revision 01. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 1999a.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Total System Performance Assessment—Site Recommendation Methods and Assumptions.* TDR–MGR–MD–000001. Revision 00. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 1999b.

Civilian Radioactive Waste Management System Management and Operating Contractor. *ANSYS Calculations in Support of Enhanced Design Alternatives.* B00000000–01717–0210–00074. Revision 00. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 1999c.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Thermal Tests Thermal-Hydrological Analysis/Model Report.* ANL–NBS–TH–000001. Revision 00. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000a.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Ventilation Model.* ANL–EBS–MD–000030. Revision 00. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000b.

Civilian Radioactive Waste Management System Management and Operating Contractor. *Repository Safety Strategy: Plan to Prepare the Postclosure Safety Case to Support Yucca Mountain Site Recommendation and Licensing Considerations.* TDR–WIS–RL–000001. Revision 03. Las Vegas, NV: Civilian Radioactive Waste Management System Management and Operating Contractor. 2000c.

Hardin, E.L. *Near-Field/Altered-Zone Models Report.* UCRL–ID–129179 DR. Livermore, CA: Lawrence Livermore National Laboratory. 1998.

Hughson, D.L., L.B. Browing, and R.W. Fedors. *Analysis of Niche Studies and Development of Bases for Total System Performance Assessment Seepage Parameters.* San Antonio, TX: Center for Nuclear Waste Regulatory Analyses. 2000.

Lichtner, P.C., M.S. Seth, and S. Painter. *MULTIFLO User's Manual MULTIFLO Version 1.2—Two-Phase Nonisothermal Coupled Thermal-Hydrologic-Chemical Flow Simulator.* Revision 2. Change 1. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses. 2000.

Mohanty, S., T.J. McCartin, and D.W. Esh. *Total-System Performance Assessment (TPA) Version 4.0 Code: Module Descriptions and User's Guide.* San Antonio, TX: Center for Nuclear Waste Regulatory Analyses. 2000.

Phillips, O.M. Infiltration of a liquid finger down a fracture into superheated rock. *Water Resources Research* 32(6): 1,665–1,670. 1996.

TRW Environmental Safety Systems, Inc. *Total System Performance Assessment—Viability Assessment Analyses—Technical Basis Document.* B00000000–01717–4301–00001. Revision 01. Las Vegas, NV: TRW Environmental Safety Systems, Inc. 1998.

U.S. Department of Energy. *Viability Assessment of a Repository at Yucca Mountain.* DOE/RW–0508. Las Vegas, NV: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. 1998.

U.S. Nuclear Regulatory Commission. *Issue Resolution Status Report. Key Technical Issue: Container Life and Source Term.* Revision 2. Washington, DC: U.S. Nuclear Regulatory Commission, Division of Waste Management. 1999.

APPENDIX

Table 1. Matrix hydraulic properties, DTN:LL980209004242.026 [from Total System Performance Assessment—Viability Assessment (TRW Environmental Safety Systems Inc., 1998)]

Model Unit	Geological Unit	Porosity	Permeability (m^2)	S_r	α (Pa^{-1})	m
TCw11	Tpcpll	0.066	5.40e-18	0.13	1.15e-6	0.2310
TCw12	Tpcpln	0.066	5.40e-18	0.13	2.01e-6	0.2447
TCw13	Tpcpv	0.140	5.69e-17	0.33	3.74e-6	0.4548
PTn21	Tpbt4	0.369	1.61e-14	0.10	3.98e-5	0.2531
PTn22	Tpy	0.234	3.30e-15	0.14	7.94e-6	0.4925
PTn23	Tpbt3	0.353	5.40e-14	0.17	5.44e-5	0.3002
PTn24	Tpp	0.469	8.80e-14	0.10	3.43e-5	0.3859
PTn25	Tpbt2	0.464	3.18e-13	0.10	1.81e-4	0.3195
TSw31	Tptrv	0.042	7.76e-17	0.11	5.84e-5	0.2304
TSw33	Tptpul	0.135	2.04e-17	0.06	6.21e-6	0.2479
TSw35	Tptpll	0.115	2.22e-17	0.08	4.01e-6	0.1983
TSw36	Tptpln	0.092	8.70e-18	0.18	2.27e-6	0.5138
TSw37	Tptpv	0.020	4.08e-18	0.50	7.39e-6	0.3709
CH1vc	Tpbt1	0.265	1.60e-12	0.04	7.60e-5	0.1592
CH2vc	Tac(v)	0.321	5.50e-14	0.06	4.12e-5	0.2291
CH3zc	Tac(z)	0.240	2.50e-18	0.20	2.16e-5	0.2119
CH4zc	Tacbt	0.169	5.49e-18	0.33	1.03e-6	0.4322
PP3vp	Tpc(3)	0.274	1.91e-15	0.07	1.66e-5	0.3142
PP2zp	Tcp(2)	0.197	1.75e-17	0.18	8.39e-6	0.3568
BF3vb	Tcb(w)	0.274	1.91e-15	0.07	1.66e-5	0.3142

Table 2. Fracture hydraulic properties, DTN:LL980209004242.026 [from Total System Performance Assessment—Viability Assessment (TRW Environmental Safety Systems Inc., 1998)]

Model Unit	Porosity	Permeability vertical (m^2)	Permeability horizontal (m^2)	S_r	α (Pa^{-1})	m	A_{mod}
TCw11	2.33e-4	2.29e-11	6.03e-12	0.01	2.37e-3	0.667	5.00e-4
TCw12	2.99e-4	1.38e-11	6.03e-12	0.01	2.37e-3	0.669	5.00e-4
TCw13	7.05e-5	2.82e-12	2.40e-13	0.01	9.12e-4	0.669	5.00e-4
PTn21	4.84e-5	5.25e-13	5.25e-13	0.01	1.10e-3	0.669	5.02e-4
PTn22	4.83e-5	1.95e-13	1.95e-13	0.01	1.85e-3	0.669	5.00e-4
PTn23	1.30e-4	2.57e-13	2.57e-13	0.01	3.45e-3	0.667	5.00e-4
PTn24	6.94e-5	6.17e-14	6.17e-14	0.01	9.13e-4	0.667	5.00e-4
PTn25	3.86e-5	7.76e-14	7.76e-14	0.10	1.81e-4	0.320	5.00e-1
TSw31	8.92e-5	1.07e-11	1.00e-12	0.01	1.44e-4	0.566	4.68e-1
TSw33	1.05e-4	2.63e-11	8.91e-13	0.01	1.73e-3	0.667	5.00e-4
TSw35	3.29e-4	3.80e-12	9.12e-13	0.01	1.26e-3	0.667	5.00e-4
TSw36	3.99e-4	1.20e-12	1.20e-12	0.01	1.32e-3	0.667	5.00e-4
TSw37	4.92e-4	1.20e-12	1.20e-12	0.01	1.19e-3	0.659	5.00e-4
CH1vc	7.14e-5	1.74e-13	1.74e-13	0.01	1.18e-3	0.669	5.00e-1
CH2vc	7.14e-5	2.88e-13	2.88e-13	0.01	1.18e-3	0.667	5.00e-1
CH3zc	1.10e-5	2.51e-14	1.17e-14	0.01	1.12e-3	0.654	9.22e-1
CH4zc	1.10e-5	2.51e-14	1.55e-14	0.01	1.14e-3	0.667	5.00e-1
PP3vp	7.14e-5	7.08e-13	6.92e-13	0.01	1.42e-3	0.667	5.00e-4
PP2zp	1.10e-5	2.51e-14	6.46e-14	0.01	1.14e-3	0.667	5.00e-1
BF3vb	7.14e-5	7.08e-13	6.92e-13	0.01	1.42e-3	0.667	5.00e-4

Table 3. Matrix thermal and physical properties, DTN:STN05071897001.002 [from TSPA-VA (TRW Environmental Safety Systems Inc., 1998)]

Unit	Thermal Conductivity—Wet (W/m-K)	Thermal Conductivity—Dry (W/m-K)	Rock Specific Heat (J/kg-K)	Rock Density (kg/m^3)
TCw11	1.76	1.02	847	2.51e+3
TCw12	1.88	1.28	837	2.51e+3
TCw13	0.98	0.54	857	2.47e+3
PTn21	0.50	0.35	1080	2.34e+3
PTn22	0.97	0.44	849	2.40e+3
PTn23	1.02	0.46	1020	2.37e+3
PTn24	0.82	0.35	1330	2.26e+3
PTn25	0.67	0.23	1220	2.37e+3
TSw31	1.00	0.37	834	2.51e+3
TSw33	1.80	0.71	883	2.51e+3
TSw35	2.02	1.20	900	2.54e+3
TSw36	1.84	1.42	865	2.56e+3
TSw37	2.08	1.69	984	2.36e+3
CH1vc	1.31	0.70	1060	2.31e+3
CH2vc	1.17	0.58	1200	2.24e+3
CH3zc	1.20	0.61	1150	2.35e+3
CH4zc	1.35	0.73	1170	2.44e+3
PP3vp	1.26	0.66	841	2.58e+3
PP2zp	1.35	0.74	644	2.51e+3
BF3vb	1.26	0.66	841	2.58e+3