OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL COVER SHEET

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2. ☐ Analysis ☐ Engineering ☐ Performance Assessment ☐ Scientific

3. ☑ Model ☐ Conceptual Model Documentation ☑ Model Documentation ☐ Model Validation Documentation

4. Title:
In-Drift Thermal-Hydrological-Chemical Model

5. Document Identifier (including Rev. No. and Change No., if applicable):
ANL-EBS-MD-000026 REV 00

6. Total Attachments:
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7. Attachment Numbers - No. of Pages in Each: See Remarks
I-~~8~~ 7, II-6, III-~~61~~ 63, IV-~~106~~ 109, V-2, VI-2, VII-3, plus 1 CD-ROM (V, VI, VII)
JTKam 1/21/2000 JBC 1/21/2000

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OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL COVER SHEET

1. QA: QA

Page: 1 of: 40

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00	Initial Issue

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

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Document Title: Water Diversion Model

Document Revision/Change: 00

Document Date: 02/01/2000

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CONTENTS

FIGURES

TABLES

1. PURPOSE

The purpose of this Analysis/Model Report (AMR) is to analyze Thermal-Hydrologic-Chemical (T-H-C) processes in the Engineered Barrier System (EBS) emplacement drift, and to provide data to support the EBS post-closure performance assessment. The work scope includes predicting the temperatures at the surface of the waste package, the drip shield, and the drift wall during waste emplacement in the repository. The flow of vapor and liquid components of water into the drift will be analyzed and the condensation potential in the drift, particularly underneath the drip shield, will be assessed. A development plan entitled *Development Plan for the In-Drift Thermal-Hydrological-Chemical Analysis* (CRWMS M&O 1999f) was prepared which included a completed a checklist for the T-H-C Model. The plan documents the AMR Number as E0065 and the corresponding work package as 12012383MX for the T-H-C Model. The model shall be a two-dimensional numerical simulation, using the NUFT computer code (Non-isothermal Unsaturated-saturated Flow and Transport) (LLNL, 1998c). The analysis also requires a preprocessor RADPRO which is used in conjunction with NUFT to compute thermal radiation. A postprocessor XTOOL is used to display the results from NUFT graphically. A description of the software is presented in Sections 2.0 and 3.0.

Revision 00 of this AMR will address only thermal and hydrologic effects and will exclude any chemical effects. This assessment considers only the performance of the "as-designed" system. Failure scenarios of the drip shield are, therefore, not considered in this AMR.

2. QUALITY ASSURANCE

This report for the In-Drift Thermal-Hydrological-Chemical Analysis Model has been prepared according to AP-3.10Q *Analysis and Models.* AP-3.10Q presents the procedure for planning, development, validation and documentation of analyses and models. A QAP-2-0 activity evaluation was performed for the preparation of this report, subject to the controls of a QA program (CRWMS M&O 1999g). The backfill material and drip shield of the EBS are classified as quality level 1 (CRWMS M&O 1999h). In addition to the procedures cited above, the following procedures are applicable to this document: AP-3.14Q, AP-3.15Q, and AP-SI.1Q.

3. COMPUTER SOFTWARE AND MODEL USAGE

The analysis is performed using the multiphase flow module **usnt** of NUFT, developed at Lawrence Livermore National Laboratory (LLNL, 1998c).

The version of NUFT used for this analysis is Ver.2.0s, which has been qualified by the Lawrence Livermore National Laboratory (LLNL) for the Yucca Mountain Site Characterization Project (LLNL, 1998d). Since LLNL is a Management and Operating (M&O) contractor, this version is regarded as transferred software in accordance with the requirements of the AP-SI.1Q *Software Qualification Procedures*. The code was obtained

from LLNL through Configuration Management (CM) and is appropriately used for the Engineered Barrier System (EBS) application, within the range of validation, according to AP-SI.1Q. However, the routine within Ver. 2.0s that computes thermal radiation has not yet been qualified. Additionally, the use of NUFT (basically designed for porous media) to model natural convection in air space is an approximation and will require validation beyond that provided in Attachment IV as more experimental data become available. This will be done in the future revisions of this AMR with the ongoing model calibration process that will result in a better prediction of the natural convection pattern in the air space.

The Computer Software Configuration Item (CSCI) and Medium Identifier (MI) numbers for Ver. 2.0s are given by CM as the letter of Certification Number provided by the LLNL, which is **LLYMP9809098** (See Attachment II). The Document Identifier (DI) number(s) and other configuration management information for NUFT are included in Attachment III.

Version 2.0s has been installed on a Sun workstation with CPU Property Tag Number 115488. An installation test has been performed to verify a sample output, based on input provided by LLNL. The test is documented in Attachment III. This version cannot output quantities of evaporation or condensation as Ver. 3.0s can. NUFT Ver.3.0s is expected to be qualified by the end of December, 1999.

NUFT is an integrated finite-difference code that solves the partial differential equations of flow and transport of different components (e.g., water, air) and phases (e.g., liquid and gas) in porous and fractured media. The components and the phases are assumed to be in local thermodynamic equilibrium. The Module **usnt** (fully coupled **unsaturated** multiple phases, multiple components model with isothermal and **non-isothermal** options) is capable of modeling fully coupled unsaturated-saturated multiple phases and multiple components under isothermal and non-isothermal conditions. Of particular importance, especially for non-isothermal problems, is the ability of NUFT to handle the appearance and disappearance of any phase due to condensation and evaporation. The results produced by **usnt** are either time histories of concentrations, saturation, and fluid pressures at different locations within the problem domain, or spatial distribution of these state variables at specified times. The theory of NUFT and its equations for analysis are described in the User's Manual (LLNL, 1998c, Appendix C) and Reference Manual (LLNL, 1998b).

RADPRO Ver. 3.13 is a preprocessor of NUFT that computes the radiation coefficients of thermal radiation between radiating and reflecting surfaces, based on user input of emissivity of the radiating surface (Daveler et al. 1998, TBV). This version assumes the emissivity of all reflecting surfaces to be 1.0 and neglects user input for this value.

The radiation coefficients generated by RADPRO are included in a file named RACON that is compatible in format with the program NUFT. Incorporating RACON into the NUFT input file enables NUFT to compute radiation underneath the drip shield as this is

the only air gap assumed to exist in the model. Additionally, radiation patterns underneath the drip shield will be plotted with RADPRO.

XTOOL Ver. 9.11.1.3, a postprocessor of NUFT (LLNL, 1998a, TBV), will be used to plot the time history of temperature, relatively humidity, liquid saturation, and vapor/liquid flow pattern as computed by NUFT. One limitation of this version of XTOOL is a restriction of adding annotation to plotted results.

RADPRO, NUFT, and XTOOL are executed on a Sun Ultra 2 Workstation CPU (tag #115488) and the results are displayed on a Sun Microsystems Monitor (tag # 115506).

The thermal radiation routine of NUFT Ver.2.0s, RADPRO and XTOOL, were developed by LLNL and are currently unqualified due to resource and schedule constraints. They are expected to be qualified for use on the Yucca Mountain Site Characterization Project in 1999. Therefore, the output and results reported in this AMR are unqualified and designated as "To Be Verified" (TBV). The input and output files for RADPRO, NUFT, and XTOOL are documented in Attachments V, VI, and VII.

Model validation is presented in Section 6.4 and will be continued as more experimental data become available for the Quarter Scale Drip Shield Test.

4. INPUTS

The following model geometry and material properties are used in the analysis. These data are qualified with Data Tracking Numbers (DTN), or references from calculations (AP-3.12Q) or input transmittals (AP-3.14Q). Boundary and initial conditions, and other assumed thermal properties of the waste package, drip shield, invert material, and lithostratigraphic units, are listed in Section 5. Inputs to computer runs are designated as (TBV) until they are qualified for the Project. All unqualified data used in this report are listed in Section 5 without any qualified references and are noted as such.

4.1 DATA AND PARAMETERS

A cross-section of lithostratigraphic units at the repository center point (N233,760m, E170,750m) is presented on page 19 of *Repository Ground Support Analysis for Viability Assessment* (CRWMS M&O 1998a). The ground-surface elevation and the repository-invert elevation for those coordinates are given as EL.1407.2m and EL. 1072.3m, *Repository Ground Support Analysis for Viability Assessment* (CRWMS M&O 1998a). Based on these elevations and the fact that the water table is approximately 340 m below the invert (CRWMS M&O 1997, p.67), the length of the section from the ground surface to the water table is calculated to be approximately 675.0 m. The thickness of the individual unit has been revised by data from Input Tracking No. SSR-NEP-99261.T (CRWMS M&O 1999c). At the time of this report, the ground surface elevation of the above-mentioned repository center point has been revised to be 4663 ft. (SSR-NEP-99261.Ta). Because of schedule constraints, this value will not be updated until the next revision of this report.

Thickness of stratigraphic units and their grain density, specific heat, and thermal conductivity are based on data from Input Tracking No. SSR-NEP-99261.T (CRWMS M&O 1999c) for the coordinates (N233,760m, E170,750m).

Because of symmetry, a two-dimensional model of NUFT is constructed to include only half of the waste package and the drift spacing (40.5 m) in accordance with the Enhanced Design Alternative (EDA) II design (Wilkins and Heath, 1999) and the two vertical edges are treated as no-flow boundaries. The model extends from the ground surface to the water table about 340 m below the repository invert level (CRWMS M&O 1997). A simulation grid for the entire section is presented in Figure 1, with the spacing varying from 0.02 to 45.0 m. Figure 2 is a section of the emplacement drift with the drip shield in place. A corresponding model grid (derived from the main grid) that represents the drift with various EBS components is shown in Figure 3.

The following hydrostratigraphic properties are derived from the EBS "drift-scale" base case for the 1-D upper-bound infiltration data package LB990861233129.002: Fracture porosity, matrix porosity, tortuosity factor, fracture bulk permeability, matrix bulk permeability, maximum and residual saturation in fractures, maximum and residual saturation in matrix, Van Genuchten alpha for fractures, Van Genuchten alpha for matrix, fracture porosity, and matrix porosity.

Additional input parameters required by NUFT are derived by the following equations (LLNL, 1988, pp. 11 and 14):

$$K_m = K_{b,m} / (1-\phi_f) \quad (1)$$

$$K_f = K_{b,f} / \phi_f \quad (2)$$

$$K_b = K_{b,m} + K_{b,f} \quad (3)$$

$$\phi_b = \phi_f + (1-\phi_f)\,\phi_m \quad (4)$$

$$\beta_v = 1/(1-\lambda) \quad (5)$$

The above abbreviations are explained on page 39.

4.1.1 Radiative Heat Transfer Properties (TBV)

Emissivity of the Simulated Waste Package 0.87 (CRWMS M&O 1999d).
Emissivities of drip shield and invert material are 1.0.
Radiant heat absorption by moisture-laden air is assumed to be negligible because gases such as water vapor are also good radiators. Therefore, the impact of this assumption in the RADPRO calculation is insignificant.

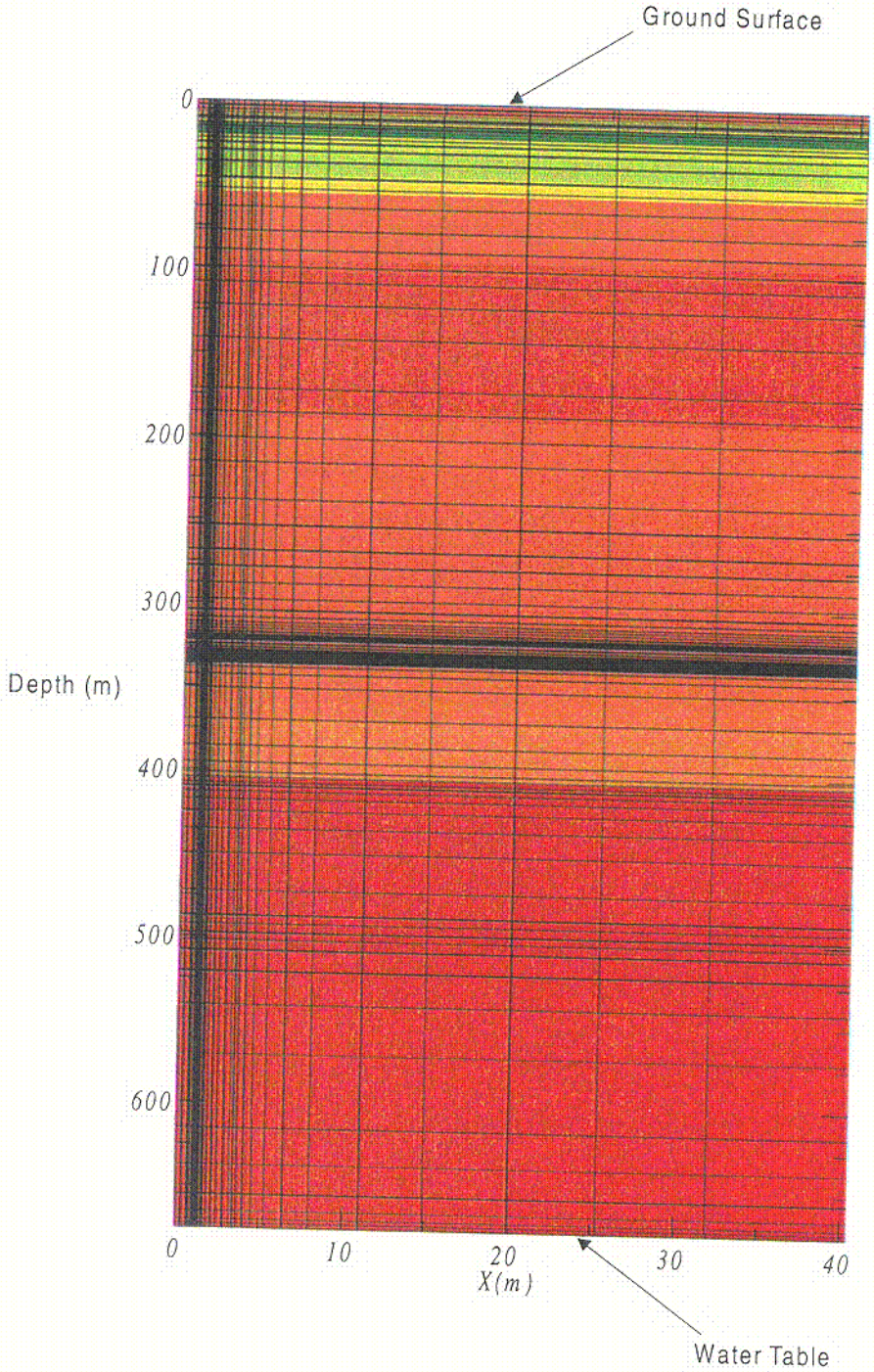
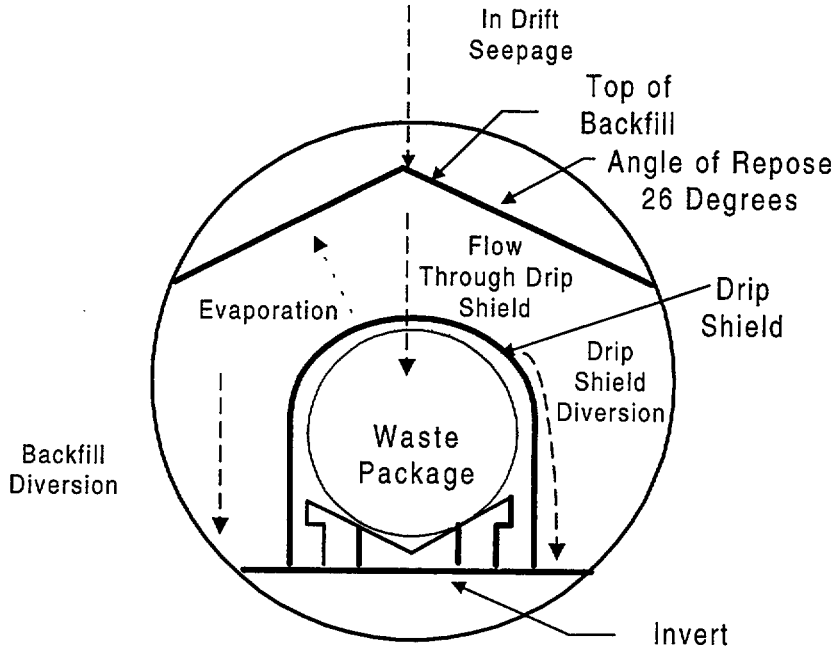


Figure 1. NUFT Simulation Grid



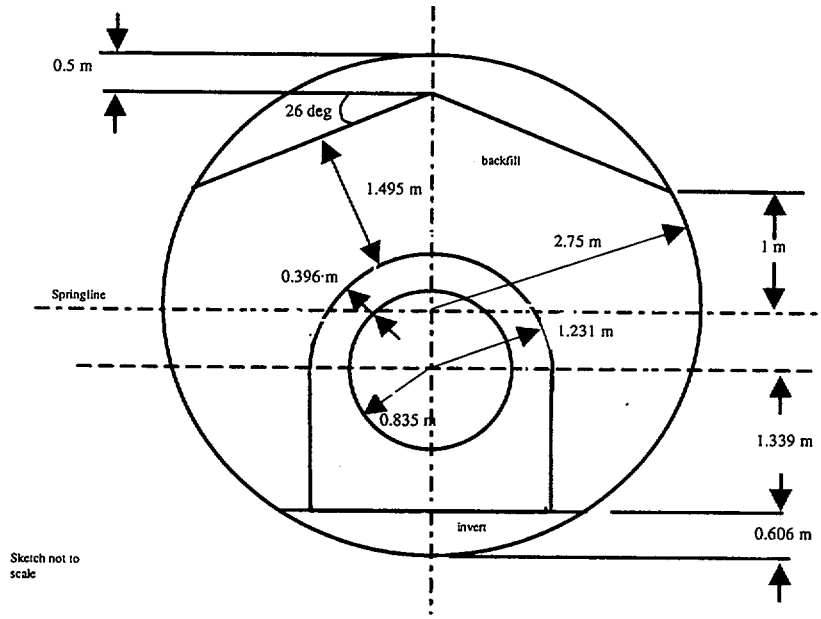


Figure 2. Conceptual Model for Diversion of Water Flow

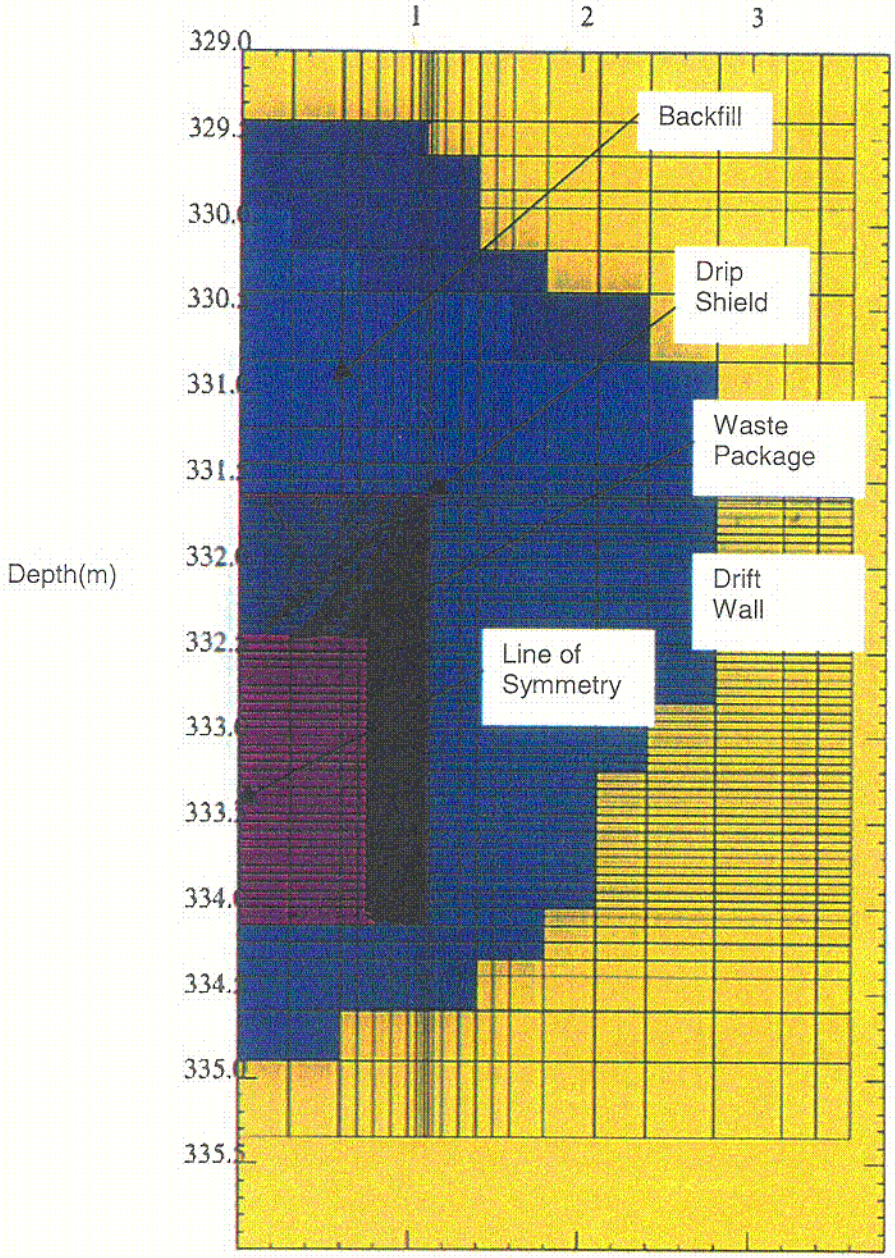


Figure 3. Detailed Grid for Full –Scale Repository Model

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4.1.2 Thermal Properties of Simulated Drift Air at 300° K (Incropera and DeWitt 1996, pg 839) (TBV)

Mass Density 1.1614 kg/m^3
Thermal Conductivity 0.0263 watt/(m-°K)
Specific Heat Capacity 1.007 kJ/kg

4.1.3 Thermal Properties of the Invert Material (DTN: SN9908T0872799.004 – indriftgeom_rev01.doc, pages 1 and 2) (TBV)

Thermal Conductivity 0.66 watt/(m-°K) Dry
Grain Density 2530 kg/m^3
Specific Heat Capacity 948 J/(kg-°K)

4.1.4 Thermal Properties of Drip Shield (DTN: SN9908T0872799.004) (TBV)

Thermal Conductivity 20.55 W/(m-°K)
Specific Heat Capacity 551.32 J/(kg-°K)
Mass Density 7900 Kg/m^3 **(Incropera and DeWitt 1996, pg 829) (TBV)**

4.1.5 Thermal Properties of Waste Package (DTN: SN9908T0872799.004) (TBV)

Mass Density 8189.2 kg/m^3
Thermal Conductivity 14.42 W/(m-°K)
Specific Heat capacity 488.86 J/(kg-°K)

4.1.6 Fluid and Thermodynamic Properties of Water and Air

Properties such as molecular weight, density, viscosity, diffusivity, enthalpy versus temperature/pressure, and specific volume as a function of temperature/pressure, are incorporated into the NUFT code (Attachment III, Software Qualification).

4.1.7 Universal Constants

The Ideal Gas Constant R (1.987 cal/(g.mol-°K)) and Gravitational Constant g (9.807 m/s^2) are accepted data incorporated into the NUFT code.

4.2 CRITERIA

Not Applicable

4.3 CODES AND STANDARDS

Not Applicable

5. ASSUMPTIONS (used in Section 6)

5.1 HYDROLOGIC PROPERTIES OF WASTE PACKAGE

The following properties are assumed from **(MO9812MWD1NUFT.000 – MOL.19990408.0013)**
Porosity = 0.010
Permeability = 0.0
Tortuosity Factor = 0.0

5.2 DRIP SHIELD AND OTHER EBS COMPONENTS

For ease of modeling, the top of the drip shield is assumed to be flat rather than curved. This assumption is discussed under "Results" in Section 6.5. The modeled thickness of the drip shield is 2 cm and the dimensions of the drift, invert material, and drip shield are shown on the simulation grid, corresponding to the EDA II design (Wilkins and Heath, 1999; CRWMS M&O 1999b).

5.3 HYDROLOGIC PROPERTIES OF DRIP SHIELD

As the drip shield is made of titanium, its hydrologic properties are assumed to be the same as those of the waste package (Section 5.1)
Porosity = 0.010
Permeability = 0.0
Tortuosity Factor = 0.0

5.4 THERMAL AND HYDROLOGIC PROPERTIES OF ATMOSPHERIC AIR

A heat capacity of 1,007 J/(kg-K) is assigned to the atmosphere above the ground surface (MO9812MWD1NUFT.000). The thermal conductivity of the atmosphere is 0.0263 W/(m-K), same as that used for air in the emplacement drift (Incropera and DeWitt 1996). A porosity of 0.990 and a bulk intrinsic permeability of 1E-8 m^2 are used for the atmosphere, according to MO9812MWD1NUFT.000.

5.5 APPROXIMATION OF DRIFT AIR

To simulate the air space underneath the drip shield, a fictitious material with a porosity of 0.990 and a saturated porous medium-equivalent permeability of 10,000 darcys is assumed to occupy the simulated drift air space underneath the drip shield. A porosity close to 1.0 is chosen because using 1.0 would lead to a singularity in the flow equations. An adjustment of thermal conductivity is addressed in Attachment IV. The selection of a single value of intrinsic permeability (1E-8 m^2) and a single value of thermal conductivity (0.0263 W/(m-K)) for the air gap will approximate the average heat transfer between the waste package and the drip shield. To account for spatial variation of heat transfer in the air gap, thermal conductivity and permeability of the pseudo-porous material would have to be selected to produce air convection pattern similar to that in the

air gap. Furthermore, the values of these parameters would change with the temperature difference between the waste package and the drip shield as the thermal loading varies. Improved parameter calibration will be implemented in a later revision of this AMR.

5.6 THERMAL LOADING OF WASTE PACKAGE

The thermal loading for the waste package is based on data from the Design Input transmittal (CRWMS M&O 1999a) and is presented in Attachment V. As the main purpose of this report is to predict flow into various EBS components of the drift during the cooling phase of the repository, the first 50 years or 100 years of thermal loading will be ignored in the analyses described in Section 6. This is done to decrease the turnaround time of the production runs. The impact of this modification will be discussed in Section 6.

Ignoring the first 100 years of thermal loading will not impact the results for revision 00A of this AMR because chemical reactions are not considered in this model.

Thermal-mechanical induced alterations in material properties are addressed in another AMR.

The simulated waste package support is not considered in this analysis and the lower surface of the waste package is assumed to be in direct contact with the invert material. This assumption ignores the convective heat transfer in the air space between the waste package and the invert material although given the geometry of the support, air movement around the support may be somewhat restricted. This air space trapped in the support system would tend to reduce the convective heat transfer to the invert material. The impact of ignoring this air gap and heat conduction by the support will be evaluated in a later revision of this AMR when the final design of the waste package support system is complete.

5.7 WATER INFLUX INTO DRIFT

This report evaluates the impact of water influx into the drift that could affect the performance of the drip shield in minimizing water contact with the waste package. The first approach involves uniformly applying an infiltration rate of 35 mm/yr on the ground surface and percolation at this rate will, at a steady or quasi-steady state, continue through the profile. This rate is based on the total percolation flux from fractures (25 mm/yr) and matrix (10 mm/yr) (MO9901RIB00044.000) at the repository level. For the sensitivity analysis, the infiltration rate will be increased to 68 mm/yr to represent the maximum expected for a long-term projection of weather changes in the repository area.

5.8 HYDROLOGIC PROPERTIES OF THE INVERT MATERIAL (SN9908T0872799.004 – MOL.19990901.0312)

Porosity = 0.545
Intrinsic Permeability (m^2) = 6.16 E-10

Van Genuchten α_v (1/Pa) = 1.2232E-3
n = 2.7
Residual saturation = 0.092

Porosity and permeability are test measurements and the other parameters are derived from curvefitting to water retention data.

5.9 BACKFILL MATERIAL

The Overton sand backfill is assumed to completely fill the outer annulus between the drip shield and the drift wall rather than leaving a relatively small air gap on top of the backfill, as depicted in Figure 3. The air gap above the backfill will facilitate natural convection that would tend to dry the crown area so less moisture would accumulate above the drip shield. The air space would also facilitate moisture runoff on the surface of the backfill away from the crown area. Thus omission of the air gap is conservative. This assumption allows any influx into the crown of the drift to be in direct contact with the backfill and, thus, would facilitate flow to the invert of the drift. Whereas in the presence of the air space above the backfill, liquid from crown of the drift could come into contact with the backfill by free fall. Additionally, as this modification only occurs in the outer rather than the inner annulus of the drip shield, this assumption will not impact the condensation potential underneath the drip shield.

5.10 THERMAL AND HYDROLOGIC PROPERTIES OF BACKFILL MATERIAL (SN9908T0872799.004 – MOL.19990901.0312)

Porosity = 0.410
Intrinsic Permeability (m^2) = 1.43E-11
Van Genuchten α_v (1/Pa) = 2.75E-4
n = 2.0
residual saturation = 0.01

Porosity and permeability are determined from test measurements and the other parameters are derived from curvefitting to water retention data.

The backfill material is chosen such that it has a permeability about an order of magnitude higher than that of the surrounding rock. As a result, capillary barrier effect would minimize the infiltration of liquid from the host rock into the backfill under unsaturated conditions.

5.11 TORTUOSITY FACTORS

A factor of 1.0 is assigned to Simulated Drift Air and Atmosphere to simulate open air space with porosity values of 0.999 and 0.990, respectively.
A factor of 0.0 is assigned to Simulated Heaters and Drip Shield since they are assumed to be air and water tight and have zero permeability.

A factor of 0.7 is assigned to the Invert Material since it is a granular material similar to the lithostratigraphic units at the repository horizon. This coefficient was estimated for a range of liquid saturation in soils by Penman (1940) and was found to be 0.66 (~ 0.7) as an average value.

5.12 BOUNDARY CONDITIONS

The boundary conditions at the ground surface and the water table are specified in the MO9812MWD1NUFT.000 data package and are presented in Table 1:

Table 1. Boundary Conditions

	Ground Surface	Water Table
Temperature (°C)	19.1	32.0
Gas-phase Pressure (Pa)	8.6×10^4	9.1×10^4
Liquid Saturation (%)	0.0	100.0

These boundary conditions will be fixed during both the initialization and production NUFT runs.

At the time this report was prepared, the temperatures and pressures for the ground surface and water table were being revised. This information will be updated in the next revision of this report.

5.13 INITIAL CONDITIONS

To specify the initial conditions of gas-phase pressure, formation temperature, and liquid saturation for the heating simulations, an ambient condition is initialized (hereby referred to as an initialization run), using a linear distribution of the boundary condition specified in Section 5.13. During the initialization run, the waste package, the drip shield, the Overton Sand Backfill, and the Invert Material are absent, as indicated in Figure 4. An infiltration rate of 35 mm/year is imposed at the ground surface as discussed in Section 5.7. The ambient liquid saturation and temperature distribution, obtained by running the model for 1.0×10^6 years in a steady or quasi-steady state, are shown in Figures 5 and 6. These ambient conditions will become the initial conditions for the production run when heating of the waste package is simulated. The production run will last for approximately 100,000 simulated years.

The initial condition adopted for the simulations represents the state prior to excavation of the drifts. When a drift is excavated, stress-relief may cause significant property changes (e.g. permeability increase due to micro-cracking) in the near-field, and water drainage from the matrix and fractures can change the initial water distribution. An assessment of whether, and how soon the in-situ initial condition would be re-established and its impact on the performance will be addressed in the Water Distribution/Removal AMR.

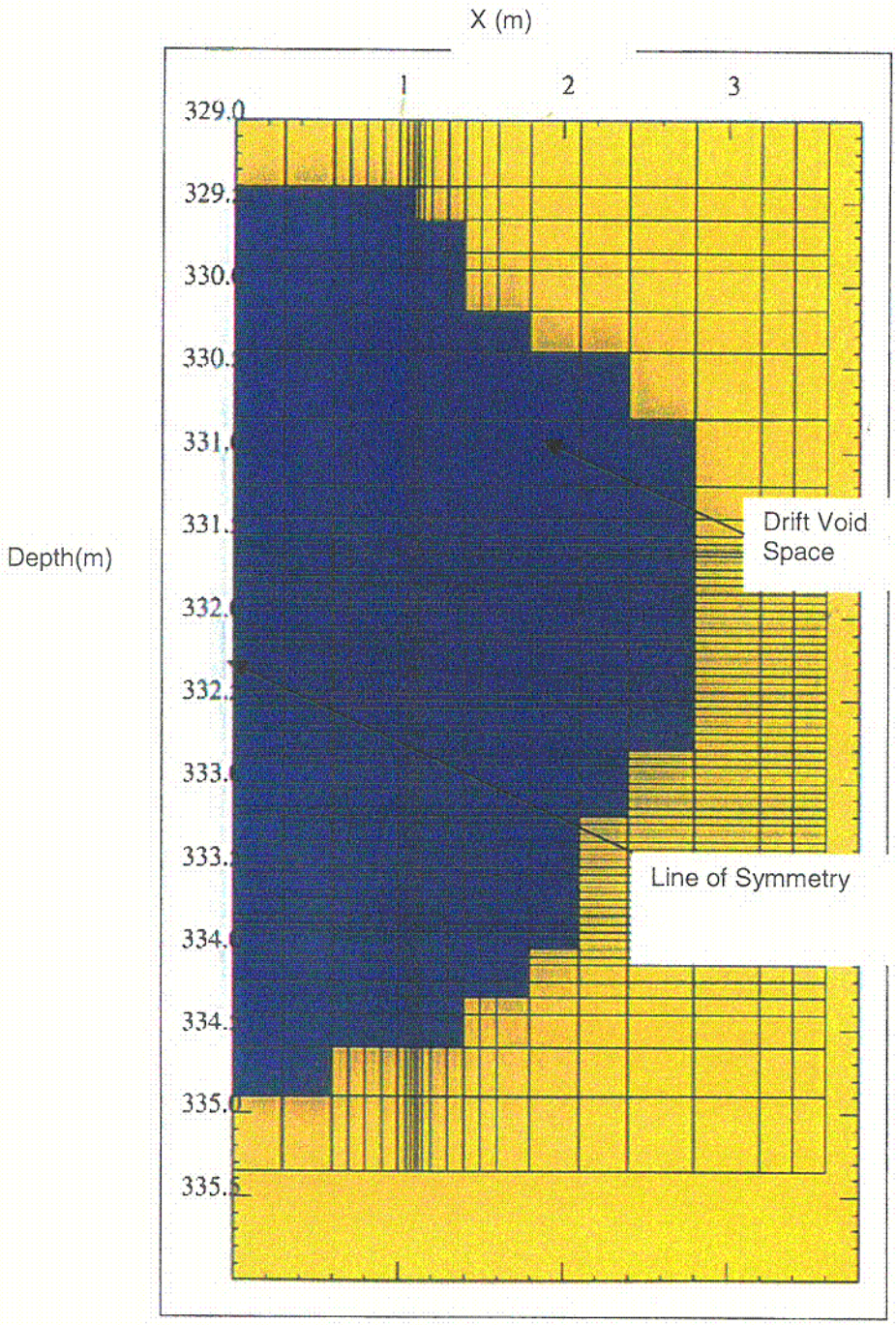

Figure 4. Detailed Grid for Initialization Run

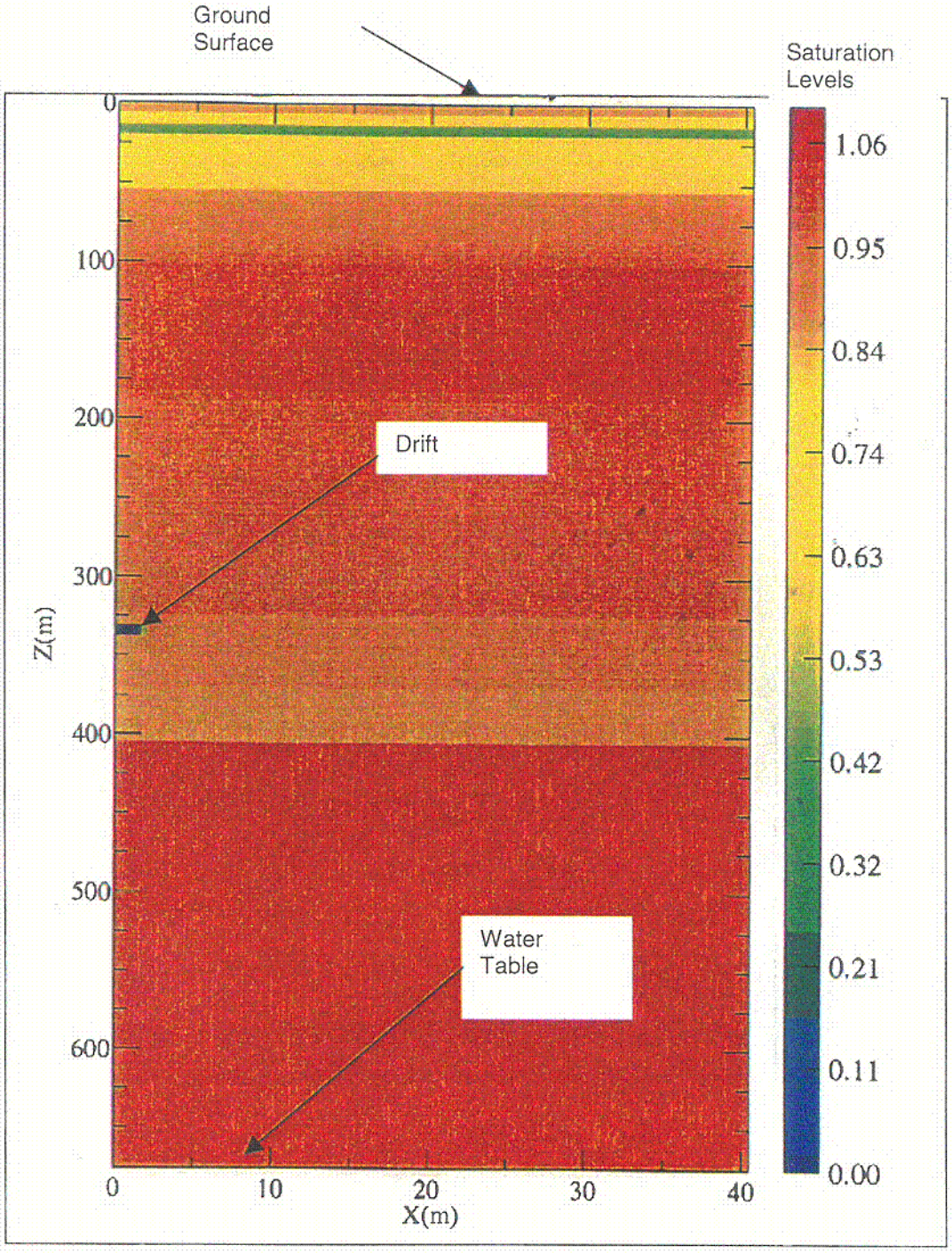

Figure 5. Initial Saturation Contours for the Two-Dimensional T-H Model with a Drip Shield at an Infiltration Rate of 35 mm per year

C4

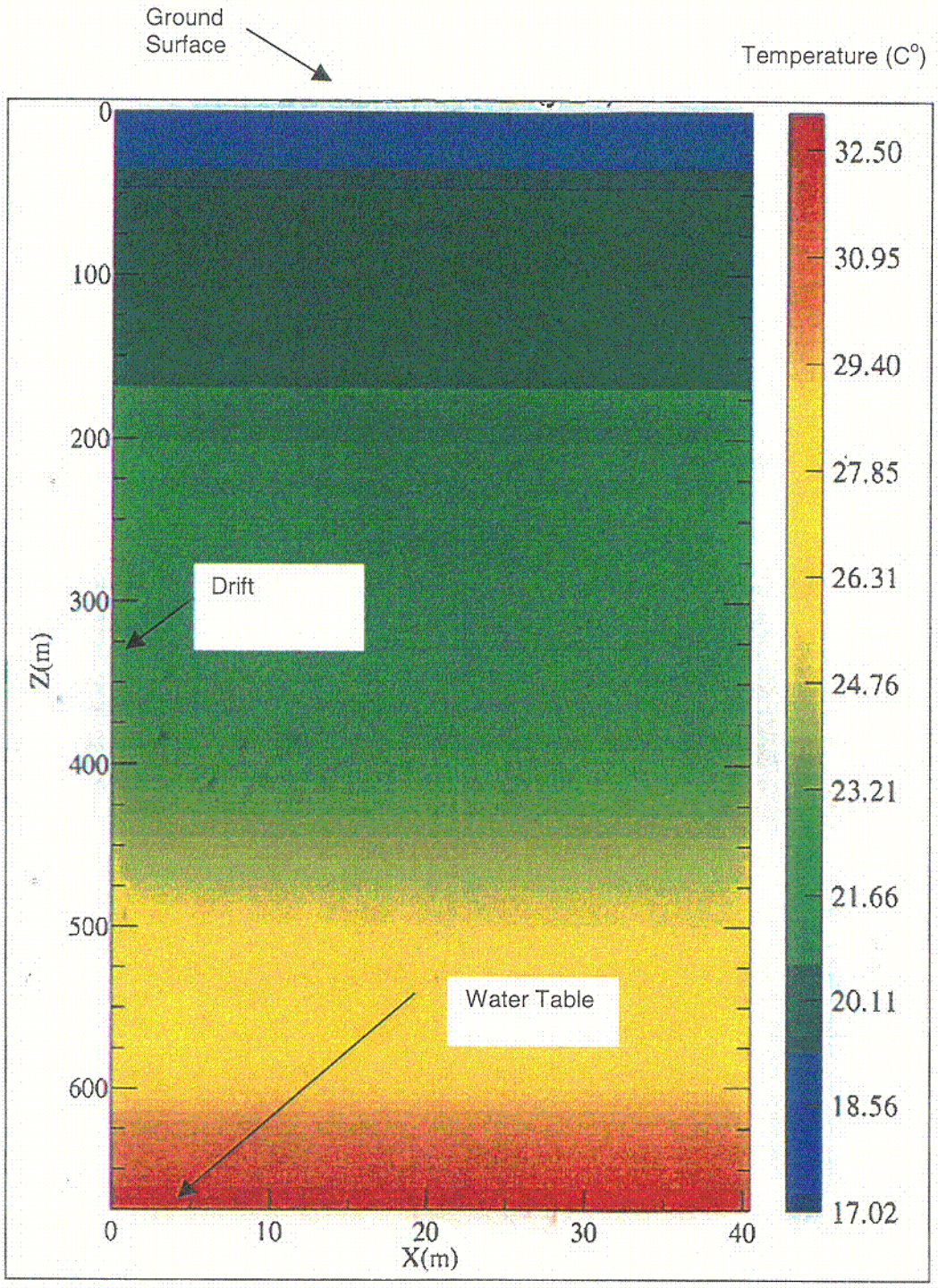

Figure 6. Initial Temperature Contours for the Two-Dimensional T-H Model with a Drip Shield After 100 years at an Infiltration Rate of 35 mm per year

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6. ANALYSIS/MODEL

The purpose of the In-Drift Thermal-Hydrological-Chemical (T-H-C) Analysis is to analyze T-H-C processes in the EBS emplacement drift and provide data to support the EBS post-closure performance assessment. Input to this model will include the unsaturated hydrologic and thermal properties of the EBS component materials and of the geologic formation around the drift. The analysis will include an evaluation of the chemical alteration of individual components, and how such alteration could change the thermal-hydrologic performance. The potential for evaporation and condensation under the drip shield will be assessed.

The output of the analysis will be a documented method for evaluating the EBS performance under the T-H-C environments that are expected to prevail in the selected License Application Design Selection (LADS) design for the potential repository. The analysis will provide input to two Engineered Barrier System (EBS) process models: the Physical and Chemical Environment Model, and the Water Distribution and Removal Model.

6.1 USE OF THE NUFT CODE TO SIMULATE NATURAL CONVECTION IN AIR SPACE

As stated in Section 3, the NUFT code was developed for simulating flow and heat transport in porous and fractured media. Using it to model fluid flow in the air space of the drifts poses a major challenge.

To justify the use of NUFT to simulate free convection in the air space, a calculation has been performed in Attachment IV to demonstrate that, by adjusting the permeability and thermal conductivity of the drift air, it would be possible to match the results of NUFT with an analytical solution to a heat transfer problem in concentric cylinders. The matching is based on average heat transfer and temperature prediction rather than a detailed mapping of the flow pattern. The adjusted permeability and thermal conductivity values for drift air are found to be 1.0E-8 m^2 and 0.0263 W/m-K, respectively, which will be used in all production runs in this report.

The validity of this approach is also described in Section 6.4 where comparison between experimental measurement from the quarter-scale test and model results is presented and discussed. The Quarter Scale Drip Shield Test (QSDST) is being conducted in accordance with the *Planning Guidance for EBS Test Number 3 – Drip Shield Test* (CRWMS, 1999e). As for the QSDST, a permeability of 1.0E-6 m^2 and a thermal conductivity of 0.0263 W/m-K were found to be appropriate for predicting the average temperature distribution. Selection of grid spacing is based on guidelines from NUFT-based modeling studies derived from the Multiscale Thermohydrologic Model AMR. A systematic grid refinement study will be performed and reported in a later revision of this AMR. To account for spatial variation of heat transfer in the air gap, thermal conductivity

and permeability of the pseudo-porous material would have to be selected to produce air convection pattern similar to that in the actual air gap. Furthermore, the values of these parameters would be appropriately selected to accommodate their variation with the temperature difference between the waste package and the drip shield as the thermal loading varies.

Calibration of parameters for the drift air properties for the QSDST as described above is based on the different thermal properties of the central heater, the drip shield, and the invert material rather than the base-case data when base-case data (Section 4.0) were not available. As a result, these assumed properties (listed in Attachment IV) were used in previous thermal analyses for predicting the temperatures of the test (Run # ymp2Ddst0 in Section 6.4). When the base-case data became available, an impact analysis was performed (Run # ymp2Ddst01 in Section 6.4) using these data. A comparison of the results from these two runs is presented in Section 6.4. No significant differences were found.

6.2 USE OF THE ECM APPROACH

An Equivalent Continuum Medium (ECM) model is constructed for NUFT analysis, using the stratigraphic units and their properties referenced in Section 4.1. However, the base-case hydrologic data (LB990861233129.002) display a strong anisotropy in permeability for the units around the drift, with fracture permeability dominating in the medium. The fractures have an almost vertical orientation (CRWMS, 1998b) which facilitates preferential downward flow rather than horizontal flow. The ECM model is used for the analysis of this AMR because ECM is the only model available in NUFT ver. 2.0, the version that was qualified at the time of this report.

6.3 THERMAL RADIATION

Before running NUFT, RADPRO is used to generate radiation coefficients for all production runs. The inputs to RADPRO consist of the relationship between all radiating and reflecting surfaces in the NUFT model and the emissivity of the radiating surface. Because of the assumption that the outer annulus is completely filled with backfill, the only area where radiation will be effective is in the air space underneath the drip shield. Input listings for these data are included in Attachment V.

6.4 ANALYSIS METHOD

A QSDST is simulated using NUFT and is described in Stage I below. The QSDST is set up in the Atlas Laboratory in Las Vegas, Nevada to mimic the performance of the EBS at the repository level with the exception that the test scale is ¼ of the actual repository dimensions. In addition, the space between the drip shield and the wall of the test cell is entirely filled with air without any porous backfill material. The temperature of a central heater is maintained at 80 degrees C. to simulate the temperature of the waste package while the temperature of the cell wall is maintained at 60 degrees C. by an outer heater system. RADPRO and NUFT are used to simulate thermal radiation and natural air

convection (using the pseudo-porous medium approximation) in both the inner (between the central heater and the drip shield) and outer (between the drip shield and the cell wall) air spaces.

In Stage II, five computer runs are made for the repository-scale model, using the material properties specified in Sections 4.1 and 4.2, hydrologic and thermal properties of the stratigraphic units are obtained from DTN: LB990861233129.002 and Input Tracking No. SSR-NEP-99261.T, respectively, and with the assumptions stated in Section 5. Boundary conditions are stated in Section 5.13 and initial conditions (pressure and saturation) are varied as follows.

6.4.1 Stage I

Analysis of thermal (T) effects only, without accounting for water evaporation and condensation in the drift. The purpose is to compare model temperature prediction with experimental results, using measurements from the EBS QSDST and the approach described in Section 6.1.

A comparison of the results from Runs # ymp2Ddst0 (using initial dataset) and ymp2Ddst01 (using final dataset), with measurements from the QSDST (Howard, 1999) and assuming the temperatures of the central and outer heaters are fixed at 80° C and 60° C, respectively, is presented in Table 2:

Table 2. Summary of Results for Sensitivity Study
(Temperatures in °C)

Location	Run#ymp2Ddst0	Run #ymp2Ddst01	QSDST
Central Heater	80	80	80
Outer Heater	60	60	60
Drip Shield	67.3 – 68.2	67.1 – 68.2	67.0 – 69.0
Invert Surface Material	63.1 – 66.8	65.5 – 66.7	66.0 – 67.8 [a]

a At junction of drip shield and invert material

The impact analysis shows there are no significant differences in the results of the runs, and model prediction matches reasonably well with the experimental measurements for the 60°-80° temperature range. Comparison between model results and measurements will be made for different temperature ranges in future revisions when experimental data are available. The overall heat flux and temperature distribution are dominated by radiant heat transfer with the exception that the heat transfer at the apex of the drip shield and the bottom of the waste package are likely to be also affected to a substantial degree by natural convective heat transfer.

The case with a drip shield shows a steeper thermal gradient between the central heater and the outer heater than the case without the drip shield because the drip shield tends to block the heat from spreading outwards.

Input listings for NUFT, RADPRO and the results from QSDST are included in Attachment IV.

6.4.2 Stage II

Analysis of In-Drift Thermal-Hydrologic (T-H) effects, including water phase changes, but excluding chemical effects.

Run #1 – ddymp2DdsR2 – Initialization Run using initial conditions in Section 5.13
Infiltration flux at ground surface = 35 mm/year
No drip shield
Simulated Duration: approximately 1.0 x 10^6 years

This run is designed to result in an ambient temperature and water distribution (steady-state shown in Figures 5 and 6) in the simulated profile, based on a maximum expected flux 35 mm/year.

Run #2 - ymp2Dds2R22 – Production Run using heat loading in Section 5.6, but skipping the first 50-year loading:
Infiltration flux at ground surface = 35 mm/year
Drip shield in-place.
Simulated Duration: approximately 100,000 years.
Initial conditions are the same as final conditions from Run #1

Run #3 - ymp2Dds2R23a – Production Run using heat loading in Section 5.6 but skipping the first 100-year loading:
Infiltration flux at ground surface = 35 mm/year
Drip shield in-place.
Simulated Duration: approximately 100,000 years.
Initial conditions are the same as final conditions from Run #1

To initiate Runs #2 and #3, RADPRO, the post-processsor of NUFT, is used to generate thermal radiation in the area below the drip shield as shown in Figure 7. Listing of input files "radymp," "radymp.con," and the output file "results99" is included in Attachment V.

Runs #2 and #3 will demonstrate whether a change in the duration of heating would cause any significant change in the results.

Run #4 – ddymp2DdsR2b – Initialization Run using initial conditions in Section 5.13
Infiltration flux at ground surface = 68 mm/year
Drip shield in-place
Simulated duration: approximately 1.0 x 10^6 years.
The 68 mm/year rate is the expected rate under long-term weather changes – almost twice the maximum rate expected in short term. This run serves as a sensitivity analysis.

Run #5 – ymp2Dds2R23b – Production Run using heat loading in Section 5.6, but skipping the first 100 years of thermal loading.

Infiltration flux at the ground surface = 68 mm /year
Drip shield in-place
Simulated duration: approximately 100,000 years
Initial conditions are the same as final conditions from Run # 4

Listing of input files for Runs 1 through 5 is included in Attachment VI. These runs do not allow for any near-field property changes during excavation for the drifts, as mentioned in Section 5.14. These issues are being considered in another AMR and will be reviewed in the next revision of this report.

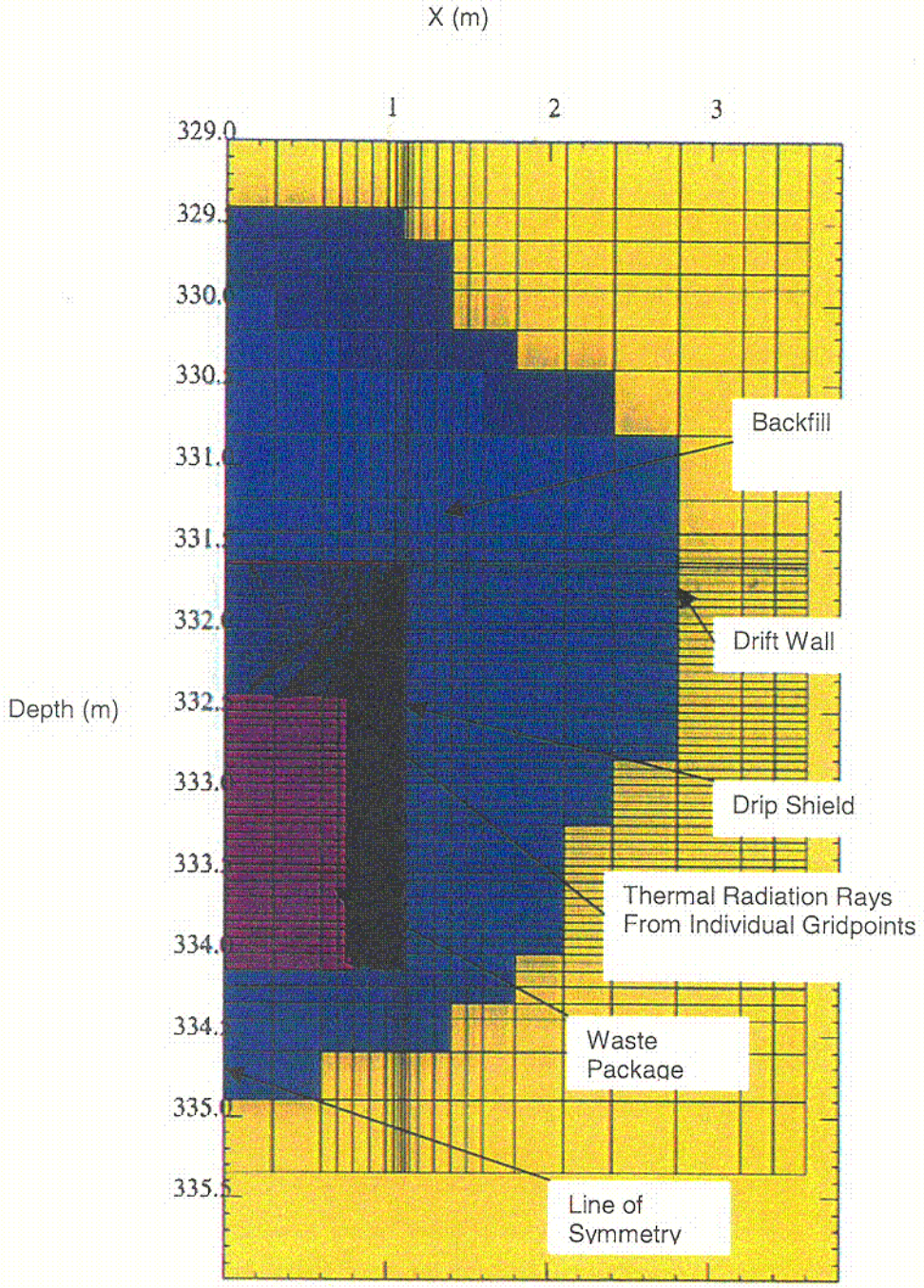

Figure 7. Detailed Grid Showing Thermal Radiation Underneath the Drip Shield

6.4.3 Stage III

Analysis of In-Drift T-H-C effects, including the deposition and dissolution of solid phases in the invert material within the drift.

Backfill/Invert materials may be altered from those of the as-placed materials by the hydrothermal regime imposed by the emplacement of waste in the repository, and changing the hydrologic properties in ways that would alter repository performance. While changes to thermal, mechanical, and sorptive properties may also be important, only hydrologic property changes are considered here. As mentioned in Section 1, the chemical effects are not addressed in this version of the AMR and will be assessed in later revisions.

6.5 RESULTS (Stage II In-Drift T-H Analysis)

1. Runs #2 and #3 show practically the same temperatures (within ½ degree C difference) on the waste package, the drip shield, and the invert material after approximately 3,000 years of simulation.
   Results from Runs #2 and #3 are presented in Attachment VII.

2. Temperature difference between the waste package, the drip shield, and invert material is less than 7 °C from 50/100 to 1,000 years, and is less than 2 °C beyond 1,000 years (Attachment VII).

3. Temperature on the surface of each component (waste package, drip shield, or invert material) varies only within 0.5 °C at any given time (Attachment VII).This will be verified in later revisions of this AMR with refined model calibration using temperature-dependent thermal conductivity and permeability for the air space beneath the drip shield, as described in Section 5.9.

4. Assuming the air space above the backfill is absent, water influx into the drift is confined mainly to the crown of the drift and is able to saturate the backfill only up to 1 percent during the first 10,000 years of cooling. From 10,000 to 15,000 years, saturation in the backfill starts to build up to 100 percent on the top surface of the drip shield. This saturated zone only has a thickness of about 0.1 m and a lateral extent of approximately 1 m. A series of plots of temperature and liquid saturation in the vicinity of the drift area are presented in Figures 8 through 11. Direction of water movement in the host rock around the drift is generally downward, as shown in Figure 12. Webb (1998) performed a pre-test analysis of the transient behavior of capillary barrier for similar types of material with an infiltration rate much higher than 35 mm/year and found that the underlying high-permeability layer was saturated only up to 5 percent. The computer runs show that because of the capillary barrier effect, most of the water flow is confined to the host rock and only an insignificant amount would infiltrate into the backfill. The effectiveness of the capillary barrier

between the hostrock and the backfill material would be reduced if fractures of significant width and low capillary suction potential are the primary pathways for water flow in the hostrock. The impact of such fractures will be assessed in a future revision of this AMR.

5. Water saturation on the flat top surface of the drip shield increases from about 0.1 at 6,000 years to about 0.6 at 15,000 years. This increase in water saturation may be the result of approximating the round surface of the drip shield by a flat surface. The effect of this approximation on saturation buildup on the top of the drip shield will be investigated in a later revision of this AMR.

6. Run # 5 (ymp2Dds2R23b) shows the same results as described above in item 3 for Run # 3 except the 60 to 80 percent saturation in the backfill immediately above the top of the drip shield occurs after 2,500 years rather than 10,000 years. This is due to a higher infiltration flux of 68 mm/yr.

7. Relative humidity in the air gap underneath the drip shield increases to about 90 percent during cooling, but never reached 100 percent for water vapor to condense. Plots of relative humidity over time at various locations beneath the drip shield are shown in Attachment VII.

8. Assuming that the waste package is in direct contact with the invert material as modeled, the invert material is predicted to be dry with temperatures slightly lower than the drip shield at all times. After 20,000 years and at the junction of the invert material with the backfill and host rock, there is an approximately 0.25m x 0.25m area in the invert material where saturation rises to 9 percent. As the amount of water influx into the invert material is predicted to be negligible, condensation is not expected to form underneath the drip shield. The impact of omitting the waste package support, placing the waste package in direct contact with the invert material and excluding natural convective heat transfer in part of the air gap will be assessed in later revisions of this AMR.

9. Radiation dominates the average heat transfer characteristics of the air gap between the waste package and the drip shield. However, at the apex of the drip shield and the bottom of the waste package, convective heat flux may become comparable to the radiant heat flux. In general, the dominance of radiant heat transfer offsets the errors due to the approximation made in modeling natural convective heat transfer in the air gap. Natural convection may be significant only in so far as it affects moisture transport within that air space.

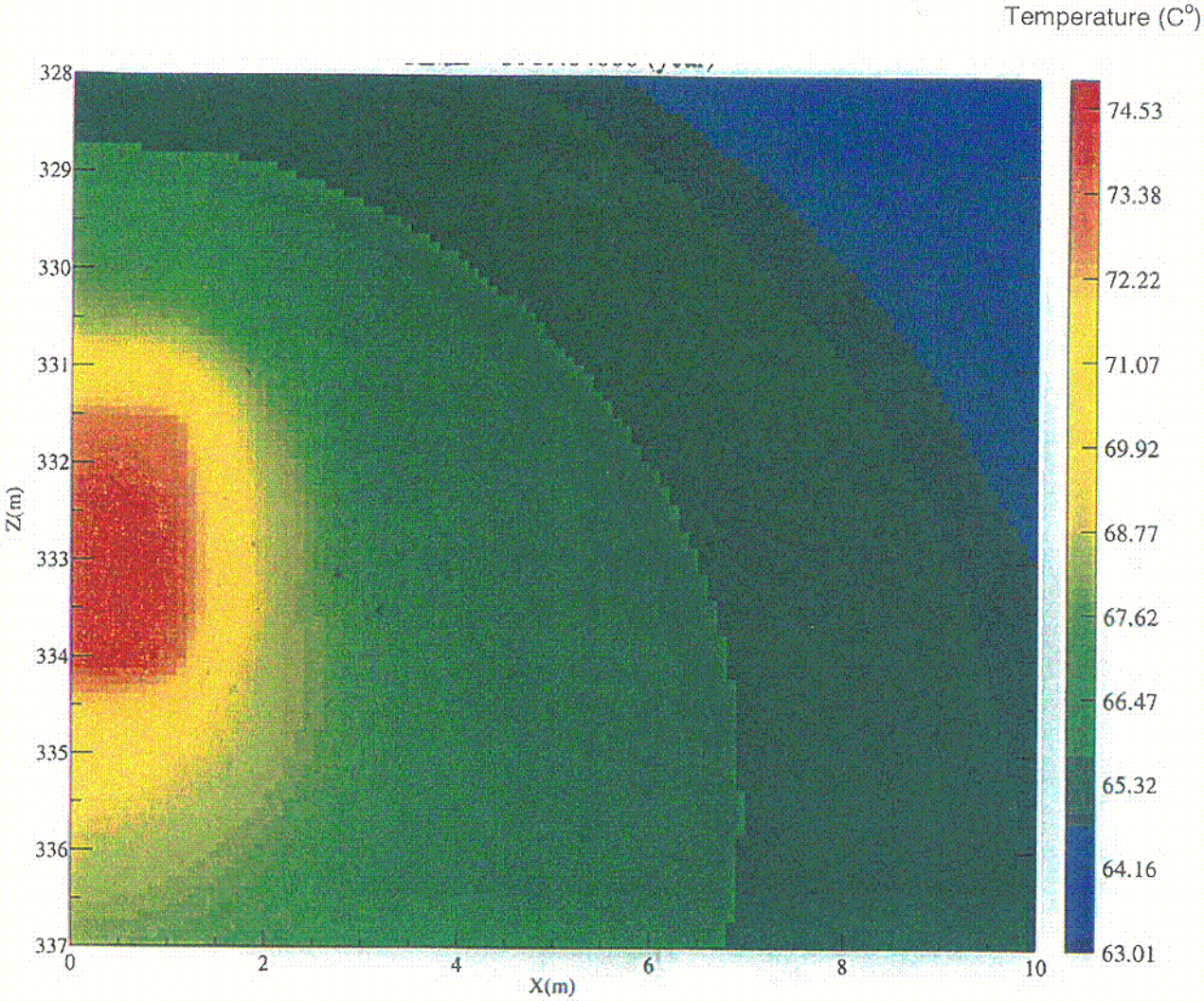

Figure 8. Temperature Contours for the Two-Dimensional T-H Model with a Drip Shield After 6,000 years at an Infiltration Rate of 35 mm per year

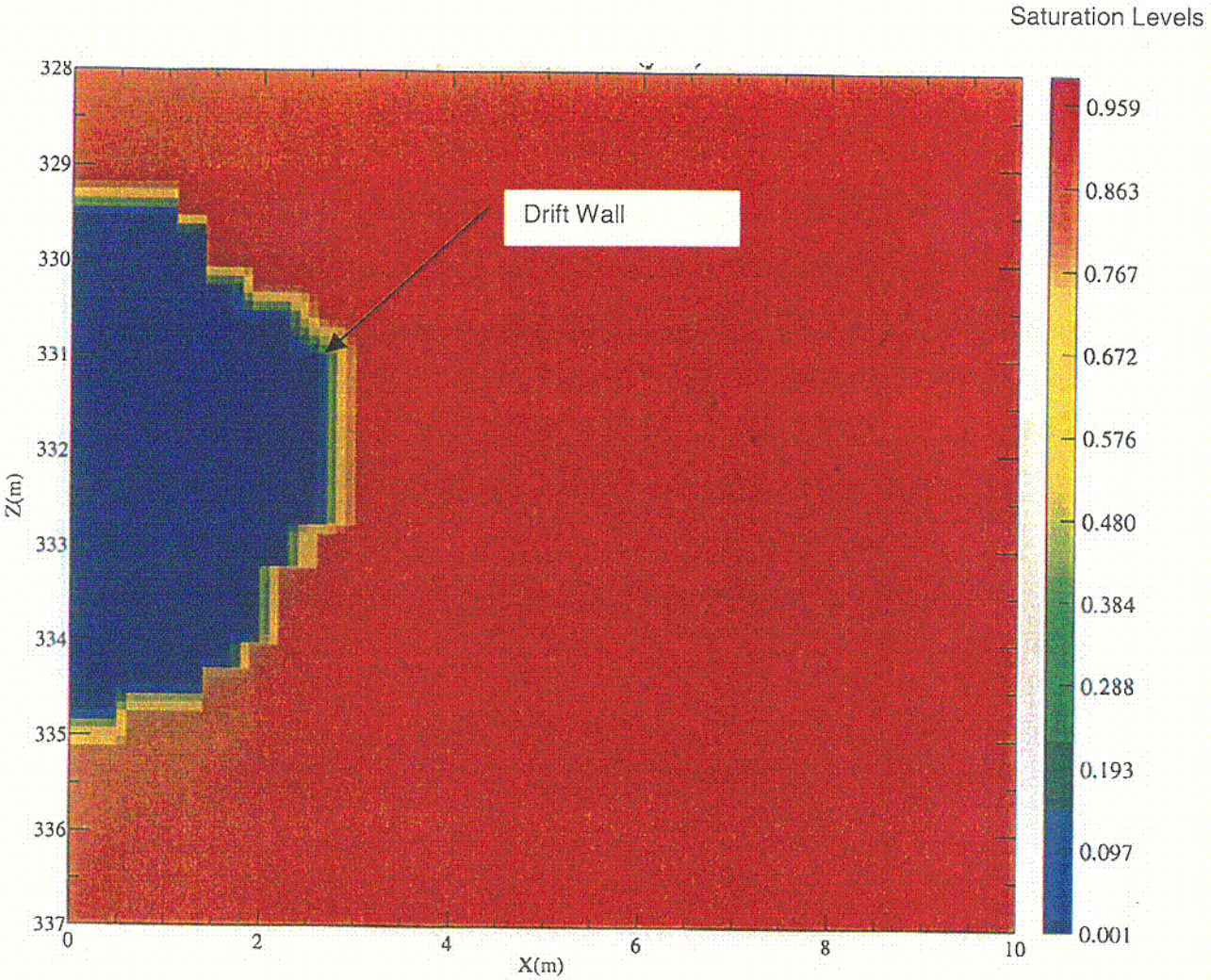

Figure 9. Saturation Contours for the Two-Dimensional T-H Model with a Drip Shield after 6,000 Years at an Infiltration Rate of 35 mm per year

C8

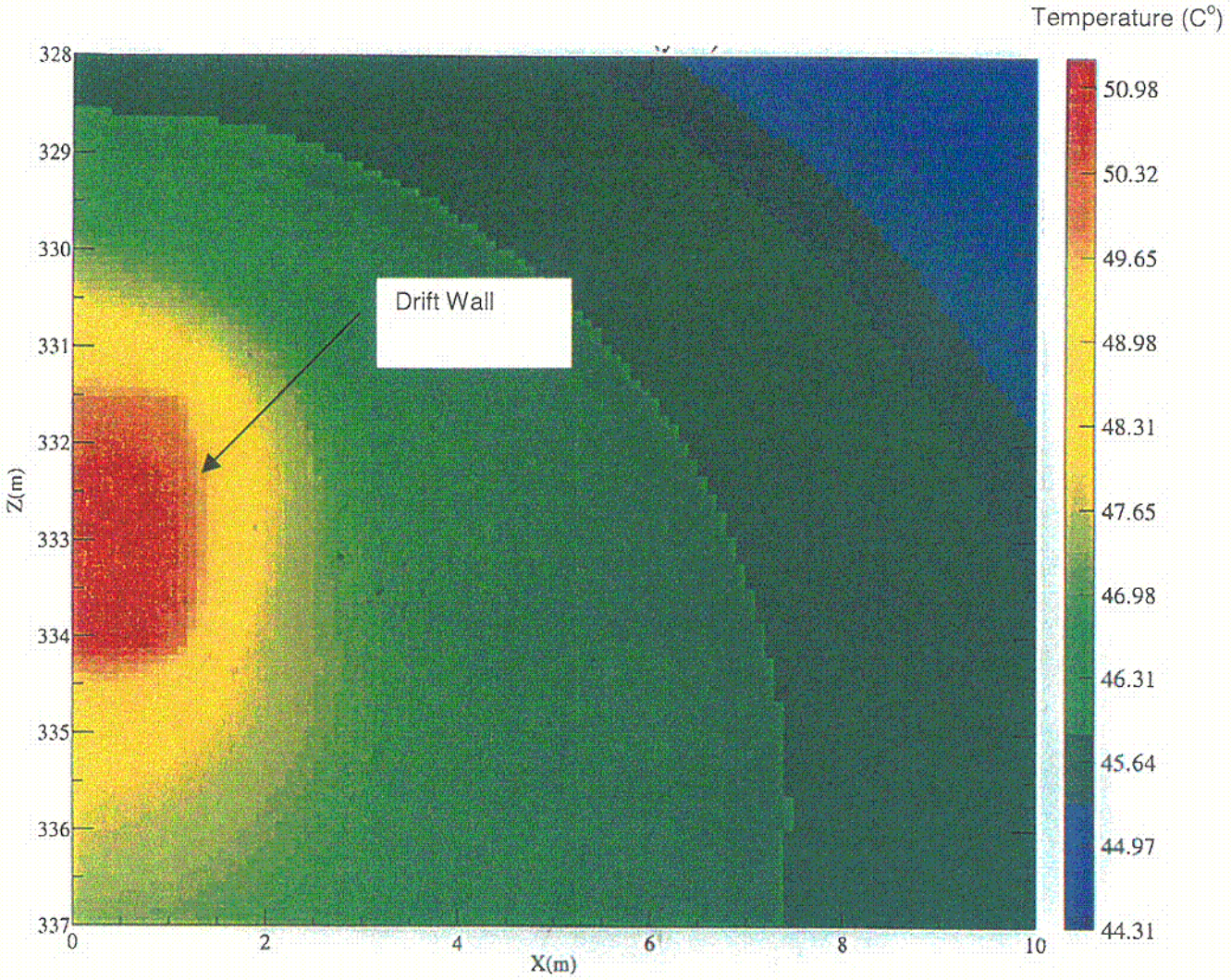

Figure 10. Temperature Contours for the Two-Dimensional T-H Model with a Drip Shield After 15,000 years at an Infiltration Rate of 35 mm per year

C9

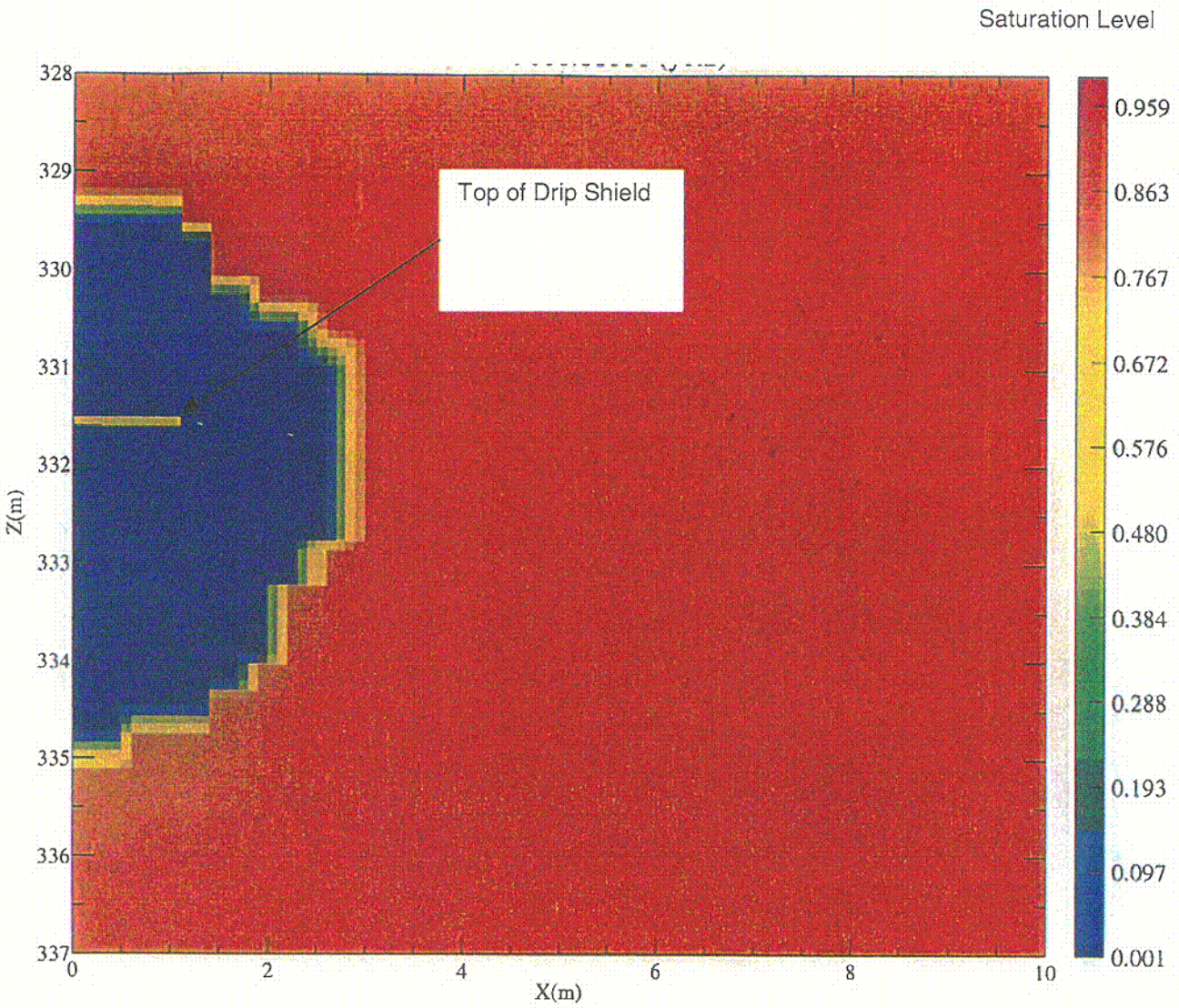

Figure 11. Saturation Contours for the Two-Dimensional T-H Model with a Drip Shield after 15,000 Years at an Infiltration Rate of 35 mm per year

C10

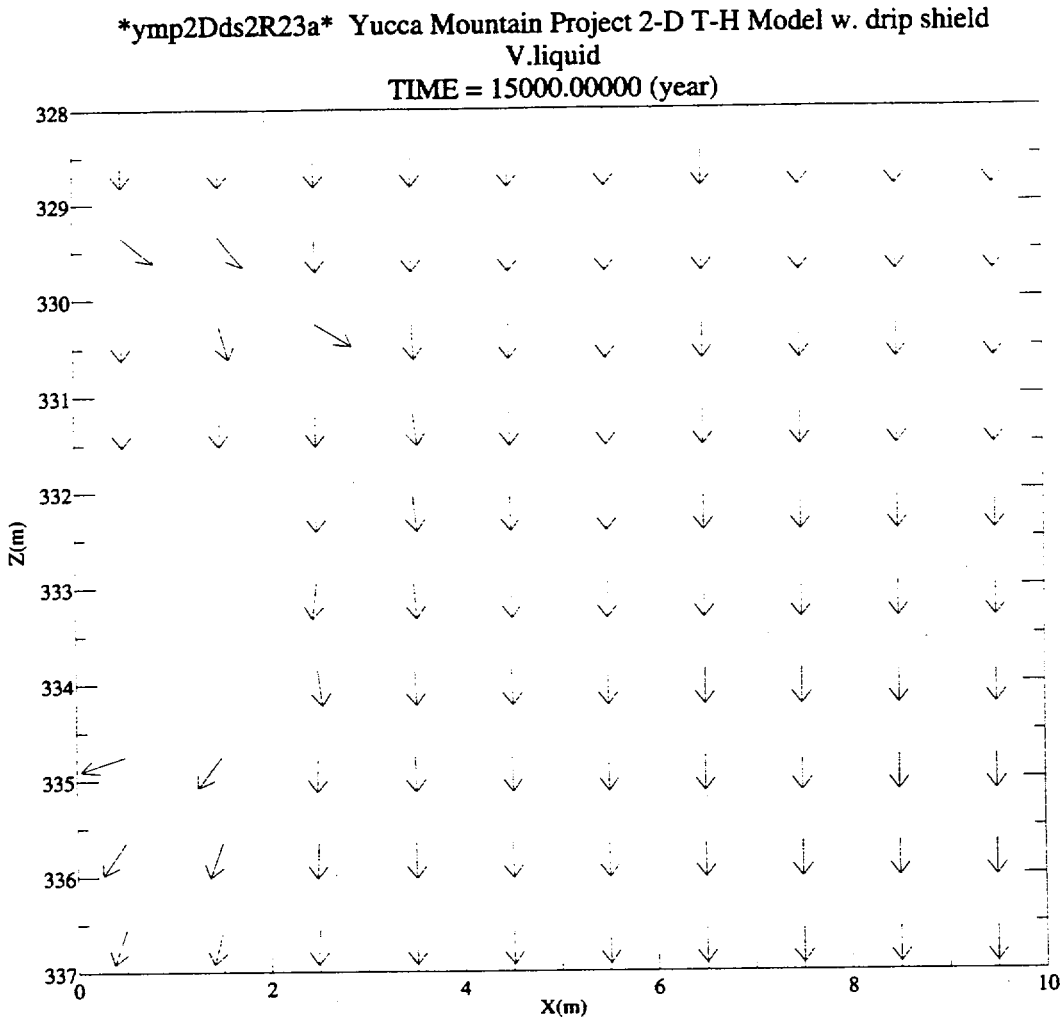

Figure 12. General Direction of Liquid Movement

7. CONCLUSIONS

1. Based on average heat transfer approximation in the air gap below the drip shield, condensation is not expected to form there during a period of 10,000 years and beyond, although there is a buildup of relative humidity to the 90 percent range. Later revision of this AMR will consider more detailed, non-uniform heat transfer in the air gap to confirm that the likelihood for condensation to form on the invert would be greater than that around the apex of the drip shield. Also, the impact of wide fractures on the effectiveness of the capillary barrier needs to be assessed (uncertainty).

2. Because of the rise in the relative humidity in the air gap underneath the drip shield during the cooling phase, the corrosion potential of the waste package and drip shield should be assessed (uncertainty).

3. There is a tendency for liquid saturation in the backfill to increase above the drip shield. Thus, leakage through the drip shield is possible if its structural integrity is in question. A failure mode analysis for the drip shield is recommended.

4. The impact of the TBVs on the conclusions are presented as follows:

   A. Fracture orientation (TBV-3492) is raised as a comment only.

   B. TBV-3497 and TBV-3498 are test description and development plan, respectively.

   C. TBV-3504 and TBV-3505 are user's and reference manuals, respectively, of NUFT Ver. 2.0.

   D. TBV-3506 is the software qualification plan for NUFT Ver. 2.0.

   E. TBV-3511 is used for illustration of the concept of a capillary barrier.

   F. The equations in TBV-3586 are well established in the earth science literature.

   G. The conclusions are not affected by using approximately twice the infiltration rate as specified in TBV-3311 and TBV-3312.

No data from the above items A through E were used in the analyses of this report and, therefore, the conclusions are not impacted. All other TBV inputs (configuration and properties of all EBS components, rock properties and stratigraphy) are unqualified and along with the unqualified software used, all results from this model are unqualified and cannot be used for procurement, fabrication, construction, or used in a verified design package without being tracked in accordance with applicable procedures. Any change in these unqualified data will require an impact analysis that may modify the conclusions of this report.

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8.4 CORRESPONDENCE

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ACRONYMS AND ABBREVIATIONS

ACRONYMS

AMR - Analysis/Model Report

CM - Configuration Management

CPU – Central Processing Unit

CRWMS M&O – Civilian Radiative Waste Management System, Maintenance & Operating Contractor

CSCI - Computer Software Configuration Item

DKM – Dual Permeability Model

DSDST – Quarter Scale Drip Shield Test

ECM – Equivalent Continuum Medium

EBS – Engineered Barrier System

EDA – Enhanced Design Alternative

LADS – License Application Design Selection

LLNL - Lawrence Livermore National Laboratory

MI - Medium Identifier

NUFT – Non-isothermal Unsaturated –saturated Flow and Transport

QSDST – Quarter Scale Drip Shield Test

TBV - To Be Verified

T-H – Thermal-Hydrological

T-H-C - Thermal-Hydrological-Chemical

ABBREVIATIONS

D_i = diameter of outer cylinder, m

D_0 = diameter of inner cylinder, m
K = permeability, m^2
k = thermal conductivity, W/m-K
L = $(D_o - D_i)/2.0$
n = Van Genuchten Beta parameter
Pr = Prandtl number
q' = heat transfer rate per unit length, W/m
Ra = Rayleigh number

Greek Letters

α = thermal diffusivity, m^2/s
α_v = Van Genuchten alpha parameter, 1/Pa
β = volumetric thermal expansion coefficient, K^{-1}
β_v = Van Genuchten Beta parameter
λ = Van Genuchten m (λ)
ϕ = porosity
ν = kinematic viscosity, m^2/s

Subscripts

b = bulk (equivalent medium)
b,f = fracture bulk
b,m = matrix bulk
c = cross-sectional
eff = effective
f = fracture (intrinsic)
L = based on characteristic length
m = matrix (intrinsic)

Superscripts

* = dimensionless quantity

ATTACHMENT I

DOCUMENT INPUT REFERENCE SHEETS

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
DOCUMENT INPUT REFERENCE SYSTEM

1. Document Identifier No./Rev.:	Change:	Title:
ANL-EBS-MD-000026 Rev. 00	ICN N/A	IN-DRIFT THERMAL-HYDROLOGICAL-CHEMICAL MODEL

Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBVDue To		
2a.	2. Technical Product Input Source Title and Identifier(s) with Version	3. Section					Unqual.	From Uncontrolled Source	Un-Confirmed
1	Daveler, S.; Nitao, J.; and Buscheck, T. 1998. *Radpro User's Guide.* Livermore, California: Lawrence Livermore National Laboratory. TIC: 245488.	Entire	TBV-3501	3	USED TO GENERATE THERMAL RADIATION	1	X	N/A	X
2	Lawrence Livermore National Laboratory 1998. *Xtool User's Guide.* Livermore, California: Lawrence Livermore National Laboratory. TIC: 245489.	Entire	TBV-3503	3	USED FOR GRAPHICAL PLOTS	1	X	N/A	X
3	CRWMS M&O 1997. *Determination of Available Volume for Repository Siting.* BCA000000-01717-0200-00007 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19971009.0699.	p. 67	TBV-3490	4.1	DEPTH TO GROUND WATER TABLE FROM DRIFT INVERT	1	X	N/A	X
4	CRWMS M&O 1998. *Repository Ground Support Analysis for Viability Assessment.* BCAA00000-01717-0200-00004 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980512.0714.	p. 19	TBV-3491	4.1	GROUND SURFACE ELEVATION OF REPOSITORY CENTER POINT	1	X	N/A	X
5	CRWMS M&O 1998. *Cross Drift Geotechnical Predictive Report: Geotechnical Baseline Report.* BABEA0000-01717-5705-00002 REV 1. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980806.0219.	p. 4-10, 4-11	TBV-3492	6.2	FRACTURE ORIENTATING	1	X	N/A	X
	Wilkins, D.R. and Heath, C.A.	Entire	N/A - Reference Only	4.1, 5.2	Drift	1	N/A	N/A	N/A

I-2

6	1999. "Direction to Transition to Enhanced Design Alternative II." Letter from Dr. D.R. Wilkins and C.A. Heath (CRWMS M&O) to Distribution, June 15, 1999, LV.NS.JLY.06/99-026, with enclosures, "Strategy for Baselining EDA II Requirements" and "Guidelines for Implementation of EDA II." ACC: MOL.19990622.0126; MOL.19990622.0127; MOL.19990622.0128.				Spacing,dimensions of drift, drip shield and other EBS components.				
8	CRWMS M&O 1999. *Waste Package Emplacement Supports and Drip Shields.* Design Input Transmittal EBS-SSR-99211.T. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990628.0132.	p. 1	TBV-3494	5.2	EDA II DESIGN-EBS COMPONENTS CONFIGURATION AND LAYOUT	1	X	N/A	X
9	CRWMS M&O 1999. *Thermal Modeling Parameters by Stratigraphic Unit.* Input Transmittal SSR-NEP-99261.T. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990910.0090; MOL.19990920.0109.	p. 1	TBV-3495	4.1	THICKNESS OF STRATIGRAPHIC UNIT	1	X	N/A	X
10	CRWMS M&O 1999. *Thermal Calculation of the Waste Package with Backfill.* BB0000000-01717-0210-00001 Rev 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981214.0073.	p. 10	TBV-3496	4.1.1	EMISSIVITY OF WASTE PACKAGE	1	X	N/A	X
12	CRWMS M&O 1999. *Development Plan for In-Drift Thermal-Hydrological-Chemical Model.* TDP-EBS-MD-000011 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991005.0213.	Entire	TBV-3498	1.0	DEVELOPMENT PLAN-SCOPE OF WORK	1	X	N/A	X
		p512,13,14;828,29,39	TBV-3585	Att	THERMAL	1	X	N/A	N/A

15	Incropera, F.P. and Dewitt, D.P. 1996. *Fundamentals of Heat and Mass Transfer.* 4th Edition. New York, New York: John Wiley & Sons. TIC: 243950.			IV,4.1.2,4.1.4	PROPERTIES OF DRIFT AIR, WASTE PACKAGE, AND DRIP SHIELD; EQUATIONS OF FREE CONVECTION FOR CONCENTRIC CYLINDERS				
16	LB990861233129.002. Drift Scale Calibrated 1-D Property Set, FY99. Submittal date: 08/06/1999.	Entire	TBV-3502	4.1	Hydrostratigraphic properties; Calibrated Fracture and Matrix Property sets	1	X	N/A	X
17	Nitao, J.J. 1988. *Numerical Modeling of the Thermal and Hydrological Environment Around a Nuclear Waste Package Using the Equivalent Continuum Approximation: Horizontal Emplacement.* UCID-21444. Livermore, California: Lawrence Livermore National Laboratory. ACC: NNA.19890317.0021.	p. 11, 14	TBV-3586	4.1	EQUATIONS RELATING POROSITY, PERMEABILITY, ALPHA, AND BETA PARAMETERS	1	X	N/A	N/A
18	Nitao, J.J. 1998. *Reference Manual for the NUFT Flow and Transport Code, Version 2.0.* UCRL-MA-130651. Livermore, California: Lawrence Livermore National Laboratory. TIC: 238072.	Entire	TBV-3504	3	USED FOR RUNNING NUFT CODE	1	X	N/A	X
19	Nitao, J.J. 1998. *User's Manual for the USNT Module of the NUFT Code, Version 2.0 (NP-Phase, NC-Component, Thermal).* Livermore, California: Lawrence Livermore National Laboratory. TIC: 238071.		TBV-3505	3	USED FOR RUNNING NUFT CODE	1	X	N/A	X
		Appendix C	N/A - Accepted Data (Fact)	3	Theory and associated equations.	1	X	N/A	X
20	Shaffer, R. 1998. *Individual Software Plan for the Qualification of NUFT, Version 2.0s.* ISP-NF-13, Rev. 2. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19981104.0140.	Entire	TBV-3506	Attachment III	SOFTWARE QUALIFICATION FOR NUFT	1	X	N/A	X

21	MO9812MWD1NUFT.000. The Niche Pattern Modified Waste Emplacement Alternative Design. Submittal date: 12/11/1998.	p. 11	TBV-3507	5.1; 5.4	HYDROLOGIC PROPERTIES OF WASTE PACKAGE; HYDROLOGIC AND THERMAL PROPERTIES OF ATMOSPHERIC AIR	1	X	N/A	X
22	Penman, H.L. 1940. "Gas and Vapor Movement in Soils I. The Diffusion of Vapours Through Porous Solids." *Journal of Agricultural Science, 30,* 437-462. Cambridge, England: The University Press. TIC: 236561.	p. 437 - 462	TBV-3508	5.11	TORTUOSITY FACTOR FOR ROCK AND SOILS	1	X	N/A	X
23	Ryder, E.E.; Finley, R.E.; George, J.T.; Ho, C.K.; Longenbaugh, R.S.; and Connolly, J.R. 1996. *Bench-Scale Experimental Determination of the Thermal Diffusivity of Crushed Tuff.* SAND94-2320. Albuquerque, New Mexico: Sandia National Laboratories. ACC: MOL.19961111.0011.	p. 5-3	TBV-3509	Attachment IV	THERMAL PROPERTIES OF INVERT MATERIAL	1	X	N/A	X
25	SN9908T0872799.004. Tabulated In-Drift Geometric and Thermal Properties used in Drift-Scale Models for TSPA-SR (Total System Performance Assessment-Site Recommendation). Submittal date: 08/30/1999.	p. 1 - 2	TBV-3471	4.1.3-4.1.5,	THERMAL PROPERTIES OF WASTE PACKAGE, DRIP SHIELD, AND SIMULATED DRIFT AIR	1	X	N/A	X
		Item 2: pg 1-16	TBV-3976	5.8, 5.10	THERMAL AND HYDROLOGIC PROPERTIES OF BACKFILL AND INVERT MATERIALS.	1	X	N/A	N/A
26	MO9901RIB00044.000. Reference Information Base Data Item - Hydrologic Characteristics: Unsaturated Zone Flow	Figure 3	TBV-3312	5.7	FRACTURE PERCOLATION FLUX AT REPOSITORY	1	X	N/A	X
		Figure 1	TBV-3311	5.7	MATRIX	1	X	N/A	X

	Characteristics. Submittal date: 01/06/1999.				PERCOLATION FLUX AT REPOSITORY				
27	Webb, S.W. 1998. *Preliminary Predictions of EBS Pilot-Scale Capillary Barrier Transient Behavior.* WA-0353. Albuquerque, New Mexico: Sandia National Laboratories. ACC: MOL.19991206.0225.	p. 5	TBV-3511	6.5	COMPARE SATURATION IN THE COARSE LAYER FOR CAPILLARY BARRIER PERFORMANCE	1	X	N/A	X
28	Howard, C. 1999. "60 Degree and 80 Degree Data - Water Turn-On Set for Tomorrow." E-mail from C. Howard to J. Kam, J. Case, S.W. Webb, R. Schreiner, and D. Chestnut (CRWMS M&O), September 13, 1999, with attachments. ACC: MOL.19991022.0536.	Entire	TBV-3587	6.4.1	Temperatures of drip shield, WP, and test cell	1	X	N/A	N/A
29	CRWMS M&O 1999. *Enhanced Design Alternative (EDA) II Repository Estimated Waste Package Types and Quantities.* Design Input Transmittal PA-WP-99184.Ta. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990809.0289.	Entire	TBV-3493	5.6	Thermal Loading of Waste Package	1	X	N/A	X
30	CRWMS M&O 1999. *Engineered Barrier System Performance Modeling (WP#12012383MX).* Activity Evaluation. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990719.0317.	Entire	N/A - Qualified/Confirmed/Controlled	2.0	Activity evaluation for quality assurance.	N/A	N/A	N/A	N/A
		7.1	TBV-0460	2.0	SYSTEM CLASSIFICATION - PREVIOUS TBV DESCRIPTION:THE QA CLASSIFICATION OF MGR SYSTEM, STRUCTURES AND COMPONENTS	1	X	N/A	N/A

32	CRWMS M&O 1999. *Classification of the MGR Ex-Container System.* ANL-XCS-SE-000001 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990928.0221.				(SSCS) ASSUMES THAT THE MGR DESIGN IS MODIFIED TO INCORPORATE THE DESIGN PROVIDED BY THE STRATEGY TO MITIGATE PRECLOSURE OFFSITE EXPOSURE (CRWMS M&O INTEROFFICE CORRESPONDENCE, C.R. HASTINGS TO DISTRIBUTION, LV.SEI.CRH.7/98-024, 1998), HEREAFTER REFERRED TO AS THE "SAFETY STRATEGY". TIS SAFETY STRATEGY PROPOSES GENERAL DESIGN GUIDANCE FOCUSED ON REDUCING THE RISKS ASSOCIATED WITH.....				
33	CRWMS M&O 1999. Planning Guidance for EBS Test Number 3 - Drip Shield Test Memo from J. Pye to Distribution. LV.EBSPM.JHP.05/99-005 ACC: MOL.19990518.0308.	Entire	N/A - Qualified/Confirmed/Controlled	6.1	Test configuration and description - Reference only	N/A	N/A	N/A	N/A

ATTACHMENT II

LETTER OF SOFTWARE CERTIFICATION FROM LLNL

Lawrence Livermore National Laboratory

LLYMP9809098
September 15, 1998

QA: N

TRW, Software Configuration Management
c/o Gregory Carlisle, SUM1/423
4460 South Arville Street, Building 1, Room 126G
Las Vegas, NV 89103

Subject: Shipment of Certified Software Package for NUFT 2.0s

Dear Greg:

This letter is to attest that NUFT 2.0s has been certified for quality affecting analyses on the YMP. The validation range of this certification is described in the enclosed documentation. This certification status is based upon the completion of all tests, reviews, and documents required by LLNL Quality Assurance Procedure 033-YMP-QP-3.2.4-2.

All of the required documentation are in the NUFT 2.0s Master File (LLNL Records Center reference number LLYMP9809098, and a copy is being shipped to Las Vegas for inclusion in the M&O Records System Facility and assignment of an ascension number. This work has been completed by LLNL and verified by on-site OQA Representatives

Therefore, pursuant to Repository Subsurface Design and WPO's requests for LLNL to transfer the referenced software (see M&O QAP-SI-3, Para. 5.10.1), and completion of the above requirements, I approve of the electronic transfer of the Certified NUFT 2.0s Software Package to these users. Upon receipt of your instructions, LLNL will transmit by e-mail the subject code and installation documentation.

Michael Fernandez

Michael W. Fernandez, (Acting)
Special Projects Technical Area Leader

II - 2

An Equal Opportunity Employer • University of California • P.O. Box 808 Livermore, California 94551-9900 • Telephone (510) 422-1100 • Twx 910-386-8339 UCLL LVMR
Yucca Mountain Project, P.O. Box 5514, L-217, Livermore, California 94551-9900 • Fax (510) 422-0540 or FTS 532-0540

MWF:

Attachment:
1) NUFT 2.0s Validation and Verification Document, Appendix 6

Enclosures:
1) NUFT 2.0s Requirements Document
2) NUFT 2.0s Release Notes, User's Manual, Reference Manual
3) NUFT 2.0s Verification and Validation Document

cc: w/o encl

James A. Blink	L-217
Thomas A. Buscheck	L-206
Gary L. Johnson	L-632
Edward J. Kansa	L-200
Wunan Lin	L-206
Cynthia B. Palmer	L-204
John F. Pelletier	L-204
Ron Shaffer	L-200
Dale G, Wilder	L-204
LLNL LRC (2)	L-217
Las Vegas, NV:	
Bryan Dunlap	M/S 423
Robert L. Howard	M/S 423
Jerry A, McNeish	M/S 423
James T. Kam	M/S 423
Thomas Doering	M/S 423

Appendix6

Task Report
Installation at Livermore

1. Name(s) of task participant(s)

Thomas Wolery

2. Date of task accomplishment

September 11, 1998

3. Name of task

Installation test on target platform in Livermore.

4. Identification of task in the V&V plan (i.e. heading reference)

Section 5.7.1, Item 2, done on target platform in Livermore.

5. Narrative description of any preconditions

1) A released installation package must be available
2) A target platform at the YMP site in Livermore must be available
3) An independent software engineer must be available in Livermore to perform and test the installation.

6. Narrative description of any important environmental influences

The test platform was a SUN Sparc Ultra1 with 128MB of memory running SUNOS 5.5.1and X-windows Version CDE102..

7. Narrative description of any other influences that affected task performance

None.

8. Narrative description of task

A copy of the NUFT installation package was obtained from email distribution (5 separate emails with enclosed attachments).

NUFT was installed using the following email instructions.

I. Receiving the NUFT Release Distribution

The NUFT Release Distribution is composed of the NUFT Executable Distribution
and files for installing the NUFT Executable Distribution on your platform.
You will receive the NUFT Release Distribution in four parts via four separate e-mails.
Each part contained within the e-mail is delineated by a line containing "Begin <part>"
and a line containing "End <part>" where <part> is the name of the part. After saving
each e-mail into a file, you should delete all lines preceding Begin <part>,
the Begin <part> line, the End <part> line, and all lines following the End <part> line.

The four e-mails are:

E-mail for the README part

The Subject field of this e-mail is: NUFT Release 2.0s README

This e-mail contains the NUFT Release Distribution README file.
The README file contains the instructions for installing the NUFT Distribution on your platform. It also contains a disposition of qualification test exceptions.

Save this e-mail as README.

E-mail for the INSTALL-SCRIPT part

The subject field of this e-mail is: NUFT Release 2.0s INSTALL-SCRIPT

This e-mail contains the NUFT Release Distribution INSTALL-SCRIPT file.
INSTALL-SCRIPT is the C-shell script you will use to install the NUFT Executable Distribution.

Save this e-mail as INSTALL-SCRIPT.

E-mail for the dist.uu part

The subject field of this e-mail is: NUFT Release 2.0s dist.uu

Note: My Eudora automatically undecoded this file.
-TJW
9/11/98

This e-mail contains the NUFT Executable Distribution dist.uu file.
dist.uu is a uuencoded file containing the NUFT Executable Distribution which contains the NUFT executable, ancillary files needed for NUFT execution, a sample input file, and user documentation files.

Save this e-mail as dist.uu

E-mail for the BOM-PROC part

The subject field of this e-mail is: NUFT Release 2.0s Bill-of-Materials

This e-mail contains a procedure for generating a bill-of-materials for the NUFT Release. The bill-of-materials lists the names and revision numbers of items used in the generation and qualification of NUFT Release 2.0s.

Save this e-mail as BOM-PROC.

II. Installing the NUFT Executable Distribution

After you have received all of the e-mails, follow the instructions in README to install NUFT.

III. Testing the NUFT Executable Distribution

The directory in which you installed the NUFT Executable Distribution contains

the NUFT input file instTEST.in and its associated output file instTEST.th.

1. cd to this directory.
2. Set the environment variable NUFTPATH to this directory.
3. Run the NUFT executable main with the input file:

   main instTEST.in

   main will produce an output file named instTEST.ex.

4. Compare instTEST.ex with instTEST.th:

   diff instTEST.ex instTEST.th

   The only difference should be in a line beginning with "$RunDate".

9. Narrative summary of task results (acceptable or not acceptable)

The installation instructions are acceptable and everything worked as predicted.

10. . Recommendations

~~None.~~ The BOM is confusing as there is nothing which says what the installer should do with it. In the absence of a problem, the answer would seem to be "nothing."

11. Author Signature

Thomas J. Wolery Date 9/11/98

ATTACHMENT III

SOFTWARE INSTALLATION

Based on the instructions provided by the LLNL to test the NUFT executable distribution, the installation test is performed as follows:

Run NUFT 2.0s with input file "instTEST.in" and compare output file "instTEST.ex" with the output file"instTEST.th" provided by the LLNL. They match each other and, therefore, installation test is completed successfully. Included in this attachment are listing of both input and output files.

X-Sender: kansa@s104.es.llnl.gov
Mime-Version: 1.0
Date: Mon, 21 Sep 1998 10:49:34 -0800
To: gansemer1@llnl.gov
From: Lynn Lewis 925 422-8949 <lewis@s139.es.llnl.gov> (by way of Lynn Lewis) (by way of Ed Kansa)
Subject: NUFT Release 2.0s BOM-PROC

----------Begin BOM-PROC----------

NUFT Release Bill-of-Materials Generation Procedure

Purpose

The objective of the NUFT Bill-of-Materials Generation Procedure is to generate a bill-of-materials for a distributed NUFT Release. The bill-of-materials lists the items used to construct and verify the NUFT Release.

Procedure Steps

Step 1.
Installation of the NUFT Release results in the creation of the directory ~/NUFT/version where version is the version identifier of the Release.

cd to this directory.

Step 2.
This directory contains the NUFT executable file main. Imbedded in main are specially formatted records containing bill-of-materials information for the Release. For each item used in the construction and qualification of the Release there is an imbedded record of the following format:

item_name version_no archive_date item_type

item_name: the file name of the item.
version_no: the version number of the item.
archive_date: the date on which the item was archived into the NUFT Release Repository.
item_type: the item's type (e.g., source file).

Run the what command on main to generate the bill-of-materials:

```
what main | grep NUFT
or,
what main | grep NUFT | awk '{printf ("$-20s %6s %s %s \n", $1, $2, $3, $4)}'
```

----------End BOM-PROC----------

III-4

X-Sender: kansa@s104.es.llnl.gov
Mime-Version: 1.0
Date: Mon, 21 Sep 1998 10:49:21 -0800
To: gansemer1@llnl.gov
From: Lynn Lewis 925 422-8949 <lewis@s139.es.llnl.gov> (by way of Lynn Lewis) (by way of Ed Kansa)
Subject: NUFT Release 2.0s INSTALL-SCRIPT

```
-----------------------------Begin INSTALL-SCRIPT-------------------------
#!/bin/csh -f -e
#
# SCCS_ID  @(#)INSTALL-SCRIPT   1.1 09/26/97 NUFT_SCRIPT_FILE
#

# for installing executable on unix workstation
# usage:  INSTALL-SCRIPT <tar-file>
#    or
#        INSTALL-SCRIPT <compressed-tar-file>
#
# note: assumes that the file VERSION in the tar file holds the version number
# if tar file is compressed, script will uncompress it
#

unalias rm

echo "Begin program for installing NUFT executable. "

# name of tar file
if($#argv != 1) then
        echo "wrong no. of arguments, usage: INSTALL-SCRIPT <tar-file>"
        echo "                        or:    INSTALL-SCRIPT
<compressed-tar-file>"
        exit 1
endif

set TARFILE = ${argv[1]}
if(! -e $TARFILE) then
        echo "missing input file : " $TARFILE
        exit 1
endif

if(${argv[1]:e} == Z) then
        if(-e $TARFILE) then
                echo "uncompressing tar file: " $TARFILE
                uncompress $TARFILE
                set TARFILE = ${argv[1]:r}
                if({$TARFILE:e} != tar) then
                        echo "bad input file : " ${argv[1]}
                        exit 1
                endif
        else
                echo "missing input file : " $TARFILE
                exit 1
        endif
else if(${argv[1]:e} != "tar") then
        echo "bad input file: " ${argv[1]}
endif

# extract version
```

```
if(! -d ~/NUFT) then
        if( -e ~/NUFT) then
                echo "cannot create NUFT directory because a file of that
name exists"
                exit 1
        endif
        echo "**creating directory ~/NUFT"
        mkdir ~/NUFT
endif

mv $TARFILE ~/NUFT
cd ~/NUFT
tar -xf $TARFILE Version
set VERSION = `cat Version`
rm Version

# set installation directory
set NUFTDIR = ~/NUFT/$VERSION

echo "**will install NUFT files into directory: " $NUFTDIR
#
if(! -e $NUFTDIR) then
        echo "**creating directory: " $NUFTDIR
        mkdir $NUFTDIR
endif

echo "**moving file " $TARFILE "to " $NUFTDIR
mv $TARFILE $NUFTDIR

cd $NUFTDIR
echo "**extracting files from " $TARFILE
tar -xf $TARFILE

# create execution shell file nuft-dist
echo "#\!/bin/csh -f" > nuft-dist
echo setenv NUFTPATH $NUFTDIR >> nuft-dist
echo '$NUFTPATH/main $argv' >> nuft-dist
echo 'exit $status' >> nuft-dist
chmod +x nuft-dist

# create execution shell file nuft-dist-ini
echo "#\!/bin/csh -f" > nuft-dist-ini
echo setenv NUFTPATH $NUFTDIR >> nuft-dist-ini
echo '$NUFTPATH/main -init on $argv' >> nuft-dist-ini
chmod +x nuft-dist-ini
echo 'exit $status' >> nuft-dist-ini

# symbolically link nuft-dist and nuft-dist-ini into ~/bin/nuft
if(! -e ~/bin) then
        mkdir ~/bin
endif
rm -f ~/bin/nuft  ~/bin/nuftini
echo "**linking " execution script ${NUFTDIR}/nuft-dist "to ~/bin/nuft"
ln -s $NUFTDIR/nuft-dist  ~/bin/nuft
ln -s $NUFTDIR/nuft-dist-ini  ~/bin/nuftini
sync
rehash
echo "****installation successful, just type nuft <input-file\> to run****"
echo "  (make sure ~/bin direction is part of your PATH variable"
echo "   usually set in your .login file)"
```

```
echo "Be sure to read addendum.doc in " ${NUFTDIR} " for updates to the
manual."
```

----------End INSTALL-SCRIPT----------

X-Sender: kansa@s104.es.llnl.gov
Mime-Version: 1.0
Date: Mon, 21 Sep 1998 10:48:52 -0800
To: gansemer1@llnl.gov
From: Lynn Lewis 925 422-8949 <lewis@s139.es.llnl.gov> (by way of Lynn Lewis) (by way of Ed Kansa)
Subject: NUFT Release 2.0s README

----------Begin README----------

```
#
# SCCS_ID  @(#)README   1.3 02/02/98 NUFT_PART
#
```

INSTRUCTIONS FOR INSTALLING NUFT
(executable and source code)
John J. Nitao
Lawrence Livermore National Laboratory
Livermore, CA 94551

INSTRUCTIONS FOR INSTALLING NUFT EXECUTABLE FROM AN EMAIL DISTRIBUTION

You will receive the NUFT executable distribution by email in uuencoded format. The following are instructions describe how to install the code.

1. Copy the contents of the email to a file in the home directory and type:

   uudecode file-name

   where file-name = name of the file.
   This will create a file of the form <version>.dist.tar.Z
   where <version> is the version no.

2. I will also be sending a file called INSTALL-SCRIPT. Copy the email to a file and call it INSTALL-SCRIPT. Be sure that there are no leading blank lines in the file. Type the following:

   csh -f INSTALL-SCRIPT <version>.dist.tar.Z

   where <version> is the version no. above.
   This will create a new subdirectory NUFT/<version> below your home directory. Note that installation of future versions will create new subdirectories. The installation will also create a subdirectory called bin below the home directory if there is not already one and will place a symbolically linked execution script called `nuft' there.

3. Look at the file addendum.doc there, which contains updates to the documentation.

4. The manual describes how to run NUFT.

INSTRUCTIONS FOR INSTALLING NUFT EXECUTABLE FROM A FILE DISTRIBUTION

1. The code is in a compressed tar file called <version>.dist.tar.Z where <version> is the version no. There will also be a file called INSTALL-SCRIPT. Copy the compressed tar file and the file INSTALL-SCRIPT to your home directory. Type the following:

```
csh -f INSTALL-SCRIPT <version>.dist.tar.Z
```

   where <version> is the version no. above. This will create a new subdirectory NUFT/<version> below your home directory. Note that installation of future versions will create new subdirectories. The installation will also create a subdirectory called bin below the home directory if there is not already one and will place a symbolically linked execution script called `nuft' there.

2. Look at the file addendum.doc there, which contains updates to the documentation.

3. The manual describes how to run NUFT.

Please save these instructions in case of future updates.

==========

Disposition of qualification test exceptions

NUFT Test Anomaly - case:vsam5:

The following extraction sets are out of tolerance with respect to standards established for the subject test.

diff:6.173 % ex set #: 1, time: 1.3216e+06, pt #: 4, value(expected, actual): (3.6807e-01, 4.2224e-01)

diff:5.591 % ex set #: 1, time: 1.3216e+06, pt #: 5, value(expected, actual): (3.7922e-01, 4.2828e-01)

diff:8.139 % ex set #: 1, time: 649290, pt #: 9, value(expected, actual): (7.3331e-01, 8.0473e-01)

diff:6.405 % ex set #: 1, time: 649290, pt #: 10, value(expected, actual): (7.4834e-01, 8.0454e-01)

diff:5.263 % ex set #: 2, time: 3.0305e+06, pt #: 3, value(expected, actual): (2.8774e+05, 3.0048e+05)

diff:5.469 % ex set #: 2, time: 3.0305e+06, pt #: 7, value(expected, actual): (2.8980e+05, 3.0293e+05)

diff:7.710 % ex set #: 2, time: 3.0305e+06, pt #: 10, value(expected, actual): (2.0861e+05, 1.8987e+05)

NUFT Test Anomaly - case:vsam6:

The following extraction sets are out of tolerance with respect to standards established for the

subject test.

```
diff:10.395 % ex set #:  1, time:  1.2545e+07, pt #:  85,
value(expected, actual):  (  1.5059e-01,   4.7679e-02)

diff:15.058 % ex set #:  1, time:  1.9104e+07, pt #:  85,
value(expected, actual):  (  1.4907e-01,   0.0000e+00)

diff:11.725 % ex set #:  1, time:  3.091e+07, pt #:  85,
value(expected, actual):  (  1.1608e-01,   0.0000e+00)

diff:6.061 % ex set #:  1, time:  5.1745e+07, pt #:  85,
value(expected, actual):  (  6.0001e-02,   0.0000e+00)
```

Code comparisons between NUFT and VTOUGH yielded excellent agreement between the two codes over a wide range of physical problems. An automated screening tool was used to compare output of the two codes on a variety of test problems.

Comparison was based on three separate criteria. With the first criterion, the percent difference in value of the dependent variable was computed for all nodes at various times. With the second criterion, the difference in each variable was normalized by the range of the variable attained in the test problem. With the third criterion, the normalized offset distance between time histories generated by the two codes was calculated for each node. A deviance that exceeded 5% on all three criteria signalled the need for closer scrutiny.

Out of the thousands of test points there were two test problems vsam5 and vsa6 that had deviances not satisfying the criterion over a small percentage of the domain. The deviances were small, less than 8.2% for vsam5, and 15% for vsam6.

These deviances arise at those points not because the two codes are giving significantly different results, but because the points are located at the foot of a sharp front in space, whose location is very sensitive to small numerical perturbations. Such a front is seen in the attached postscript file, vsam6.profile.ps, which shows a comparison of liquid saturation profiles from NUFT and VTOUGH, generated in vsam6. A small change in location of the front can yield large differences in solution variables at the given point in space.

Therefore, the tests between NUFT and VTOUGH were deemed to show good agreement between the two codes over the problems tested.

---------- END OF README.DOC ----------

----------End README----------

X-Sender: kansa@s104.es.llnl.gov
Mime-Version: 1.0
Date: Mon, 21 Sep 1998 10:49:08 -0800
To: gansemer1@llnl.gov
From: Lynn Lewis 925 422-8949 <lewis@s139.es.llnl.gov> (by way of Lynn Lewis) (by way of Ed Kansa)
Subject: E-mail of NUFT Release 2.0s - Release Notes Revision 0

You will be receiving by e-mail the NUFT Release Distribution for Release 2.0s. Release 2.0s has been qualified for use on SUN platforms running SUNOS 5.5.1.

This e-mail describes how you will be receiving the distribution, how to install it on your platform, and how to test your installation. It also contains notes regarding Release 2.0s.

I. Receiving the NUFT Release Distribution

The NUFT Release Distribution is composed of the NUFT Executable Distribution and files for installing the NUFT Executable Distribution on your platform. You will receive the NUFT Release Distribution in four parts via four separate e-mails. Each part contained within the e-mail is delineated by a line containing
"Begin <part>" and a line containing "End <part>" where <part> is the name of the part.
After saving each e-mail into a file, you should delete all lines preceding Begin <part>,
the Begin <part> line, the End <part> line, and all lines following the End <part> line.

The four e-mails are:

E-mail for the README part

The Subject field of this e-mail is: NUFT Release 2.0s README

This e-mail contains the NUFT Release Distribution README file.
The README file contains the instructions for installing the NUFT Distribution on your platform. It also contains a disposition of qualification test exceptions.

Save this e-mail as README.

E-mail for the INSTALL-SCRIPT part

The subject field of this e-mail is: NUFT Release 2.0s INSTALL-SCRIPT

This e-mail contains the NUFT Release Distribution INSTALL-SCRIPT file.
INSTALL-SCRIPT is the C-shell script you will use to install the NUFT Executable Distribution.

Save this e-mail as INSTALL-SCRIPT.

E-mail for the dist.uu part

The subject field of this e-mail is: NUFT Release 2.0s dist.uu

This e-mail contains the NUFT Executable Distribution dist.uu file. dist.uu is a uuencoded file containing the NUFT Executable Distribution which contains the NUFT executable, ancillary files needed for NUFT execution, and installation test input and expected output files.

Save this e-mail as dist.uu

E-mail for the BOM-PROC part

The subject field of this e-mail is: NUFT Release 2.0s Bill-of-Materials

This e-mail contains a procedure for generating a bill-of-materials for the NUFT Release. The bill-of-materials lists the names and revision numbers of items used in the generation and qualification of NUFT Release 2.0s.

Save this e-mail as BOM-PROC.

II. Installing the NUFT Executable Distribution

After you have received all of the e-mails, follow the instructions in README to install NUFT.

III. Testing the NUFT Executable Distribution

The directory in which you installed the NUFT Executable Distribution contains the NUFT input file instTEST.in and its associated output file instTEST.th.

1. cd to this directory.
2. Set the environment variable NUFTPATH to this directory.
3. Run the NUFT executable main with the input file:

```
./main instTEST.in
```

   main will produce an output file named instTEST.ex.

4. Compare instTEST.ex with instTEST.th:

```
diff instTEST.ex instTEST.th
```

   The only difference should be in a line containing SCCS_ID and a line beginning with "$RunDate".

IV. NUFT Release 2.0s Notes

IV.A. User Documentation

The following user documents will be shipped separately:

Reference Manual for the NUFT Flow and Transport Code, Version 2.0.
UCRL-MA-130651

User's Manual for the USNT Module of the NUFT Code, Version 2.0.
UCRL-MA-130653

IV.B. NUFT Release 2.0s Bill-of-Materials

The following files are not listed in the Bill-of-Materials but are part of NUFT Release 2.0s:

bmrk018_0_2.0s.rst: revision 1.1
Restart file produced by the execution of the bmrk018_0 test problem.

tools_version_2.0s.doc: revision 1.1
Bill-of-Materials file for tools used to produce Release 2.0s.

The following files were updated for Release 2.0s but their revision numbers were not updated in the Bill-of-Materials:

instTEST.th: revision 1.4

The following files are listed in the Bill-of-Materials but are not part of this distribution:

ref.ps
us1.ps
usnt.ps

ref.ps and usnt.ps are user documentation files which are being shipped separately.

IV.C Limitations and Assumptions in the Use of NUFT Release 2.0s

---

The use of this code for quality affecting activities is contingent upon the receiving organization completing the installation test and returning the completed LLNL Software Installation and Checkout Form to the LLNL Software Configuration Management Coordinator.

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The use of NUFT on Yucca Mountain quality affecting analyses requires the use of appropriately qualified data.

NUFT user organizations are responsible for ensuring that the software is appropriately applied. This includes, for example controls to ensure:
1) appropriate distribution of NUFT within their organization,
2) that individual users are appropriately qualified and trained,
3) that NUFT is applied correctly to the intended problems, and
4) that results NUFT produces are properly interpreted.

Dependable results can only be achieved by skilled practitioners. For example, professional judgment is required to select the proper mesh and compatible boundary conditions to adequately simulate the physical phenomena being analyzed

at a particular geologic site. More generally, results depend upon initial values, boundary conditions, mesh selection, time step selection, accurate characterization of physical parameters, and choice of modeled phenomena, and only an expert can perform reasonability checks that determine if the numerical solution approximates reality. More than one individual may be required to prepare the NUFT input file.

NUFT is intended to be used by civil engineers, hydrologists, physicists and/or geologists with expertise in numerical solution of PDEs, who can be expected to intervene if the solutions produced are anomalous or unrealistic. At least one user should have a background in application of numerical methods to analyze non-isothermal groundwater flow. Such experts typically use a combination of test problems and successive inclusion of model phenomena to understand and gain confidence in solutions produced by PDE solvers. Significant erroneous variation in input values or input values out of range will produce erroneous calculational results that a competent user will recognize and remedy. The user is charged with inspecting the NUFT output file to ensure that the actual input parameter values used in the calculations agree with the user's expectations.

NUFT 2.0s demonstrates isothermal and nonisothermal, multi-phase fluid flow in one-, two- or three-dimensions in a cartesian coordinate system. It is capable of producing the full range of liquid saturations (S) from initially unsaturated (S=0) to fully saturated (S=1). Water mass fraction in the gas phase shall be modeled over the full range >from dry (0) to wet (1). The calculation of relative humidity is not valid when liquid saturation is exactly 1.

NUFT 2.0s is capable of analyzing the following phenomena:

flow (mass transport or infiltration) in unsaturated media

flow (mass transport) in saturated media

coupled mass and energy (heat) transport in geologic media by conduction, convection and diffusion with multiple gas and liquid fluid phases, including phase change

NUFT 2.0s is capable of analyzing these problems for the following different conceptual models of geologic media representative of the Yucca mountain site:

porous media

fractured media

fractured porous media

In intended applications:

all phenomena may be analyzed in one, two, or three dimensions.

NUFT normally will be applied to analyze time-varying transients. Some transient problems may approach a quasi-steady state or steady state solution.

To perform these calculations, NUFT incorporates thermophysical fluid properties for air, water vapor and water. Fluid properties are interpolated from equations that were derived from the ASME steam tables. The properties of air follow the ideal gas law. Fluid mixtures are represented by a scaled linear combination of the individual properties obtained from the ideal gas law and the steam tables.
Calculations can be performed over the range of temperature and pressure conditions anticipated in repository analyses (temperatures of 6 to 500 C, pressures of 2.67x103 to 1.03x107 Pa).

NUFT 2.0s uses two different formulations to compute mass fraction of water in the gas phase. The variable is X.water.gas for the first formulation, and Xd.water.gas for the second. The code is qualified only for the second formulation.

Table 1 summarizes NUFT functional capabilities certified in release 2.0s.

Table 1. Certified functional capabilities of release 2.0s

A. Flow processes

Pressure-driven gas flow

Pressure-driven liquid flow

Gravity effects

Capillary forces

Viscous forces

B. Constitutive relations

Vapor pressure lowering

Van Genuchten characteristic curve

Temperature dependent capillary pressure

C. Phase change/diffusion

Phase change

Phase (dis)appearance

Binary diffusion in gas

D. Heat transport

Conduction

Single phase convection

Two phase convection (including heat pipe)

E. Dimensionally

1-D

2-D

3-D

F. Other

Automatic timestepping

Restart capability

NUFT 2.0s executes the complete set of benchmark problems in approximately 10 min. when executed on a SUN SPARC workstation running in multi-user mode. Typical individual test problems executed in one or a few minutes. Execution time for practical problems is expected to be on the order of a few hours.

For benchmark test problems, NUFT satisfies at least one of the following criteria:

1) Parameter value is within 5% of the results for the same problem from

either VTOUGH or the analytical solution,
2) Parameter value is within 5% of a normalized distance to a standard time history curve, or
3) Parameter value is within 5% of a parameter variation from standardized data normalized to the parameter range.

NUFT 2.0s possesses additional functional capabilities that are not certified for quality affecting use in this release. These include:

a) A contaminate transport option and dual permeability (DKM) option which provides for separate permeabilities for fractures and matrix,
b) Non-cartesian co-ordinate system, and
c) Radiant heat transfer capability.

Please report any problems with the use of NUFT 2.0s to the LLNL Code Sponsor

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```
;; SCCS_ID  @(#)instTEST.in   1.1 01/27/98 NUFT_INPUT_FILE


(usnt
  (title "*instTEST* CODE DEMONSTRATION: PHASE TRANSITIONS, COMPONENT
(DIS-)APPEARANCES      ")

     (title "instTEST" )
     (modelname nuft)
     (time 0.0 )
;;     (tstop  1.0e4)
     (tstop  2.0e3)
      (dt 10.)
;;     (dtmax 750.)
;;     (dtmin 100.)
     (stepmax 1000000 )

 ;;     (tolerdt  (P 1.e3)(S 0.05)(C 0.2)(T 10))
    (tolerdt  (P 6.e4)(S .2)(X 0.2)(T 5))
    (reltolerdt 0.0 0.0 0.0 0.0 0.0 0.0)

;;     (tolerconv (P 1.e3)(C 1.e-5)(S 0.005)(T 0.1))
     (tolerconv (P 1.e2)(X 1.e-5)(S 0.01)(T 0.01))
     (reltolerconv (P 0.005)(X 0.000)(S 0.000)(T 0.001))

;;     (tolerconv 1.e1 1.e-3 1.e-3 1.e-4 1.e-4 0.01)
;;     (reltolerconv 0.001 0.01 0.01 0.001 0.001 0.001)

     ;;; activate following line for preconditioned conjugate gradient
     ;;; method:
;;(linear-solver pcg)
(pcg-parameters  (precond comb) (north 10) (toler 1.e-4)  ;;JJN
                           (abstoler 1.e-5)
                           (itermax 30)(direct 1 0 1))

     (vapor-pressure-lowering off)

 ;; following comes before vtough.pkg so it will override
 ;; same as in vtough.pkg but with no temp. dep. capillary
 ;; pressure

     ;; phase properties
     (phaseprop
          (liquid
             (rhoP rhoPLiqWat)
             (viscosity visLiqWat)
             (enthP enthPLinearMix)
           (pcTemFac 1.0)   ;; no temp-dep factor
          )
          (gas
             (rhoP rhoPZFacStm)
             (viscosity visGasAirWat)
             (enthP enthPLinearMix)
          )
      ) ;; end phaseprop
```

```
;; adjust partitioning coeff for air to match vtough
;; change C from 6.65e9 to 1.0e10

  (compprop
          (water
                (intrinsic (MoleWt 18.))
                (gas
                        (Keq KeqWatVapor)
                  (freeDiffusivity binGasKinetic (power 1.8)(D0 2.13e-
5))
                        (enthC enthCWatVap))
                (liquid (freeDiffusivity 1.e-9) (Keq 1.0)
                        (enthC enthCLiqWat)
                        (rhoC rhoCLiqWat))
           )
          (air
                (intrinsic (MoleWt 29.))
                (gas (Keq KeqStd (C 1.0e10)(D 0.0))
                  (freeDiffusivity binGasKinetic (power 1.8)(D0 2.13e-
5))
                        (enthC enthCConstCp (Cp 1009.0)(Tref 0.0) (Hv
0.0)) )
                (liquid (freeDiffusivity 1.e-9)   (Keq 1.0) (enthC 0.0)
)
          )

     );;end component properties


  (include-pkg "vtough.pkg")

  (rocktab
    (TRANS
      (porosity 0.500) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.000e+03) (solid-density 2.650e+03)
      (tcond tcondLin (solid 2.100000)(liquid 2.100000)(gas 2.100000))
      (K0 1.000e-14) (K1 0.000e+00) (K2 0.000e+00)
      (tort (gas 0.000e+00) (liquid 0.0))
      (kr (gas krTable (table  ;; tabulate Corey's curve
            0.0  0.0
            .05  0.0
            .051 7.277e-9
            .052 5.817e-8
            .055 9.068e-7
            .058 3.706e-6
            .06  7.228e-6
            .08  1.921e-4
            .1   8.75e-4
            .15  6.723e-3
            .2   2.17e-2
            .25  .04930
            .3   9.19e-2
            .35  .1513
            .4   .228
```

```
          .45   .3227
          .5    .434
          .55   .5602
          .6    .699
          .625  .7721
          .64   .8169
          .65    .847
          .66    .8774
          .67    .9079
          .68    .9385
          .69    .9692
          .695   .9846
          .698   .9938
          .7     1.0
          1.0    1.0)
         )

        (liquid krTable (table   ;; tabulate Corey's curve
          0.0   0.0
          .3    0.0
          .325  2.188e-6
          .35   3.501e-5
          .375  1.773e-4
          .390  3.676e-4
          .4    5.60e-4
          .5    8.96e-3
          .6    4.54e-2
          .7    .143
          .8    .350
          .85   .513
          .9    .726
          .91   .776
          .92   .828
          .93   .882
          .94   .940
          .945  .9696
          .948  .9877
          .949  .9939
          .95   1.000
          1.0    1.0)
        )

    )
    (pc (liquid 0.0))
)

 (RCK7
    (porosity 0.500) (Kd (air 0.0)(water 0.0))
    (KdFactor (water 0.0) (air 0.0))
    (Cp 1.000e+03) (solid-density 2.650e+03)
    (tcond tcondLin (solid 0.0)(liquid 0.0)(gas 0.0))
    (K0 0.0) (K1 0.000e+00) (K2 0.000e+00)
    (tort (gas 0.000e+00) (liquid 0.0))
    (kr (gas 0.0) (liquid 0.0))
    (pc (liquid 0.0))
)
```

```
(SHOME
  (porosity 0.500) (Kd (air 0.0)(water 0.0))
  (KdFactor (water 0.0) (air 0.0))
  (Cp 1.000e+03) (solid-density 2.650e+03)
  (tcond tcondLin (solid 1.800000)(liquid 2.100000)(gas 1.800000))
  (K0 1.000e-14) (K1 0.000e+00) (K2 0.000e+00)
  (tort (gas 1.000e-01) (liquid 0.0))
  (kr (gas krTable (table
        0.0  0.0
        .1   0.0
0.101   0.1598E-07
0.102   0.1277E-06
0.103   0.4307E-06
0.104   0.1020E-05
0.105   0.1990E-05
0.106   0.3435E-05
0.107   0.5450E-05
0.108   0.8127E-05
0.109   0.1156E-04
0.110   0.1584E-04
0.112   0.2732E-04
0.114   0.4329E-04
0.116   0.6449E-04
0.118   0.9163E-04
0.120   0.1254E-03
0.122   0.1666E-03
0.124   0.2159E-03
0.126   0.2739E-03
0.128   0.3414E-03
0.130   0.4190E-03
0.132   0.5075E-03
0.134   0.6075E-03
0.136   0.7196E-03
0.138   0.8446E-03
0.140   0.9830E-03
0.142   0.1136E-02
0.144   0.1303E-02
0.146   0.1486E-02
0.148   0.1685E-02
0.150   0.1900E-02
0.152   0.2133E-02
0.154   0.2383E-02
0.156   0.2653E-02
0.158   0.2941E-02
0.160   0.3249E-02
0.162   0.3577E-02
0.164   0.3926E-02
0.166   0.4296E-02
0.168   0.4689E-02
0.170   0.5104E-02
0.172   0.5542E-02
0.174   0.6004E-02
0.176   0.6490E-02
0.178   0.7001E-02
```

0.180	0.7537E-02
0.182	0.8099E-02
0.184	0.8687E-02
0.186	0.9302E-02
0.188	0.9944E-02
0.190	0.1061E-01
0.192	0.1131E-01
0.194	0.1204E-01
0.196	0.1280E-01
0.198	0.1358E-01
0.200	0.1440E-01
0.202	0.1525E-01
0.204	0.1613E-01
0.206	0.1704E-01
0.208	0.1798E-01
0.210	0.1895E-01
0.212	0.1996E-01
0.214	0.2100E-01
0.216	0.2208E-01
0.218	0.2319E-01
0.220	0.2433E-01
0.222	0.2551E-01
0.224	0.2672E-01
0.226	0.2797E-01
0.228	0.2926E-01
0.230	0.3058E-01
0.232	0.3194E-01
0.234	0.3334E-01
0.236	0.3477E-01
0.238	0.3625E-01
0.240	0.3776E-01
0.242	0.3931E-01
0.244	0.4090E-01
0.246	0.4252E-01
0.248	0.4419E-01
0.250	0.4590E-01
0.252	0.4765E-01
0.254	0.4944E-01
0.256	0.5127E-01
0.258	0.5314E-01
0.260	0.5505E-01
0.262	0.5700E-01
0.264	0.5900E-01
0.266	0.6104E-01
0.268	0.6312E-01
0.270	0.6524E-01
0.272	0.6741E-01
0.274	0.6962E-01
0.276	0.7188E-01
0.278	0.7417E-01
0.280	0.7652E-01
0.282	0.7890E-01
0.284	0.8133E-01
0.286	0.8381E-01
0.288	0.8633E-01
0.290	0.8889E-01
0.292	0.9150E-01

0.294	0.9416E-01
0.296	0.9686E-01
0.298	0.9961E-01
0.300	0.1024E+00
0.302	0.1052E+00
0.304	0.1081E+00
0.306	0.1111E+00
0.308	0.1140E+00
0.310	0.1171E+00
0.312	0.1201E+00
0.314	0.1232E+00
0.316	0.1264E+00
0.318	0.1296E+00
0.320	0.1329E+00
0.322	0.1362E+00
0.324	0.1395E+00
0.326	0.1430E+00
0.328	0.1464E+00
0.330	0.1499E+00
0.332	0.1534E+00
0.334	0.1570E+00
0.336	0.1607E+00
0.338	0.1644E+00
0.340	0.1681E+00
0.342	0.1719E+00
0.344	0.1757E+00
0.346	0.1796E+00
0.348	0.1835E+00
0.350	0.1875E+00
0.352	0.1915E+00
0.354	0.1956E+00
0.356	0.1997E+00
0.358	0.2039E+00
0.360	0.2081E+00
0.362	0.2124E+00
0.364	0.2167E+00
0.366	0.2210E+00
0.368	0.2254E+00
0.370	0.2299E+00
0.372	0.2344E+00
0.374	0.2390E+00
0.376	0.2435E+00
0.378	0.2482E+00
0.380	0.2529E+00
0.382	0.2576E+00
0.384	0.2624E+00
0.386	0.2673E+00
0.388	0.2721E+00
0.390	0.2771E+00
0.392	0.2820E+00
0.394	0.2871E+00
0.396	0.2921E+00
0.398	0.2972E+00
0.400	0.3024E+00
0.402	0.3076E+00
0.404	0.3129E+00
0.406	0.3182E+00

0.408	0.3235E+00
0.410	0.3289E+00
0.412	0.3343E+00
0.414	0.3398E+00
0.416	0.3453E+00
0.418	0.3509E+00
0.420	0.3565E+00
0.422	0.3622E+00
0.424	0.3679E+00
0.426	0.3736E+00
0.428	0.3794E+00
0.430	0.3852E+00
0.432	0.3911E+00
0.434	0.3970E+00
0.436	0.4030E+00
0.438	0.4090E+00
0.440	0.4151E+00
0.442	0.4211E+00
0.444	0.4273E+00
0.446	0.4334E+00
0.448	0.4397E+00
0.450	0.4459E+00
0.452	0.4522E+00
0.454	0.4585E+00
0.456	0.4649E+00
0.458	0.4713E+00
0.460	0.4778E+00
0.462	0.4842E+00
0.464	0.4908E+00
0.466	0.4973E+00
0.468	0.5039E+00
0.470	0.5106E+00
0.472	0.5173E+00
0.474	0.5240E+00
0.476	0.5307E+00
0.478	0.5375E+00
0.480	0.5443E+00
0.482	0.5512E+00
0.484	0.5581E+00
0.486	0.5650E+00
0.488	0.5720E+00
0.490	0.5790E+00
0.492	0.5860E+00
0.494	0.5930E+00
0.496	0.6001E+00
0.498	0.6073E+00
0.500	0.6144E+00
0.502	0.6216E+00
0.504	0.6288E+00
0.506	0.6360E+00
0.508	0.6433E+00
0.510	0.6506E+00
0.512	0.6579E+00
0.514	0.6653E+00
0.516	0.6727E+00
0.518	0.6801E+00
0.520	0.6875E+00

```
0.522    0.6950E+00
0.524    0.7025E+00
0.526    0.7100E+00
0.528    0.7175E+00
0.530    0.7251E+00
0.532    0.7327E+00
0.534    0.7403E+00
0.536    0.7479E+00
0.538    0.7556E+00
0.540    0.7632E+00
0.542    0.7709E+00
0.544    0.7787E+00
0.546    0.7864E+00
0.548    0.7941E+00
0.550    0.8019E+00
0.552    0.8097E+00
0.554    0.8175E+00
0.556    0.8253E+00
0.558    0.8331E+00
0.560    0.8410E+00
0.562    0.8488E+00
0.564    0.8567E+00
0.566    0.8646E+00
0.568    0.8725E+00
0.570    0.8804E+00
0.572    0.8883E+00
0.574    0.8963E+00
0.576    0.9042E+00
0.578    0.9122E+00
0.580    0.9201E+00
0.582    0.9281E+00
0.584    0.9361E+00
0.586    0.9440E+00
0.588    0.9520E+00
0.590    0.9600E+00
0.592    0.9680E+00
0.594    0.9760E+00
0.596    0.9840E+00
0.598    0.9920E+00
 .599     .996
0.600    0.1000E+01
 1.0    1.0)
          )

          (liquid krTable (table
0.0        0.0
0.4        0.0
0.401    0.1600E-10
0.402    0.2560E-09
0.403    0.1296E-08
0.404    0.4096E-08
0.405    0.9999E-08
0.406    0.2073E-07
0.407    0.3841E-07
0.408    0.6553E-07
0.409    0.1050E-06
0.410    0.1600E-06
```

0.412	0.3318E-06
0.414	0.6147E-06
0.416	0.1049E-05
0.418	0.1680E-05
0.420	0.2560E-05
0.422	0.3748E-05
0.424	0.5309E-05
0.426	0.7312E-05
0.428	0.9835E-05
0.430	0.1296E-04
0.432	0.1678E-04
0.434	0.2138E-04
0.436	0.2688E-04
0.438	0.3336E-04
0.440	0.4096E-04
0.442	0.4979E-04
0.444	0.5997E-04
0.446	0.7164E-04
0.448	0.8494E-04
0.450	0.1000E-03
0.452	0.1170E-03
0.454	0.1361E-03
0.456	0.1574E-03
0.458	0.1811E-03
0.460	0.2074E-03
0.462	0.2364E-03
0.464	0.2684E-03
0.466	0.3036E-03
0.468	0.3421E-03
0.470	0.3842E-03
0.472	0.4300E-03
0.474	0.4798E-03
0.476	0.5338E-03
0.478	0.5923E-03
0.480	0.6554E-03
0.482	0.7234E-03
0.484	0.7966E-03
0.486	0.8752E-03
0.488	0.9595E-03
0.490	0.1050E-02
0.492	0.1146E-02
0.494	0.1249E-02
0.496	0.1359E-02
0.498	0.1476E-02
0.500	0.1600E-02
0.502	0.1732E-02
0.504	0.1872E-02
0.506	0.2020E-02
0.508	0.2177E-02
0.510	0.2343E-02
0.512	0.2518E-02
0.514	0.2702E-02
0.516	0.2897E-02
0.518	0.3102E-02
0.520	0.3318E-02
0.522	0.3545E-02
0.524	0.3783E-02

0.526	0.4033E-02
0.528	0.4295E-02
0.530	0.4570E-02
0.532	0.4858E-02
0.534	0.5159E-02
0.536	0.5474E-02
0.538	0.5803E-02
0.540	0.6147E-02
0.542	0.6505E-02
0.544	0.6880E-02
0.546	0.7270E-02
0.548	0.7677E-02
0.550	0.8100E-02
0.552	0.8541E-02
0.554	0.8999E-02
0.556	0.9476E-02
0.558	0.9971E-02
0.560	0.1049E-01
0.562	0.1102E-01
0.564	0.1157E-01
0.566	0.1215E-01
0.568	0.1275E-01
0.570	0.1336E-01
0.572	0.1400E-01
0.574	0.1467E-01
0.576	0.1535E-01
0.578	0.1606E-01
0.580	0.1680E-01
0.582	0.1756E-01
0.584	0.1834E-01
0.586	0.1915E-01
0.588	0.1999E-01
0.590	0.2085E-01
0.592	0.2174E-01
0.594	0.2266E-01
0.596	0.2361E-01
0.598	0.2459E-01
0.600	0.2560E-01
0.602	0.2664E-01
0.604	0.2771E-01
0.606	0.2881E-01
0.608	0.2995E-01
0.610	0.3112E-01
0.612	0.3232E-01
0.614	0.3356E-01
0.616	0.3483E-01
0.618	0.3614E-01
0.620	0.3748E-01
0.622	0.3886E-01
0.624	0.4028E-01
0.626	0.4174E-01
0.628	0.4324E-01
0.630	0.4477E-01
0.632	0.4635E-01
0.634	0.4797E-01
0.636	0.4963E-01
0.638	0.5134E-01

0.640	0.5308E-01
0.642	0.5487E-01
0.644	0.5671E-01
0.646	0.5859E-01
0.648	0.6052E-01
0.650	0.6250E-01
0.652	0.6452E-01
0.654	0.6660E-01
0.656	0.6872E-01
0.658	0.7089E-01
0.660	0.7311E-01
0.662	0.7539E-01
0.664	0.7772E-01
0.666	0.8010E-01
0.668	0.8254E-01
0.670	0.8503E-01
0.672	0.8758E-01
0.674	0.9018E-01
0.676	0.9284E-01
0.678	0.9556E-01
0.680	0.9834E-01
0.682	0.1012E+00
0.684	0.1041E+00
0.686	0.1070E+00
0.688	0.1101E+00
0.690	0.1132E+00
0.692	0.1163E+00
0.694	0.1195E+00
0.696	0.1228E+00
0.698	0.1262E+00
0.700	0.1296E+00
0.702	0.1331E+00
0.704	0.1366E+00
0.706	0.1403E+00
0.708	0.1440E+00
0.710	0.1478E+00
0.712	0.1516E+00
0.714	0.1555E+00
0.716	0.1595E+00
0.718	0.1636E+00
0.720	0.1678E+00
0.722	0.1720E+00
0.724	0.1763E+00
0.726	0.1807E+00
0.728	0.1852E+00
0.730	0.1897E+00
0.732	0.1944E+00
0.734	0.1991E+00
0.736	0.2039E+00
0.738	0.2088E+00
0.740	0.2138E+00
0.742	0.2189E+00
0.744	0.2240E+00
0.746	0.2293E+00
0.748	0.2347E+00
0.750	0.2401E+00
0.752	0.2456E+00

0.754	0.2513E+00
0.756	0.2570E+00
0.758	0.2628E+00
0.760	0.2687E+00
0.762	0.2748E+00
0.764	0.2809E+00
0.766	0.2871E+00
0.768	0.2934E+00
0.770	0.2999E+00
0.772	0.3064E+00
0.774	0.3130E+00
0.776	0.3198E+00
0.778	0.3266E+00
0.780	0.3336E+00
0.782	0.3407E+00
0.784	0.3479E+00
0.786	0.3552E+00
0.788	0.3626E+00
0.790	0.3701E+00
0.792	0.3778E+00
0.794	0.3856E+00
0.796	0.3934E+00
0.798	0.4015E+00
0.800	0.4096E+00
0.802	0.4178E+00
0.804	0.4262E+00
0.806	0.4347E+00
0.808	0.4434E+00
0.810	0.4521E+00
0.812	0.4610E+00
0.814	0.4700E+00
0.816	0.4792E+00
0.818	0.4884E+00
0.820	0.4979E+00
0.822	0.5074E+00
0.824	0.5171E+00
0.826	0.5269E+00
0.828	0.5369E+00
0.830	0.5470E+00
0.832	0.5572E+00
0.834	0.5676E+00
0.836	0.5782E+00
0.838	0.5888E+00
0.840	0.5997E+00
0.842	0.6107E+00
0.844	0.6218E+00
0.846	0.6331E+00
0.848	0.6445E+00
0.850	0.6561E+00
0.852	0.6678E+00
0.854	0.6797E+00
0.856	0.6918E+00
0.858	0.7040E+00
0.860	0.7164E+00
0.862	0.7289E+00
0.864	0.7416E+00
0.866	0.7545E+00

```
 0.868    0.7675E+00
 0.870    0.7807E+00
 0.872    0.7941E+00
 0.874    0.8076E+00
 0.876    0.8214E+00
 0.878    0.8352E+00
 0.880    0.8493E+00
 0.882    0.8636E+00
 0.884    0.8780E+00
 0.886    0.8926E+00
 0.888    0.9074E+00
 0.890    0.9223E+00
 0.892    0.9375E+00
 0.894    0.9528E+00
 0.896    0.9683E+00
 0.898    0.9841E+00
 0.900    0.1000E+01
 1.0      1.0
            )
      )
      )

      (pc (liquid pcTable (table 0.2 1.0e5  1.0  0.0)))
    )
  )  ;; end rocktab



     (output
        ;; outputs all results into extool file "instTEST.ex"
      (extool (variables S.liquid P T Xd.water.gas)
        (range "*")(file-ext ".ex")
      (outtimes 100.11        381.07        1138.1        1894.0
2000.0          )
      )
        (forcetimes (outtimes 100.11        381.07        1138.1
1894.0        2000.0         ))

       );; end output
 ;;
=========================================================================
=====

      (mesh-file  "instTEST.mesh")  ;; MUST include node coordinates
(fake accepted)

;;-------------------------------------------------------------------------
-


     (srctab

      (compflux (comp air) (range "F7*") (name AIR)
               (table     0.0  5.e-3     1.e30 5.e-3)
            (enthalpy  0.0  9.882e4  1.0e30 9.882e4)
      )
```

```
(totalflux
       (range "F8*") (name WEL)
         (table     0.0  -1.5e-2     1.e30 -1.5e-2)
       (enthalpy-internal)
)


(compflux (comp energy) (range "F9*") (name HOT)
         (table     0.0  2.0e6    1.e30 2.0e6)
)

(compflux (comp energy) (range "F10*") (name COL)
      (table  0.0 -5.0e5   1.0e30 -5.0e5)
)

(compflux  (comp water)
       (range "sho1") (name p1)
         (table     0.0  -1.0    1.e30 -1.0)
       (enthalpy  0.0 1.0e6  1.0e30 1.0e6)
)

(totalflux
       (range "sho3*") (name p3)
         (table
            0.      -0.1
            1.e2    -0.2
            2.e2    -0.3
            4.e3    -1.1
           )
       (enthalpy-internal)
)

(totalflux
       (range "sho4*") (name p4)
         (table
            0.      -0.1
            1.e2    -0.2
            2.e2    -0.3
            4.e3    -1.1
           )
       (enthalpy-internal)
)

(totalflux
       (range "sho5*") (name p5)
         (table
            0.      -0.1
            1.e2    -0.2
            2.e2    -0.3
            4.e3    -1.1
           )
       (enthalpy-internal)
)

(compflux (comp water)
       (range "sho6*") (name p6)
         (table
```

```
            0.      -0.1
            1.e2    -0.2
            2.e2    -0.3
            4.e3    -1.1
           )
        (enthalpy
            0.      1.e6
            1.e2    2.e6
            2.e2    3.e6
            4.e3    1.1e7
           )
)

(compflux (comp water)
        (range "sho7*") (name p7)
          (table
            0.      -0.1
            1.e2    -0.2
            2.e2    -0.3
            4.e3    -1.1
           )
        (enthalpy
            0.      1.e6
            1.e2    2.e6
            2.e2    3.e6
            4.e3    1.1e7
           )
)

(compflux (comp water)
        (range "sho8*") (name p8)
          (table
            0.      -0.1
            1.e2    -0.2
            2.e2    -0.3
            4.e3    -1.1
           )
        (enthalpy
            0.      1.e6
            1.e2    2.e6
            2.e2    3.e6
            4.e3    1.1e7
           )

)

(compflux (comp water) (range "sho10*") (name p10)
          (table
            0.      1.1
            1.e2    1.0
            2.e2    0.9
            3.e3    0.1
           )
        (enthalpy
            0.      1.0e6
            1.e2    1.2e6
            2.e2    1.4e6
```

```
            3.e3    3.0e6
           )
 )


 );; end srctab


          ;;initial conditions
(state
  (P by-key ("*" 1.e5)
       ("F2*" 1.e6)
       ("F4*" 99.e5)
       ("F5*" 1.e6)
       ("F6*" 10.e6)
       ("F8*" 1.e7)
       ("F10*" 40.e5)
       ("sho*" 45.e5)
       ("sho11*" 50.e5)
       ("sho12*" 40.e5)
   )


  (T by-key ("*" 250.0)
       ("F1*" 20)
       ("F2*" 170)
       ("F3*" 99.5)
       ("F4*" 310)
       ("F5*" 100)
       ("F6*" 100)
       ("F7*" 20)
       ("F8*" 300)
       ("F9*" 90)
       ("F10*" 280)
       ("sho11*" 240)
       ("sho12*" 100)
   )
  (S.liquid by-key ("*" 0.5)
       ("F*" 0.0)
       ("F2*" 1.0)
       ("F3*" .999)
       ("F4*" .001)
       ("F5*" 1.00)
       ("F6*" 0.0)
       ("F7*" 1.0)
       ("F8*" 1.0)
       ("F9*" .01)
       ("F10*" 0)
       ("sho11*" 1.0)
       ("sho12*" 1.0)
   )

  (X.air  by-key("*" -1)
       ("F1*" 1.0)
       ("F2*" 0)
       ("F5*" 0)
       ("F6*" 1.0)
```

```
            ("F7*" 0)
            ("F8*" 0)
            ("F10*" 0)
            ("sho11*" 0)
            ("sho12*" 0)
        )

    )  ;; end state

 )  ;; end input
```

```
         1
*instTEST* *instTEST* CODE DEMONSTRATION: PHASE TRANSITIONS, COMPONENT
(DIS-)APP
         10
instTEST.mesh
NUFT version 2.0s (SUN/SOLARIS)
0
VARIABLE
$end_internal_grid
$OperatingSystem  SunOS s116.es.llnl.gov 5.5.1 Generic_103640-17 sun4u
sparc SUNW,Ultra-2
$C-Compiler  cc: WorkShop Compilers 4.2 30 Oct 1996 C 4.2
$FortranCompiler  f77: WorkShop Compilers 4.2 04 Mar 1997 FORTRAN 77
4.2 patch 104529-01
$RunID
$RunDate  Wed Oct  7 13:27:02 1998
         4
S.liquid
P
T
Xd.water.gas
         0
        22
F1
F2
F3
F4
F5
F6
F7
F8
F9
F10
sho1
sho2
sho3
sho4
sho5
sho6
sho7
sho8
sho9
sho10
sho11
```

```
sho12
         0
THIST
EVAR S.liquid
T *
E *

THIST
EVAR P
T *
E *

THIST
EVAR T
T *
E *

THIST
EVAR Xd.water.gas
T *
E *

1.001100e+02
         1
        22
7.852671e-05
1.000000e+00
9.993419e-01
7.377989e-04
9.994621e-01
0.000000e+00
9.998663e-01
1.000000e+00
9.826758e-03
0.000000e+00
4.744532e-01
5.000000e-01
4.959984e-01
4.959984e-01
4.959984e-01
4.958759e-01
4.958759e-01
4.958759e-01
5.000000e-01
5.271134e-01
1.000000e+00
1.000000e+00
1.001100e+02
         2
        22
1.023493e+05
8.283809e+05
1.081390e+05
9.885707e+06
3.257638e+06
9.945619e+06
6.186299e+05
```

```
9.804890e+06
1.503488e+05
3.959572e+06
4.486063e+06
4.500000e+06
4.310127e+06
4.310127e+06
4.310127e+06
4.473379e+06
4.473379e+06
4.473379e+06
4.500000e+06
4.547374e+06
5.000000e+06
4.000000e+06
1.001100e+02
         3
        22
2.000804e+01
1.699869e+02
9.959462e+01
3.098949e+02
1.001012e+02
9.998018e+01
2.000604e+01
2.999485e+02
1.046708e+02
2.762718e+02
2.501686e+02
2.500000e+02
2.490053e+02
2.490053e+02
2.490053e+02
2.496656e+02
2.496656e+02
2.496656e+02
2.500000e+02
2.502641e+02
2.400000e+02
1.000000e+02
1.001100e+02
         4
        22
1.435223e-02
0.000000e+00
8.845663e-01
9.968048e-01
1.993420e-02
0.000000e+00
2.356927e-03
0.000000e+00
7.097492e-01
1.000000e+00
8.581914e-01
8.516356e-01
8.804877e-01
8.804877e-01
```

```
8.804877e-01
8.518287e-01
8.518287e-01
8.518287e-01
8.516356e-01
8.451904e-01
0.000000e+00
0.000000e+00
3.810700e+02
         1
        22
3.109399e-04
9.997623e-01
1.000000e+00
0.000000e+00
9.981650e-01
0.000000e+00
9.993912e-01
1.000000e+00
8.508368e-03
0.000000e+00
4.026491e-01
5.000000e-01
4.724331e-01
4.724331e-01
4.724331e-01
4.700885e-01
4.700885e-01
4.700885e-01
5.000000e-01
5.953230e-01
1.000000e+00
1.000000e+00
3.810700e+02
         2
        22
1.023996e+05
7.918920e+05
1.309590e+06
9.824781e+06
7.550708e+06
9.861865e+06
2.269005e+06
9.255739e+06
4.525704e+05
3.844732e+06
4.460633e+06
4.500000e+06
3.610396e+06
3.610396e+06
3.610396e+06
4.006486e+06
4.006486e+06
4.006486e+06
4.500000e+06
4.881107e+06
5.000000e+06
```

```
4.000000e+06
3.810700e+02
          3
         22
2.006424e+01
1.699836e+02
9.997610e+01
3.095724e+02
1.002920e+02
9.994965e+01
2.002495e+01
2.998040e+02
1.453157e+02
2.658107e+02
2.506764e+02
2.500000e+02
2.430540e+02
2.430540e+02
2.430540e+02
2.427376e+02
2.427376e+02
2.427376e+02
2.500000e+02
2.537867e+02
2.400000e+02
1.000000e+02
3.810700e+02
          4
         22
1.439544e-02
1.000000e+00
0.000000e+00
9.968257e-01
8.598807e-03
0.000000e+00
6.425773e-04
0.000000e+00
8.904919e-01
1.000000e+00
8.741152e-01
8.516356e-01
9.707206e-01
9.707206e-01
9.707206e-01
8.403445e-01
8.403445e-01
8.403445e-01
8.516356e-01
8.337838e-01
0.000000e+00
0.000000e+00
1.138100e+03
          1
         22
9.358275e-04
9.990619e-01
1.000000e+00
```

```
0.000000e+00
9.975332e-01
0.000000e+00
9.982459e-01
9.981583e-01
0.000000e+00
2.109789e-03
2.082555e-01
5.000000e-01
3.811381e-01
3.811381e-01
3.811381e-01
3.702028e-01
3.702028e-01
3.702028e-01
5.000000e-01
7.581263e-01
1.000000e+00
1.000000e+00
1.138100e+03
         2
        22
1.025346e+05
7.918608e+05
6.859643e+06
9.605245e+06
9.714702e+06
9.815591e+06
6.262273e+06
8.544895e+06
2.283117e+06
3.266972e+06
4.468203e+06
4.500000e+06
2.182671e+06
2.182671e+06
2.182671e+06
1.824922e+06
1.824922e+06
1.824922e+06
4.500000e+06
6.301704e+06
5.000000e+06
4.000000e+06
1.138100e+03
         3
        22
2.021513e+01
1.699820e+02
1.009156e+02
3.092995e+02
1.003868e+02
9.993279e+01
2.007319e+01
2.995997e+02
2.532881e+02
2.386095e+02
```

```
2.523518e+02
2.500000e+02
2.168330e+02
2.168330e+02
2.168330e+02
1.954678e+02
1.954678e+02
1.954678e+02
2.500000e+02
2.669475e+02
2.400000e+02
1.000000e+02
1.138100e+03
         4
        22
1.451124e-02
1.000000e+00
0.000000e+00
9.967777e-01
6.697130e-03
0.000000e+00
2.333674e-04
1.000000e+00
9.746793e-01
1.000000e+00
9.048214e-01
8.516356e-01
9.999687e-01
9.999687e-01
9.999687e-01
7.004050e-01
7.004050e-01
7.004050e-01
8.516356e-01
7.967007e-01
0.000000e+00
0.000000e+00
1.894000e+03
         1
        22
1.559655e-03
9.983628e-01
1.000000e+00
0.000000e+00
9.975060e-01
0.000000e+00
9.972538e-01
9.946459e-01
0.000000e+00
9.130210e-03
1.223378e-02
5.000000e-01
2.663046e-01
2.663046e-01
2.663046e-01
2.456169e-01
2.456169e-01
```

```
2.456169e-01
5.000000e-01
8.884758e-01
1.000000e+00
1.000000e+00
1.894000e+03
         2
        22
1.026695e+05
7.918296e+05
8.635787e+06
9.535363e+06
9.809192e+06
9.813510e+06
9.782362e+06
8.540448e+06
2.884947e+06
2.070810e+06
4.564631e+06
4.500000e+06
8.741924e+05
8.741924e+05
8.741924e+05
3.218248e+05
3.218248e+05
3.218248e+05
4.500000e+06
8.666722e+06
5.000000e+06
4.000000e+06
1.894000e+03
         3
        22
2.036545e+01
1.699803e+02
1.012153e+02
3.092125e+02
1.003909e+02
9.993204e+01
2.011848e+01
2.995629e+02
3.666415e+02
2.141328e+02
2.546612e+02
2.500000e+02
1.741155e+02
1.741155e+02
1.741155e+02
7.877259e+01
7.877259e+01
7.877259e+01
2.500000e+02
2.807639e+02
2.400000e+02
1.000000e+02
1.894000e+03
         4
```

```
        22
1.462627e-02
1.000000e+00
0.000000e+00
9.967618e-01
6.633281e-03
0.000000e+00
1.497489e-04
1.000000e+00
9.736734e-01
1.000000e+00
9.254393e-01
8.516356e-01
9.999710e-01
9.999710e-01
9.999710e-01
9.262210e-02
9.262210e-02
9.262210e-02
8.516356e-01
7.106032e-01
0.000000e+00
0.000000e+00
2.000000e+03
         1
        22
1.647124e-03
9.982647e-01
1.000000e+00
0.000000e+00
9.975055e-01
0.000000e+00
9.971245e-01
9.941535e-01
0.000000e+00
9.885142e-03
0.000000e+00
5.000000e-01
2.487727e-01
2.487727e-01
2.487727e-01
2.279385e-01
2.279385e-01
2.279385e-01
5.000000e-01
9.034904e-01
1.000000e+00
1.000000e+00
2.000000e+03
         2
        22
1.026884e+05
7.918252e+05
8.762933e+06
9.530462e+06
9.810718e+06
9.813477e+06
```

```
1.024802e+07
8.539824e+06
2.967109e+06
1.932167e+06
2.502021e+06
4.500000e+06
7.252230e+05
7.252230e+05
7.252230e+05
2.664558e+05
2.664558e+05
2.664558e+05
4.500000e+06
9.146202e+06
5.000000e+06
4.000000e+06
2.000000e+03
         3
        22
2.038651e+01
1.699801e+02
1.012364e+02
3.092062e+02
1.003910e+02
9.993202e+01
2.012466e+01
2.995578e+02
3.825406e+02
2.106326e+02
2.619213e+02
2.500000e+02
1.663800e+02
1.663800e+02
1.663800e+02
5.378607e+01
5.378607e+01
5.378607e+01
2.500000e+02
2.825559e+02
2.400000e+02
1.000000e+02
2.000000e+03
         4
        22
1.464236e-02
1.000000e+00
0.000000e+00
9.967607e-01
6.632259e-03
0.000000e+00
1.429915e-04
1.000000e+00
9.735802e-01
1.000000e+00
8.323939e-01
8.516356e-01
9.999977e-01
```

9.999977e-01
9.999977e-01
3.554000e-02
3.554000e-02
3.554000e-02
8.516356e-01
6.901467e-01
0.000000e+00
0.000000e+00

```
"input" user: 0.35 s. sys: 0.01 s.; called 1 times
"init." user: 0.05 s. sys: 0 s.; called 1 times
"output" user: 0.01 s. sys: 0.02 s.; called 318 times
"char. funs" user: 0.28 s. sys: 0.02 s.; called 4233 times
"build eqts" user: 5.44 s. sys: 0.04 s.; called 705 times
"lin.eqt.soln." user: 0.41 s. sys: 0 s.; called 705 times
total user cpu time: 6.86 s., sys. cpu time: 0.27 s.
total wall clock time: 7.28781 s.

         1
*instTEST SCCS_ID  "@(#)instTEST.th 1.3 01/29/98 NUFT_EXPOUT_FILE" CODE
DEMONSTRATION: PHASE TRANSITIONS, COMPONENT (DIS-)APP
         10
instTEST.mesh
NUFT version 12-11-97b (SUN/SOLARIS)
0
VARIABLE
$end_internal_grid
$OperatingSystem  SunOS s13.es.llnl.gov 5.5.1 Generic_103640-01 sun4u
sparc SUNW,Ultra-2
$C-Compiler  cc: WorkShop Compilers 4.2 30 Oct 1996 C 4.2
$FortranCompiler  f77: WorkShop Compilers 4.2 30 Oct 1996 FORTRAN 77
4.2
$RunID
$RunDate  Wed Jan 28 18:57:29 1998
         4
S.liquid
P
T
Xd.water.gas
         0
        22
F1
F2
F3
F4
F5
F6
F7
F8
F9
F10
sho1
sho2
sho3
sho4
sho5
sho6
sho7
sho8
sho9
sho10
sho11
sho12
         0
THIST
EVAR S.liquid
```

```
T *
E *

THIST
EVAR P
T *
E *

THIST
EVAR T
T *
E *

THIST
EVAR Xd.water.gas
T *
E *

1.001100e+02
         1
        22
7.852671e-05
1.000000e+00
9.993419e-01
7.377989e-04
9.994621e-01
0.000000e+00
9.998663e-01
1.000000e+00
9.826758e-03
0.000000e+00
4.744532e-01
5.000000e-01
4.959984e-01
4.959984e-01
4.959984e-01
4.958759e-01
4.958759e-01
4.958759e-01
5.000000e-01
5.271134e-01
1.000000e+00
1.000000e+00
1.001100e+02
         2
        22
1.023493e+05
8.283809e+05
1.081390e+05
9.885707e+06
3.257638e+06
9.945619e+06
6.186299e+05
9.804890e+06
1.503488e+05
3.959572e+06
4.486063e+06
```

```
4.500000e+06
4.310127e+06
4.310127e+06
4.310127e+06
4.473379e+06
4.473379e+06
4.473379e+06
4.500000e+06
4.547374e+06
5.000000e+06
4.000000e+06
1.001100e+02
         3
        22
2.000804e+01
1.699869e+02
9.959462e+01
3.098949e+02
1.001012e+02
9.998018e+01
2.000604e+01
2.999485e+02
1.046708e+02
2.762718e+02
2.501686e+02
2.500000e+02
2.490053e+02
2.490053e+02
2.490053e+02
2.496656e+02
2.496656e+02
2.496656e+02
2.500000e+02
2.502641e+02
2.400000e+02
1.000000e+02
1.001100e+02
         4
        22
1.435223e-02
0.000000e+00
8.845663e-01
9.968048e-01
1.993420e-02
0.000000e+00
2.356927e-03
0.000000e+00
7.097492e-01
1.000000e+00
8.581914e-01
8.516356e-01
8.804877e-01
8.804877e-01
8.804877e-01
8.518287e-01
8.518287e-01
8.518287e-01
```

```
8.516356e-01
8.451904e-01
0.000000e+00
0.000000e+00
3.810700e+02
         1
        22
3.109399e-04
9.997623e-01
1.000000e+00
0.000000e+00
9.981650e-01
0.000000e+00
9.993912e-01
1.000000e+00
8.508368e-03
0.000000e+00
4.026491e-01
5.000000e-01
4.724331e-01
4.724331e-01
4.724331e-01
4.700885e-01
4.700885e-01
4.700885e-01
5.000000e-01
5.953230e-01
1.000000e+00
1.000000e+00
3.810700e+02
         2
        22
1.023996e+05
7.918920e+05
1.309590e+06
9.824781e+06
7.550708e+06
9.861865e+06
2.269005e+06
9.255739e+06
4.525704e+05
3.844732e+06
4.460633e+06
4.500000e+06
3.610396e+06
3.610396e+06
3.610396e+06
4.006486e+06
4.006486e+06
4.006486e+06
4.500000e+06
4.881107e+06
5.000000e+06
4.000000e+06
3.810700e+02
         3
        22
```

```
2.006424e+01
1.699836e+02
9.997610e+01
3.095724e+02
1.002920e+02
9.994965e+01
2.002495e+01
2.998040e+02
1.453157e+02
2.658107e+02
2.506764e+02
2.500000e+02
2.430540e+02
2.430540e+02
2.430540e+02
2.427376e+02
2.427376e+02
2.427376e+02
2.500000e+02
2.537867e+02
2.400000e+02
1.000000e+02
3.810700e+02
         4
        22
1.439544e-02
1.000000e+00
0.000000e+00
9.968257e-01
8.598807e-03
0.000000e+00
6.425773e-04
0.000000e+00
8.904919e-01
1.000000e+00
8.741152e-01
8.516356e-01
9.707206e-01
9.707206e-01
9.707206e-01
8.403445e-01
8.403445e-01
8.403445e-01
8.516356e-01
8.337838e-01
0.000000e+00
0.000000e+00
1.138100e+03
         1
        22
9.358275e-04
9.990619e-01
1.000000e+00
0.000000e+00
9.975332e-01
0.000000e+00
9.982459e-01
```

```
9.981583e-01
0.000000e+00
2.109789e-03
2.082555e-01
5.000000e-01
3.811381e-01
3.811381e-01
3.811381e-01
3.702028e-01
3.702028e-01
3.702028e-01
5.000000e-01
7.581263e-01
1.000000e+00
1.000000e+00
1.138100e+03
         2
        22
1.025346e+05
7.918608e+05
6.859643e+06
9.605245e+06
9.714702e+06
9.815591e+06
6.262273e+06
8.544895e+06
2.283117e+06
3.266972e+06
4.468203e+06
4.500000e+06
2.182671e+06
2.182671e+06
2.182671e+06
1.824922e+06
1.824922e+06
1.824922e+06
4.500000e+06
6.301704e+06
5.000000e+06
4.000000e+06
1.138100e+03
         3
        22
2.021513e+01
1.699820e+02
1.009156e+02
3.092995e+02
1.003868e+02
9.993279e+01
2.007319e+01
2.995997e+02
2.532881e+02
2.386095e+02
2.523518e+02
2.500000e+02
2.168330e+02
2.168330e+02
```

```
2.168330e+02
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1.954678e+02
1.954678e+02
2.500000e+02
2.669475e+02
2.400000e+02
1.000000e+02
1.138100e+03
         4
        22
1.451124e-02
1.000000e+00
0.000000e+00
9.967777e-01
6.697130e-03
0.000000e+00
2.333674e-04
1.000000e+00
9.746793e-01
1.000000e+00
9.048214e-01
8.516356e-01
9.999687e-01
9.999687e-01
9.999687e-01
7.004050e-01
7.004050e-01
7.004050e-01
8.516356e-01
7.967007e-01
0.000000e+00
0.000000e+00
1.894000e+03
         1
        22
1.559655e-03
9.983628e-01
1.000000e+00
0.000000e+00
9.975060e-01
0.000000e+00
9.972538e-01
9.946459e-01
0.000000e+00
9.130210e-03
1.223378e-02
5.000000e-01
2.663046e-01
2.663046e-01
2.663046e-01
2.456169e-01
2.456169e-01
2.456169e-01
5.000000e-01
8.884758e-01
1.000000e+00
```

```
1.000000e+00
1.894000e+03
          2
         22
1.026695e+05
7.918296e+05
8.635787e+06
9.535363e+06
9.809192e+06
9.813510e+06
9.782362e+06
8.540448e+06
2.884947e+06
2.070810e+06
4.564631e+06
4.500000e+06
8.741924e+05
8.741924e+05
8.741924e+05
3.218248e+05
3.218248e+05
3.218248e+05
4.500000e+06
8.666722e+06
5.000000e+06
4.000000e+06
1.894000e+03
          3
         22
2.036545e+01
1.699803e+02
1.012153e+02
3.092125e+02
1.003909e+02
9.993204e+01
2.011848e+01
2.995629e+02
3.666415e+02
2.141328e+02
2.546612e+02
2.500000e+02
1.741155e+02
1.741155e+02
1.741155e+02
7.877259e+01
7.877259e+01
7.877259e+01
2.500000e+02
2.807639e+02
2.400000e+02
1.000000e+02
1.894000e+03
          4
         22
1.462627e-02
1.000000e+00
0.000000e+00
```

```
9.967618e-01
6.633281e-03
0.000000e+00
1.497489e-04
1.000000e+00
9.736734e-01
1.000000e+00
9.254393e-01
8.516356e-01
9.999710e-01
9.999710e-01
9.999710e-01
9.262210e-02
9.262210e-02
9.262210e-02
8.516356e-01
7.106032e-01
0.000000e+00
0.000000e+00
2.000000e+03
         1
        22
1.647124e-03
9.982647e-01
1.000000e+00
0.000000e+00
9.975055e-01
0.000000e+00
9.971245e-01
9.941535e-01
0.000000e+00
9.885142e-03
0.000000e+00
5.000000e-01
2.487727e-01
2.487727e-01
2.487727e-01
2.279385e-01
2.279385e-01
2.279385e-01
5.000000e-01
9.034904e-01
1.000000e+00
1.000000e+00
2.000000e+03
         2
        22
1.026884e+05
7.918252e+05
8.762933e+06
9.530462e+06
9.810718e+06
9.813477e+06
1.024802e+07
8.539824e+06
2.967109e+06
1.932167e+06
```

```
2.502021e+06
4.500000e+06
7.252230e+05
7.252230e+05
7.252230e+05
2.664558e+05
2.664558e+05
2.664558e+05
4.500000e+06
9.146202e+06
5.000000e+06
4.000000e+06
2.000000e+03
         3
        22
2.038651e+01
1.699801e+02
1.012364e+02
3.092062e+02
1.003910e+02
9.993202e+01
2.012466e+01
2.995578e+02
3.825406e+02
2.106326e+02
2.619213e+02
2.500000e+02
1.663800e+02
1.663800e+02
1.663800e+02
5.378607e+01
5.378607e+01
5.378607e+01
2.500000e+02
2.825559e+02
2.400000e+02
1.000000e+02
2.000000e+03
         4
        22
1.464236e-02
1.000000e+00
0.000000e+00
9.967607e-01
6.632259e-03
0.000000e+00
1.429915e-04
1.000000e+00
9.735802e-01
1.000000e+00
8.323939e-01
8.516356e-01
9.999977e-01
9.999977e-01
9.999977e-01
3.554000e-02
3.554000e-02
```

3.554000e-02
8.516356e-01
6.901467e-01
0.000000e+00
0.000000e+00

Lynn Lewis <lewis16@llnl.gov> on 10/07/98 08:17:18 PM

To: John Nitao <nitao@s13.es.llnl.gov>
cc: Jim Kam/YM/RWDOE, kansa1@llnl.gov, "Ronald J. 'Ron' Shaffer" <shaffer2@popeye.llnl.gov>
Subject: Re: NUFT Installation Test

This is the correct expected output for 2.0s. However, in the future, we need to modify the production distribution package script to include the ACTUAL output "instTEST_<rel_no>.ex" (instTEST_2.0s.ex in this instance) instead of "instTEST.th".

>Ron, Lynn,
>
>I received this email from a NUFT user in Las Vegas.
>
> John Nitao
>
>> From: Jim_Kam@notes.ymp.gov
>> Date: Wed, 07 Oct 1998 15:10:29 -0700
>> MIME-version: 1.0
>> Content-disposition: inline
>> X-Lotus-FromDomain: CRWMS
>> Content-Type: text/plain; charset=us-ascii
>> Content-Length: 397
>>
>> John,
>>
>> I've installed NUFT 2.0s and am testing the installation with the input
>> file "instTEST.in". In comparing the run output "instTEST.ex" with the
>> documented output "instTEST.th", I have realized the NUFT version stated
>> on "instTEST.th" is version 12-11-97b. Is this ver. the same as 2.0s as
>> stated on "instTEST.ex" ? If so, do we need to clarify this in the
>> documentation ?
>>
>>
>> Jim
>>
>>
>>
>>

Lynn Lewis
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email: lewis16@llnl.gov

The CSCI, DI and MI identifiers were not provided by LLNL to properly identify their software code - NUFT V2.0s
I have taken the following tack with dealing with no identification numbers being provided by the Labs -

To identify the Media (MI number) and the whole NUFT V2.0s delivery - use the Letter of Certification number provided by the Lab
- in this case the number for NUFT V2.0s is: **LLYMP9809098**

To identifiy the CSCI number provided by the Lab - I am using the Letter of Certification number also
in thi case that number again is: **LLYMP9809098**

To identify the Documentation (DI number[s]) - use the Date the Document was approved as provided by the Lab
- this case the following group of DI numbers apply to the documents LLNL provided - DI numbers used are in red

"NUFT V2.0S Release 2.0s README - February 02, 1998
"NUFT V2.0S Release 2.0s Release Notes, Revision 0 - September 18,1998
"NUFT V2.0S Release 2.0s INSTALL SCRIPT - September 26,1998
"NUFT V2.0S Release 2.0s BOM-PROC - September 18,1998
"NUFT V2.0S Release 2.0s DIST.UU - September 18,1998

"NUFT V2.0S Software Certification Checklist - July 24, 1998
"NUFT V2.0S Individual Software Plan for the Qualification of NUFT V2.0S - ISP-NF-13, Revision 2
"NUFT V2.0S Records Package Transmittal Form / TOC - LLYMP9808119

"NUFT V2.0S Requirements Document (RD) for the Prediction of Thermo-hydrologic Behavior - NUFT 2.0 - September 4, 1998, Revision 1

"NUFT V2.0S NUFT V2.0S Software Verification and Validation Plan - September 09, 1998, Revision 1

"NUFT V2.0S NUFT Configuration Management System (CMS) Developer's Guide - May 04, 1998

"NUFT V2.0S User's Manual for the USNT Module of the NUFT Code, Version 2.0 (NP-Phase, NC-Component, Thermal) - UCRL-MA-130653

"NUFT V2.0S Reference Manual for the NUFT Flow and transport Code, Version 2.0 - UCRL-MA-130651

"NUFT V2.0S Verification and Validation Document (VDD) for NUFT Veriosn 2.0s, Revision 1 - September 11, 1998

Lynn Lewis 925 422-8949 <lewis@s139.es.llnl.gov> (by way of Lynn Lewis) (by way of Ed Kansa) on 10/07/98 08:10:42 AM

To: Jim Kam/YM/RWDOE
cc:
Subject: E-mail of NUFT Release 2.0s - Release Notes Revision 0

You will be receiving by e-mail the NUFT Release Distribution for Release 2.0s. Release 2.0s has been qualified for use on SUN platforms running SUNOS 5.5.1.

This e-mail describes how you will be receiving the distribution, how to install it on your platform, and how to test your installation. It also contains notes regarding Release 2.0s.

I. Receiving the NUFT Release Distribution

The NUFT Release Distribution is composed of the NUFT Executable Distribution and files for installing the NUFT Executable Distribution on your platform. You will receive the NUFT Release Distribution in four parts via four separate e-mails. Each part contained within the e-mail is delineated by a line containing
"Begin <part>" and a line containing "End <part>" where <part> is the name of the part.
After saving each e-mail into a file, you should delete all lines preceding Begin <part>,
the Begin <part> line, the End <part> line, and all lines following the End <part> line.

The four e-mails are:

E-mail for the README part

The Subject field of this e-mail is: NUFT Release 2.0s README

This e-mail contains the NUFT Release Distribution README file.
The README file contains the instructions for installing the NUFT Distribution on your platform. It also contains a disposition of qualification test exceptions.

Save this e-mail as README.

E-mail for the INSTALL-SCRIPT part

The subject field of this e-mail is: NUFT Release 2.0s INSTALL-SCRIPT

This e-mail contains the NUFT Release Distribution INSTALL-SCRIPT file.
INSTALL-SCRIPT is the C-shell script you will use to install the NUFT Executable Distribution.

Save this e-mail as INSTALL-SCRIPT.

E-mail for the dist.uu part

The subject field of this e-mail is: NUFT Release 2.0s dist.uu

This e-mail contains the NUFT Executable Distribution dist.uu file. dist.uu is a uuencoded file containing the NUFT Executable Distribution which contains the NUFT executable, ancillary files needed for NUFT execution, and installation test input and expected output files.

Save this e-mail as dist.uu

E-mail for the BOM-PROC part

The subject field of this e-mail is: NUFT Release 2.0s Bill-of-Materials

This e-mail contains a procedure for generating a bill-of-materials for the NUFT Release. The bill-of-materials lists the names and revision numbers of items used in the generation and qualification of NUFT Release 2.0s.

Save this e-mail as BOM-PROC.

II. Installing the NUFT Executable Distribution

After you have received all of the e-mails, follow the instructions in README to install NUFT.

III. Testing the NUFT Executable Distribution

The directory in which you installed the NUFT Executable Distribution contains the NUFT input file instTEST.in and its associated output file instTEST.th.

1. cd to this directory.
2. Set the environment variable NUFTPATH to this directory.
3. Run the NUFT executable main with the input file:

```
./main instTEST.in
```

   main will produce an output file named instTEST.ex.

4. Compare instTEST.ex with instTEST.th:

```
diff instTEST.ex instTEST.th
```

   The only difference should be in a line containing SCCS_ID and a line beginning with "$RunDate".

IV. NUFT Release 2.0s Notes

IV.A. User Documentation

The following user documents will be shipped separately:

Reference Manual for the NUFT Flow and Transport Code, Version 2.0.
UCRL-MA-130651

User's Manual for the USNT Module of the NUFT Code, Version 2.0.
UCRL-MA-130653

IV.B. NUFT Release 2.0s Bill-of-Materials

The following files are not listed in the Bill-of-Materials but are part of NUFT Release 2.0s:

bmrk018_0_2.0s.rst: revision 1.1
Restart file produced by the execution of the bmrk018_0 test problem.

tools_version_2.0s.doc: revision 1.1
Bill-of-Materials file for tools used to produce Release 2.0s.

The following files were updated for Release 2.0s but their revision numbers were not updated in the Bill-of-Materials:

instTEST.th: revision 1.4

The following files are listed in the Bill-of-Materials but are not part of this distribution:

ref.ps
us1.ps
usnt.ps

ref.ps and usnt.ps are user documentation files which are being shipped separately.

IV.C Limitations and Assumptions in the Use of NUFT Release 2.0s

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The use of this code for quality affecting activities is contingent upon the receiving organization completing the installation test and returning the completed LLNL Software Installation and Checkout Form to the LLNL Software Configuration Management Coordinator.

Edward Kansa
Lawrence Livermore National Laboratory
P.O. Box 808, L-200
Livermore, CA 94550
phone: 925-423-0151
email: kansa1@llnl.gov
fax: 925-423-6907

The use of NUFT on Yucca Mountain quality affecting analyses requires the use of appropriately qualified data.

NUFT user organizations are responsible for ensuring that the software is appropriately applied. This includes, for example controls to ensure:
1) appropriate distribution of NUFT within their organization,
2) that individual users are appropriately qualified and trained,
3) that NUFT is applied correctly to the intended problems, and
4) that results NUFT produces are properly interpreted.

Dependable results can only be achieved by skilled practitioners. For example, professional judgment is required to select the proper mesh and compatible boundary conditions to adequately simulate the physical phenomena being analyzed
at a particular geologic site. More generally, results depend upon initial values, boundary conditions, mesh selection, time step selection, accurate characterization of physical parameters, and choice of modeled phenomena, and only an
expert
can perform reasonability checks that determine if the numerical solution approximates reality. More than one individual may be required to prepare the NUFT input
file.

NUFT is intended to be used by civil engineers, hydrologists, physicists and/or geologists with expertise in numerical solution of PDEs, who can be expected to intervene if the solutions produced are anomalous or unrealistic. At least
one user should have a background in application of numerical methods to analyze
non-isothermal groundwater flow. Such experts typically use a combination of test
problems
and successive inclusion of model phenomena to understand and gain confidence in
solutions
produced by PDE solvers. Significant erroneous variation in input values or input
values out of range will produce erroneous calculational results that a competent user will
recognize and remedy. The user is charged with inspecting the NUFT output file to ensure
that the actual input parameter values used in the calculations agree with the user's
expectations.

NUFT 2.0s demonstrates isothermal and nonisothermal, multi-phase fluid flow in one-, two- or three-dimensions in a cartesian coordinate system. It is capable of producing the full range of liquid saturations (S) from initially unsaturated (S=0) to fully saturated (S=1). Water mass fraction in the gas phase shall be
modeled over the full range >from dry (0) to wet (1). The calculation of relative
humidity is not valid when liquid saturation is exactly 1.

NUFT 2.0s is capable of analyzing the following phenomena:

flow (mass transport or infiltration) in unsaturated media

flow (mass transport) in saturated media

coupled mass and energy (heat) transport in geologic media by conduction, convection and diffusion with multiple gas and liquid fluid phases, including phase change

NUFT 2.0s is capable of analyzing these problems for the following different conceptual models of geologic media representative of the Yucca mountain site:

porous media

fractured media

fractured porous media

In intended applications:

all phenomena may be analyzed in one, two, or three dimensions.

NUFT normally will be applied to analyze time-varying transients. Some transient problems may approach a quasi-steady state or steady state solution.

To perform these calculations, NUFT incorporates thermophysical fluid properties for air, water vapor and water. Fluid properties are interpolated from equations that were derived from the ASME steam tables. The properties of air follow the ideal gas law. Fluid mixtures are represented by a scaled linear combination of the individual properties obtained from the ideal gas law and the steam tables.
Calculations can be performed over the range of temperature and pressure conditions anticipated in repository analyses (temperatures of 6 to 500 C, pressures of 2.67x103 to 1.03x107 Pa).

NUFT 2.0s uses two different formulations to compute mass fraction of water in the gas phase. The variable is X.water.gas for the first formulation, and Xd.water.gas for the second. The code is qualified only for the second formulation.

Table 1 summarizes NUFT functional capabilities certified in release 2.0s.

Table 1. Certified functional capabilities of release 2.0s

A. Flow processes

Pressure-driven gas flow

Pressure-driven liquid flow

Gravity effects

Capillary forces

Viscous forces

B. Constitutive relations

Vapor pressure lowering

Van Genuchten characteristic curve

Temperature dependent capillary pressure

C. Phase change/diffusion

Phase change

Phase (dis)appearance

Binary diffusion in gas

D. Heat transport

Conduction

Single phase convection

Two phase convection (including heat pipe)

E. Dimensionally

1-D

2-D

3-D

F. Other

Automatic timestepping

Restart capability

NUFT 2.0s executes the complete set of benchmark problems in approximately 10 min. when executed on a SUN SPARC workstation running in multi-user mode. Typical individual test problems executed in one or a few minutes. Execution time for practical problems is expected to be on the order of a few hours.

For benchmark test problems, NUFT satisfies at least one of the following criteria:

1) Parameter value is within 5% of the results for the same problem from either VTOUGH or the analytical solution,
2) Parameter value is within 5% of a normalized distance to a standard time history curve, or
3) Parameter value is within 5% of a parameter variation from standardized data normalized to the parameter range.

NUFT 2.0s possesses additional functional capabilities that are not certified for quality affecting use in this release. These include:

a) A contaminate transport option and dual permeability (DKM) option which provides for separate permeabilities for fractures and matrix,
b) Non-cartesian co-ordinate system, and
c) Radiant heat transfer capability.

Please report any problems with the use of NUFT 2.0s to the LLNL Code Sponsor

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ATTACHMENT IV

MODEL CALIBRATION

Material Properties:

Thermal properties of Simulated Drift Air at 300° K (Incropera and DeWitt 1996, pg.839)
Mass density 1.1614 kg/m^3
Thermal Conductivity 0.0263 W/(m-K)
Specific Heat Capacity 1.07 kJ/kg

Thermal properties of the Invert Material
Thermal Conductivity 0.66 W/(m-K) dry (Ryder et al. 1996, pg.5-3). This thermal conductivity is in the midpoint of the range mentioned in the reference.
Grain Density 2530 kg/m^3
Specific Heat Capacity 948 J/(kg-K)

Thermal properties of Drip Shield from ANSI 304 Stainless Steel @ 300° K (Incropera & DeWitt 1996, pg.829)
Mass Density 7900 kg/m^3
Thermal Conductivity 14.9 W/(m-K)
Specific Heat Capacity 477 J/(kg-K)

Thermal properties of Waste Package @ 300° K (Incropera & DeWitt 1996, pg.828)
Mass Density 7854 kg/m^3
Thermal Conductivity 60.5 W/(m-K)
Specific Heat Capacity 434 J/(kg-K)

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

NOTICE:

SPECIAL HANDLING INSTRUCTIONS

QA: QA

Document Identifier: ANL-EBS-MD-000026

Document Title: Water Diversion Model

Document Revision/Change: 00

Document Date: 02/01/2000

This document requires special handling in accordance with AP-6.1Q.

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EVALUATION OF THE NUFT CODE TO SIMULATE NATURAL CONVECTION

NUFT is developed for simulating flow and heat transport in porous and fractured media and, therefore, has limitations when used to model natural convection in air space, such as that underneath the drip shield. Recognizing these limitations, it may still be possible to use it for predicting the gross average temperature and heat transfer rate below the drip shield by assigning some pseudo porous medium properties to the air space so the model results would match an analytical solution.

A heat transfer problem in concentric cylinders with an analytical solution is selected for validating NUFT. Accordingly, a NUFT model has been developed to approximate the concentric cylinders with concentric rectangular cylinders using the drip shield and the heater as the outer and inner cylinders, respectively. The model scale corresponds approximately to the pilot quarter-scale test for canister #3. The purpose of this calculation is to adjust the thermal conductivity (due to boundary layer effect) and permeability of air in the air space between the heater and the drip shield such that the model results may come into agreement with an accepted, analytical solution to a natural convection problem for concentric cylinders. Since this NUFT model is designed for simulating natural convection only, radiation has been eliminated altogether. Attached is a grid layout for this problem.

It was found that by using an air intrinsic permeability of 1E-06 m^2 and a thermal conductivity of 0.0263 W/(m-K) as input to NUFT, the model results become consistent with the closed-form solution to a similar problem. Below is a calculation to substantiate this finding.

Following the approach and using the equations with the same notations in Example 9.5 (Incropera & Dewitt, "Introduction to Heat Transfer" pg. 477) for heat transfer in concentric cylinders, the NUFT problem is defined as follows:

Rectangular area enclosed by heater = 0.1368 sq. m.
Diameter of cylinder with equivalent area = 0.417 m.

Rectangular area enclosed by drip shield = 0.4056 sq. m.
Diameter of cylinder with equivalent area = 0.719 m.

Therefore,
D_0 = 0.719 m
D_i = 0.417m.
L = 0.151 m.

Thermal loading curves for Cases 1 and 2 are included.

Case 1.

At 15 days of simulation.
T_0 = 108.9 C
T_i = 119.2 C

Then $T_i - T_0 = \Delta T = 10.3$ C.
Average T = 114.1 C. = 387.1 K.

Air properties at 387 K,

$k = 0.033$ W/m.K
$\beta = 0.0026$
$\nu = 2.494E\text{-}5$
$\alpha = 3.606E\text{-}5$
$Pr = \nu / \alpha = 0.69$

$$Ra_L = g\beta (T_i - T_0) L^3 / (\nu\alpha) = 1.005E+6$$

$$Ra_c^* = [\ln(D_0/D_i)]^4 \, Ra_L / [L^3 (D_i^{-3/5} + D_0^{-3/5})^5] = 1.234E+5$$

$$k_{eff} = 0.386 \, [Pr / (0.861 + Pr)]^{1/4} \, (Ra_c^*)^{1/4} \, k = 0.195$$

$$q' = 2\pi \cdot \Delta T \cdot k_{eff} / [\ln(D_0 / D_i)] = 23.2 \text{ W/m (vs. 25.0 W/m from NUFT input)}$$

Note the theoretical heat transfer rate per unit length of cylinder is calculated to be close to the steady rate at the end of the curve. The model results show that after approximately 12 days, the temperature difference between the heater and the drip shield stays fairly constant around 18 – 19C. although there is a slight rising trend in temperature for both of them.

Case 2.
Next, run the model with a lower thermal loading than that in case 1 so a smaller temperature difference will result.

At 15 days of simulation,
T_0 = 79.67 C
T_I = 84.64 C therefore, ΔT = 4.97 C
Average T =82.15 C = 355.1 K

$k = 0.030$ W/m.K
$\beta = 0.0029\ K^{-1}$
$\nu = 2.092E\text{-}5\ m^2/s$
$\alpha = 2.990E\text{-}5\ m^2/s$

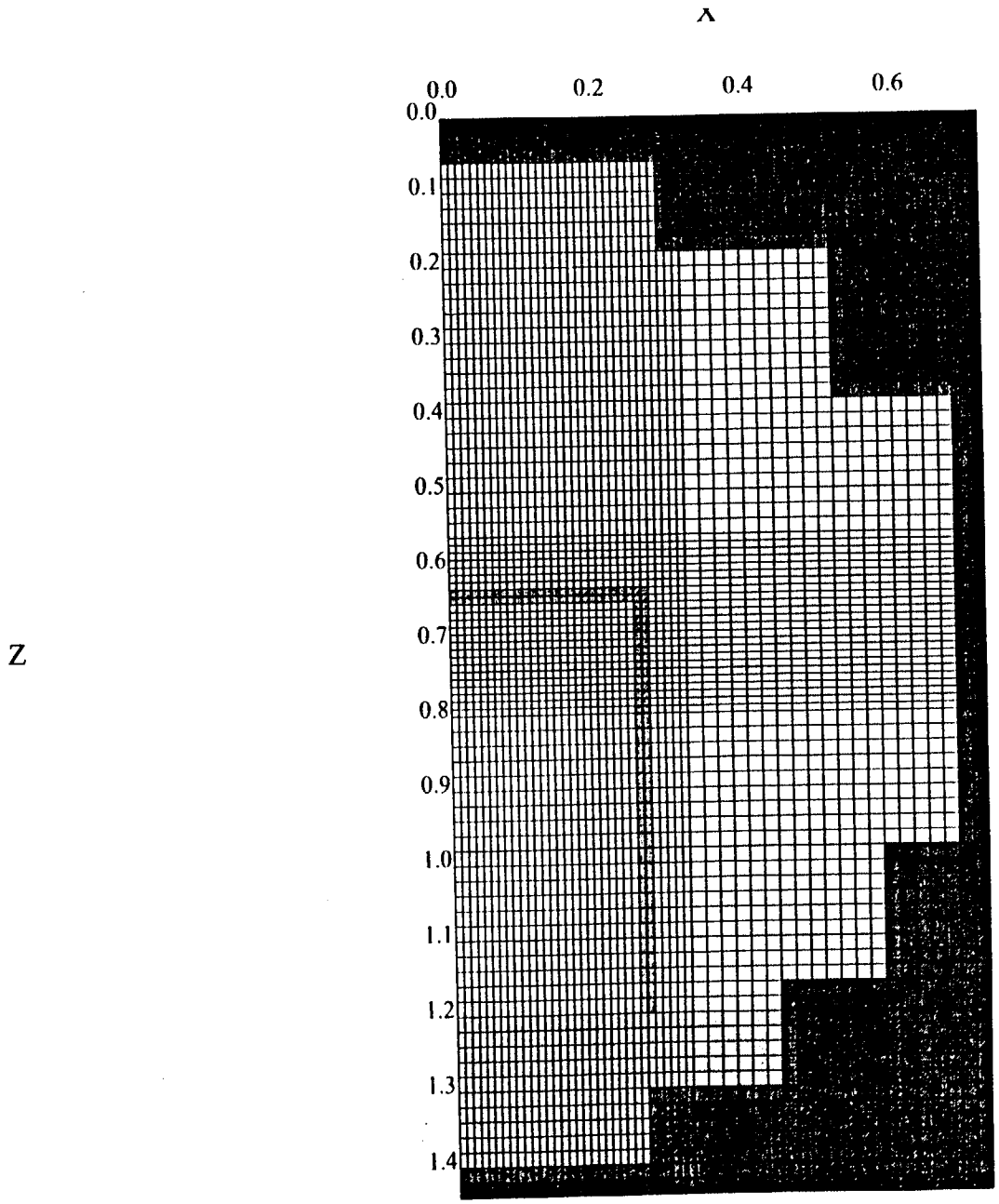
$Pr = 0.70$

$Ra_L = 7.775E+5$
$Ra_c^* = 9.548E+4$

$k_{eff} = 0.1666$

$q' = 9.55$ W/m (vs. 10.0 W/m from NUFT input)

)



Input file: radymp2Ddst9
Connection file:

IV-11

```
  (usnt
  (title " 2-D T-H Model drip shield for 1/4 scale test-insul/heat
source")
  (modelname usnt)
  (include-pkg "vtough.pkg")
  (tstop   2.0380e+06)
  (time 0)
  (stepmax 1000000)
  (dtmax  2.0380e+06)
  (dt 1e3)

;; Run ymp2Ddst91
;; Check free convection in cylinder with no radiation.
;; dry condition and no
;; water application. and no invert mat.
;; Drift air K = 1E-06 and Tcond 0.026
;; Peak thermal loading at 25 W/m


  (output
     (field (format tabular) (variables S.liquid P T RH C.water.gas )
          (file-ext ".var")
          (outtimes  0.2d .5d 1d 1.5d 2d 3d 5d 7d 9d 11d 15d 20d 22d
))

 ;; Compute fluxes

   ;;      (flux-history
   ;;       (variable Qrad)
   ;;       ( crange ("ht*" "sh*"))
   ;;       (file-ext ".rad")
   ;;      )

    ;;     (flux-history
    ;;      (variable Qrad)
    ;;      (crange ("ht*" "in*"))
    ;;      ( file-ext ".ra1")
    ;;     )



   ;;     (flux-history
   ;;      (variable Qcond)
   ;;      (crange ("ht*" "dr2*"))
   ;;      (file-ext ".con")
   ;;     )



   ;;    (flux-history
   ;;     (variable Qd.energy)
   ;;     (crange ("ht*" "sh*"))
   ;;     (file-ext ".dif")
   ;;     )


   ;; (flux-field
```

```
   ;;  (file-ext ".ad1")
   ;;  (format list)
   ;;  (variables qa.energy)
   ;;  (crange ("dr*" "sh*"))
   ;;  (outtimes 0.2y 0.5y 0.7y  1y 5y  9y ))

      (extool (variables T RH S.liquid X.air.gas P Qrad Qcond Qd.energy
V.liquid V.gas )
              (file-ext ".ext")(range "*")
(outtimes 0 0.2d 0.5d 1d 1.5d 2d 3d 5d 7d 8d 10d 12d 15d 18d 20d 22d )
  ))

  (rocktab
    (heatr
      (porosity 0.010) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 4.340e+02) (solid-density 7.854e+03)
      (tcond tcondLin (solid  60.50000)(liquid  60.500000)(gas
60.500000))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
      (tort (gas 0.000e+00) (liquid 0.0))
      (kr (gas 1.0)
          (liquid 1.0))
      (pc (liquid 0.0))
    )

    (drift
      (porosity 0.999) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.007e+03) (solid-density 1.1614)
      (tcond tcondLin (solid  0.02600)(liquid  0.02600)(gas  0.02600))
      (K0 1.000e-06) (K1 1.000e-06) (K2 1.000e-06)
;; JJN     (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krPower (power 4) (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
    )


    (shield
      (porosity 0.010) (Kd (air 0.0) (water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 4.7700e+2) (solid-density 7.900e+03)
      (tcond tcondLin (solid 14.90) (liquid 14.90) (gas 14.90))
      (K0 0.000) (K1 0.000) (K2 0.000)
      (tort (gas 0.000) (liquid 0.000))
      (kr  (gas 1.0)
           (liquid 1.0))
      (pc  (liquid 0.0))
    )

    (atm
      (porosity 0.990) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.000e+08) (solid-density 1.000e+00)
      (tcond tcondLin (solid 0.000000)(liquid 0.000000)(gas 0.000000))
```

```
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
;;JJN      (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krlLinear (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
    )

    (insul
      (porosity 0.990) (Kd (air 0.0) (water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 0.7) (solid-density 2.40e+01)
      (tcond tcondLin (solid 0.000) (liquid 0.000) (gas 0.000))
      (K0 0.00) (K1 0.0) ( K2 0.00)
      (tort (gas 1.00e+00)  (liquid 0.00))
      (kr (gas      krgLinear (Smax 1.000e+00) (Sr 0.000e+00))
          (liquid   krlLinear (Smax 1.000e+00) (Sr 0.000e+00)))
      (pc (liquid 0.0))
  )

 )

  ;; Set Boundary Conditions


  ;; (bctab
  ;;   (atmos
  ;;       (range "at*") (clamped)
  ;;   )
  ;;   (Heater
  ;;       (range "ht*") (clamped)
  ;;   )
  ;; )


  ;; Define Initial Conditions


     (state
        (P by-key ("*" 1.e5))

        (S.liquid by-key ("at*" 0.0)
                         ("dr1*" 0.0)
                         ("dr*" 0.0)
                         ("sh*" 0.0)
                         ("ht*" 0.0)
                         ("ins*" 0.0)
        )

        (T by-key ("*" 60.0)
        )


        (X.air by-key ("*" -1.0)  ("at*" 0.999) ("dr*" 0.999) ("dr1*"
0.999)
                      ("ht*" 1.0) ("sh*" 1.0) ("ins*" 0.999))
```

```
      ) ;; end state

   (input-mass-fraction on)

(linear-solver d4vband)
;;    (linear-solver pcg)
   (ilu-degree 1)
   (pcg-parameters (precond d4)(toler 1e-4)(itermax 100)(north 15))

     (srctab
       (compflux
       (comp energy)
       (name REPO)
       (range "ht*")
       (allocate-by-element ("*" 0.5))
       (table
          0.0000e+00   10.       2.00e+01    1.20e+01  2.000e+02
1.40e+01
          6.3072e+03  1.60e+01  1.2614e+04  1.80e+01  1.260e+05
2.00e+01
          3.1533e+05  2.30e+01  4.1533e+05  2.50e+01  1.038e+06
2.50e+01
          2.0380e+06  2.50e+01
         ) ;; end table
        (allocate-by-volume)
       ) ;; end compflux

    ;; (compflux
    ;; (comp water)
    ;; (name infil)
    ;; (range "*#*:1:2")
    ;; (mult-by-area z)
    ;; (table
    ;;     0.0              1.5847e-07 ;; 5.0 mm/yr
    ;;     1.0e30           1.5847e-07
    ;;    )  ;; end table

    ;;  (enthalpy   0.0   6.84E+04   1E+30   6.84E+04  ) ;; 16.3 C

    ;;    )  ;;  end compflux
       ) ;;  end srctab

(genmsh
   (down 0. 0. 1.0)
   (coord rect)
```

```
(dx          32*0.01   20*0.02   )

(dy               1)

(dz
             28*0.02    24*0.01   32*0.02        )

(mat
   (at       atm      1    nx   1    ny    1    2)
   (ins      insul    1    29   1    ny    3    3)
   (at       atm      30   nx   1    ny    3    3)
   (dr1      drift    1    29   1    ny    4    4)
   (dr       drift    1    28   1    ny    5    9)
   (dr1      drift    29   29   1    ny    5    9)
   (at       atm      31   nx   1    ny    4    8)
   (at       atm      44   nx   1    ny    10   18)
   (ins      insul    30   30   1    ny    4    9)
   (ins      insul    43   43   1    ny    10   19)
   (ins      insul    31   42   1    ny    9    9)
   (at       atm      43   nx   1    ny    9    9)
   (ins      insul    44   50   1    ny    19   19)
   (at       atm      51   nx   1    ny    19   19)
   (dr       drift    1    29   1    ny    10   10)
   (dr1      drift    30   42   1    ny    10   10)
   (dr       drift    1    41   1    ny    11   19)
   (dr1      drift    42   42   1    ny    11   19)
   (dr       drift    1    42   1    ny    20   20)
   (dr1      drift    43   50   1    ny    20   20)
   (dr       drift    1    49   1    ny    21   35)
   (dr1      drift    50   50   1    ny    21   35)
   (at       atm      52   nx   1    ny    20   61)
   (ins      insul    51   51   1    ny    20   61)
   (sh       shield   1    27   1    ny    36   37)
   (dr       drift    28   49   1    ny    36   37)
   (dr1      drift    50   50   1    ny    36   37)
   (sh       shield   26   27   1    ny    38   72)
   (dr       drift    1    25   1    ny    38   48)
   (dr       drift    28   49   1    ny    38   48)
   (dr1      drift    50   50   1    ny    38   48)
   (ht       heatr    1    17   1    ny    49   67)
   (ht       heatr    1     8   1    ny    68   70)
   (dr       drift    18   25   1    ny    49   72)
   (dr       drift    9    17   1    ny    68   72)
   (dr       drift    1     8   1    ny    71   72)
   (dr       drift    28   49   1    ny    49   60)
   (dr1      drift    50   50   1    ny    49   60)
   (dr       drift    28   45   1    ny    61   61)
   (dr1      drift    46   50   1    ny    61   61)
   (dr       drift    28   44   1    ny    62   69)
   (dr1      drift    45   45   1    ny    62   69)
   (at       atm      47   52   1    ny    63   70)
   (ins      insul    46   50   1    ny    62   62)
   (ins      insul    46   46   1    ny    63   70)
   (at       atm      51   52   1    ny    62   62)
   (dr       drift    28   38   1    ny    70   70)
```

```
(dr1     drift   39  45   1   ny   70   70)
(dr      drift   28  37   1   ny   71   72)
(dr1     drift   38  38   1   ny   71   72)
(at      atm     40  52   1   ny   72   72)
(dr      drift   1   38   1   ny   73   77)
(at      atm     40  52   1   ny   72   77)
(ins     insul   39  45   1   ny   71   71)
(at      atm     46  52   1   ny   71   71)
(ins     insul   39  39   1   ny   72   77)
(ins     insul   27  38   1   ny   78   78)
(at      atm     39  52   1   ny   78   78)
(ins     insul   27  27   1   ny   79   82)
(ins     insul   1   26   1   ny   83   83)
(at      atm     27  nx   1   ny   83   83)
(dr      drift   1   26   1   ny   78   82)
(at      atm     28  52   1   ny   79   82)
(at      atm     1   nx   1   ny   84   84)

  )

)  ;; end of genmsh

) ;; end of model input
```

```
  (usnt
  (title " 2-D T-H Model drip shield for 1/4 scale test-insul/heat
source")
  (modelname usnt)
  (include-pkg "vtough.pkg")
  (tstop   2.0380e+06)
  (time 0)
  (stepmax 1000000)
  (dtmax  2.0380e+06)
  (dt 1e3)

;; Run ymp2Ddst92
;; Check free convection in cylinder with no radiation.
;; dry condition and no
;; water application. and no invert mat.
;; Drift air K = 1E-06 and Tcond 0.026
;; Peak thermal loading @ 10 W/m


  (output
     (field (format tabular) (variables S.liquid P T RH C.water.gas )
          (file-ext ".var")
          (outtimes  0.2d .5d 1d 1.5d 2d 3d 5d 7d 9d 11d 15d 20d 22d
))

 ;; Compute fluxes

   ;;      (flux-history
   ;;       (variable Qrad)
   ;;       ( crange ("ht*" "sh*"))
   ;;       (file-ext ".rad")
   ;;      )

    ;;     (flux-history
    ;;      (variable Qrad)
    ;;      (crange ("ht*" "in*"))
    ;;      ( file-ext ".ra1")
    ;;     )



   ;;     (flux-history
   ;;      (variable Qcond)
   ;;      (crange ("ht*" "dr2*"))
   ;;      (file-ext ".con")
   ;;     )



   ;;    (flux-history
   ;;     (variable Qd.energy)
   ;;     (crange ("ht*" "sh*"))
   ;;     (file-ext ".dif")
   ;;     )


   ;; (flux-field
```

```
   ;;  (file-ext ".ad1")
   ;;  (format list)
   ;;  (variables qa.energy)
   ;;  (crange ("dr*" "sh*"))
   ;;  (outtimes 0.2y 0.5y 0.7y  1y 5y  9y ))

      (extool (variables T RH S.liquid X.air.gas P Qrad Qcond Qd.energy
V.liquid V.gas )
              (file-ext ".ext")(range "*")
(outtimes 0 0.2d 0.5d 1d 1.5d 2d 3d 5d 7d 8d 10d 12d 15d 18d 20d 22d )
  ))

  (rocktab
    (heatr
      (porosity 0.010) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 4.340e+02) (solid-density 7.854e+03)
      (tcond tcondLin (solid  60.50000)(liquid  60.500000)(gas
60.500000))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
      (tort (gas 0.000e+00) (liquid 0.0))
      (kr (gas 1.0)
          (liquid 1.0))
      (pc (liquid 0.0))
    )

    (drift
      (porosity 0.999) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.007e+03) (solid-density 1.1614)
      (tcond tcondLin (solid  0.02600)(liquid  0.02600)(gas  0.02600))
      (K0 1.000e-06) (K1 1.000e-06) (K2 1.000e-06)
;; JJN     (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krPower (power 4) (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
    )


    (shield
      (porosity 0.010) (Kd (air 0.0) (water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 4.7700e+2) (solid-density 7.900e+03)
      (tcond tcondLin (solid 14.90) (liquid 14.90) (gas 14.90))
      (K0 0.000) (K1 0.000) (K2 0.000)
      (tort (gas 0.000) (liquid 0.000))
      (kr  (gas 1.0)
           (liquid 1.0))
      (pc  (liquid 0.0))
    )

    (atm
      (porosity 0.990) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.000e+08) (solid-density 1.000e+00)
      (tcond tcondLin (solid 0.000000)(liquid 0.000000)(gas 0.000000))
```

```
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
;;JJN      (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krlLinear (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
    )

    (insul
      (porosity 0.990) (Kd (air 0.0) (water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 0.7) (solid-density 2.40e+01)
      (tcond tcondLin (solid 0.000) (liquid 0.000) (gas 0.000))
      (K0 0.00) (K1 0.0) ( K2 0.00)
      (tort (gas 1.00e+00)  (liquid 0.00))
      (kr (gas      krgLinear (Smax 1.000e+00) (Sr 0.000e+00))
          (liquid   krlLinear (Smax 1.000e+00) (Sr 0.000e+00)))
      (pc (liquid 0.0))
  )

 )

  ;; Set Boundary Conditions


  ;; (bctab
  ;;   (atmos
  ;;       (range "at*") (clamped)
  ;;   )
  ;;   (Heater
  ;;       (range "ht*") (clamped)
  ;;   )
  ;; )


  ;; Define Initial Conditions


     (state
        (P by-key ("*" 1.e5))

        (S.liquid by-key ("at*" 0.0)
                         ("dr1*" 0.0)
                         ("dr*" 0.0)
                         ("sh*" 0.0)
                         ("ht*" 0.0)
                         ("ins*" 0.0)
        )

        (T by-key ("*" 60.0)
        )


        (X.air by-key ("*" -1.0)  ("at*" 0.999) ("dr*" 0.999) ("dr1*"
0.999)
                      ("ht*" 1.0) ("sh*" 1.0) ("ins*" 0.999))
```

```
      ) ;; end state

   (input-mass-fraction on)

(linear-solver d4vband)
;;    (linear-solver pcg)
   (ilu-degree 1)
   (pcg-parameters (precond d4)(toler 1e-4)(itermax 100)(north 15))

     (srctab
       (compflux
       (comp energy)
       (name REPO)
       (range "ht*")
       (allocate-by-element ("*" 0.5))
       (table
          0.0000e+00   1.0      2.00e+01    0.20e+01  2.000e+02
0.40e+01
          6.3072e+03  0.60e+01  1.2614e+04  0.80e+01  1.260e+05
1.00e+01
          3.1533e+05  1.00e+01  4.1533e+05  1.00e+01  1.038e+06
1.00e+01
          2.0380e+06  1.00e+01
         ) ;; end table
        (allocate-by-volume)
       ) ;; end compflux

    ;; (compflux
    ;; (comp water)
    ;; (name infil)
    ;; (range "*#*:1:2")
    ;; (mult-by-area z)
    ;; (table
    ;;     0.0              1.5847e-07 ;; 5.0 mm/yr
    ;;     1.0e30           1.5847e-07
    ;;    )  ;; end table

    ;;  (enthalpy   0.0   6.84E+04   1E+30   6.84E+04  ) ;; 16.3 C

    ;;    )  ;;  end compflux
       ) ;;  end srctab

 (genmsh
    (down 0. 0. 1.0)
    (coord rect)
```

```
(dx          32*0.01  20*0.02  )

(dy               1)

(dz
             28*0.02   24*0.01  32*0.02       )

(mat
   (at       atm      1   nx   1   ny    1    2)
   (ins      insul    1   29   1   ny    3    3)
   (at       atm      30  nx   1   ny    3    3)
   (dr1      drift    1   29   1   ny    4    4)
   (dr       drift    1   28   1   ny    5    9)
   (dr1      drift    29  29   1   ny    5    9)
   (at       atm      31  nx   1   ny    4    8)
   (at       atm      44  nx   1   ny   10   18)
   (ins      insul    30  30   1   ny    4    9)
   (ins      insul    43  43   1   ny   10   19)
   (ins      insul    31  42   1   ny    9    9)
   (at       atm      43  nx   1   ny    9    9)
   (ins      insul    44  50   1   ny   19   19)
   (at       atm      51  nx   1   ny   19   19)
   (dr       drift    1   29   1   ny   10   10)
   (dr1      drift    30  42   1   ny   10   10)
   (dr       drift    1   41   1   ny   11   19)
   (dr1      drift    42  42   1   ny   11   19)
   (dr       drift    1   42   1   ny   20   20)
   (dr1      drift    43  50   1   ny   20   20)
   (dr       drift    1   49   1   ny   21   35)
   (dr1      drift    50  50   1   ny   21   35)
   (at       atm      52  nx   1   ny   20   61)
   (ins      insul    51  51   1   ny   20   61)
   (sh       shield   1   27   1   ny   36   37)
   (dr       drift    28  49   1   ny   36   37)
   (dr1      drift    50  50   1   ny   36   37)
   (sh       shield   26  27   1   ny   38   72)
   (dr       drift    1   25   1   ny   38   48)
   (dr       drift    28  49   1   ny   38   48)
   (dr1      drift    50  50   1   ny   38   48)
   (ht       heatr    1   17   1   ny   49   67)
   (ht       heatr    1    8   1   ny   68   70)
   (dr       drift    18  25   1   ny   49   72)
   (dr       drift    9   17   1   ny   68   72)
   (dr       drift    1    8   1   ny   71   72)
   (dr       drift    28  49   1   ny   49   60)
   (dr1      drift    50  50   1   ny   49   60)
   (dr       drift    28  45   1   ny   61   61)
   (dr1      drift    46  50   1   ny   61   61)
   (dr       drift    28  44   1   ny   62   69)
   (dr1      drift    45  45   1   ny   62   69)
   (at       atm      47  52   1   ny   63   70)
   (ins      insul    46  50   1   ny   62   62)
   (ins      insul    46  46   1   ny   63   70)
   (at       atm      51  52   1   ny   62   62)
   (dr       drift    28  38   1   ny   70   70)
```

```
(dr1     drift   39  45  1   ny   70  70)
(dr      drift   28  37  1   ny   71  72)
(dr1     drift   38  38  1   ny   71  72)
(at      atm     40  52  1   ny   72  72)
(dr      drift   1   38  1   ny   73  77)
(at      atm     40  52  1   ny   72  77)
(ins     insul   39  45  1   ny   71  71)
(at      atm     46  52  1   ny   71  71)
(ins     insul   39  39  1   ny   72  77)
(ins     insul   27  38  1   ny   78  78)
(at      atm     39  52  1   ny   78  78)
(ins     insul   27  27  1   ny   79  82)
(ins     insul   1   26  1   ny   83  83)
(at      atm     27  nx  1   ny   83  83)
(dr      drift   1   26  1   ny   78  82)
(at      atm     28  52  1   ny   79  82)
(at      atm     1   nx  1   ny   84  84)

  )

)  ;; end of genmsh

) ;; end of model input
```

```
;;
  (usnt
  (title " 2-D T-H Model no drip sh. for 1/4  scale test-fixed
temp.@Bound.")
  (modelname usnt)
  (include-pkg "vtough.pkg")
  (tstop   1.1533e+06)
  (time 0)
  (stepmax 1000000)
  (dtmax  1.1533e+06)
  (dt 1e3)


  (output
     (field (format tabular) (variables Vmag.gas P.gas T )
          (file-ext ".var")
          (outtimes 0.5d 1d 1.5d 2d 3d 5d 10d 13d))
   ;;  (field (format contour) (variables V.air.gas)
    ;;       (file-ext  ".vel")
    ;;       (outtimes 0.2d 0.5d 1d 1.5d 2d 3d 5d))

 ;; Compute fluxes

     (flux-history
    (variable Qrad)
    ( crange ("ht*" "dr2*"))
    (file-ext ".rad")
    )

   ;; (flux-history
    ;; (variable Qrad)
    ;; (crange ("sh*" "dr1*"))
    ;; ( file-ext ".ra1")
    ;;)



     (flux-history
      (variable Qd.energy)
      (crange ("ht*" "dr2*"))
      (file-ext ".dif")
     )



        (flux-history
         (variable Qa.energy)
         (crange ("dr2*" "dr*"))
         (file-ext ".adv")
         )


       (flux-field
        (file-ext ".vel")
        (format list)
        (variables V.gas)
        (crange ("dr2*" "dr*"))
```

```
        (outtimes 0.2d 0.5d 0.7d  1d 3d  5d 13d ))

       (extool (variables T RH S.liquid X.air.gas P Qrad Qcond Qd.energy
V.liquid V.gas )
               (file-ext ".ext")(range "*")
(outtimes 0 0.2d  0.5d 1d 1.5d 2d 3d 5d 10d 13d
        )
  ))

  (rocktab
    (heatr
      (porosity 0.010) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 4.340e+02) (solid-density 7.854e+03)
      (tcond tcondLin (solid  60.500000)(liquid  60.500000)(gas
60.500000))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
      (tort (gas 0.000e+00) (liquid 0.0))
      (kr (gas 1.0)
          (liquid 1.0))
      (pc (liquid 0.0))
    )

    (drift
      (porosity 0.999) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.007e+03) (solid-density 1.1614)
      (tcond tcondLin (solid 0.026300)(liquid 0.026300)(gas 0.026300))
      (K0 1.000e-06) (K1 1.000e-06) (K2 1.000e-06)
;; JJN     (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krPower (power 4) (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
    )

    (invert
      (porosity 0.545) (Kd (air 0.0) (water 0.0))
      (KdFactor (water 0.0) ( air 0.0))
      (Cp 939.0) (solid-density 1.150e+03)
      (tcond tcondLin (solid 0.66) (liquid 0.66) (gas 0.66))
      (Kx 1.000e-10) (Ky 1.00e-10) (Kz 1.00e-10)
      (tort (gas 0.700) (liquid 0.0))
      (kr (gas krgEffCont) (liquid krlEffCont))
      (pc (liquid pcEffCont (alpham 8.0E-08) (alphaf 1.0E-02)
      (betam 1.4) (betaf 1.4)
      (Km 1.0E-20) (Kf 1.0E-07)
      (phim 1.0E-01) (phif 1.0E-03)
      (Sresm 0.1073) (Sresf 0.0)
      (Smaxm 0.7)))
    )

    (shield
      (porosity 0.010) (Kd (air 0.0) (water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 4.7700e+2) (solid-density 7.900e+03)
      (tcond tcondLin (solid 14.90) (liquid 14.90) (gas 14.90))
```

```
      (K0 0.000) (K1 0.000) (K2 0.000)
      (tort (gas 0.000) (liquid 0.000))
      (kr  (gas 1.0)
           (liquid 1.0))
      (pc  (liquid 0.0))
    )

    (atm
      (porosity 0.990) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.000e+08) (solid-density 1.000e+00)
      (tcond tcondLin (solid 0.170000)(liquid 0.170000)(gas 0.170000))
      (K0 1.000e-08) (K1 0.000e+00) (K2 0.000e+00)
;;JJN      (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krlLinear (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
    )
  )


  ;; Set Boundary Conditions


   (bctab
     (atmos
         (range "at*") (clamped)
     )
     (Heater
         (range "ht*") (clamped)
     )
   )


  ;; Define Initial Conditions


     (state
        (P by-key ("*" 1.e5))

        (S.liquid by-key ("at*" 0.0)
                         ("dr1*" 0.0)
                         ("dr*" 0.0)
                         ("ht*" 0.0)
                         ("in*" 0.1073)
                         ("dr2*" 0.0)
        )

        (T by-key ("at*" 60.0)
                  ("ht*" 80.0)
                  ("dr*" 25.0)
                  ("dr1*" 25.0)
                  ("in*" 25.0)
                  ("dr2*" 25.0)
        )
```

```
        (X.air by-key ("*" -1.0)  ("at*" 0.999) ("dr*" 0.999) ("dr1*"
0.999)
                        ("ht*" 1.0) ("dr2*" 0.999) )

       ) ;; end state


   (input-mass-fraction on)


(linear-solver d4vband)
;;   (linear-solver pcg)
   (ilu-degree 1)
   (pcg-parameters (precond d4)(toler 1e-4)(itermax 100)(north 15))





   ;;(srctab
   ;;  (compflux
   ;;  (comp energy)
   ;;  (name REPO)
   ;;  (range "ht*")
   ;;  (allocate-by-element ("*" 0.5))
   ;;  (table
   ;;     0.0000e+00  6.00e+02  6.3072e+07  5.80e+02  1.2614e+08
5.55e+02
   ;;     1.8922e+08  5.34e+02  2.5229e+08  5.14e+02  3.1536e+08
4.97e+02
   ;;     9.4608e+08  3.60e+02  1.5768e+09  2.75e+02  2.2075e+09
2.19e+02
   ;;     2.8382e+09  1.82e+02  4.7304e+09  1.26e+02  7.8840e+09
9.29e+01
   ;;     1.1038e+10  7.64e+01  1.4191e+10  6.59e+01  1.7345e+10
5.76e+01
   ;;     2.0498e+10  5.12e+01  2.3652e+10  4.57e+01  2.6806e+10
4.12e+01
   ;;     2.9959e+10  3.77e+01  6.3072e+10  1.95e+01  1.2614e+11
1.36e+01
   ;;     1.8922e+11  1.18e+01  2.5229e+11  1.03e+01  3.1536e+11
9.29e+00

   ;;     ) ;; end table
   ;;    (allocate-by-volume)
   ;;  ) ;; end compflux


    ;; (compflux
    ;; (comp water)
    ;; (name infil)
    ;; (range "*#*:1:2")
    ;; (mult-by-area z)
    ;; (table
```

```
 ;;      0.0              1.5847e-07 ;; 5.0 mm/yr
 ;;      1.0e30           1.5847e-07
 ;;     )  ;; end table

 ;;  (enthalpy   0.0   6.84E+04   1E+30   6.84E+04  ) ;; 16.3 C

 ;;     )  ;;  end compflux
;;  ) ;;  end srctab


(genmsh
   (down 0. 0. 1.0)
   (coord rect)

   (dx          32*0.01  20*0.02  )


   (dy               1)


   (dz
                28*0.02   24*0.01  32*0.02       )

   (mat
      (at       atm     1   nx   1   ny     1    3)
      (dr1      drift   1   29   1   ny     4    4)
      (dr       drift   1   28   1   ny     5    9)
      (dr1      drift   29  29   1   ny     5    9)
      (at       atm     30  nx   1   ny     4    9)
      (at       atm     43  nx   1   ny    10   19)
      (dr       drift   1   29   1   ny    10   10)
      (dr1      drift   30  42   1   ny    10   10)
      (dr       drift   1   41   1   ny    11   19)
      (dr1      drift   42  42   1   ny    11   19)
      (dr       drift   1   42   1   ny    20   20)
      (dr1      drift   43  50   1   ny    20   20)
      (dr       drift   1   49   1   ny    21   35)
      (dr1      drift   50  50   1   ny    21   35)
      (at       atm     51  nx   1   ny    20   61)
      (dr       drift   1   27   1   ny    36   37)
      (dr       drift   28  49   1   ny    36   37)
      (dr1      drift   50  50   1   ny    36   37)
      (dr       drift   26  27   1   ny    38   72)
      (dr       drift   1   25   1   ny    38   47)
      (dr2      drift   1   18   1   ny    48   48)
      (dr       drift   19  25   1   ny    48   48)
      (dr       drift   28  49   1   ny    38   48)
      (dr1      drift   50  50   1   ny    38   48)
      (ht       heatr   1   17   1   ny    49   67)
      (ht       heatr   1    8   1   ny    68   70)
      (dr       drift   19  25   1   ny    49   72)
      (dr       drift   10  17   1   ny    69   72)
      (dr       drift   1    8   1   ny    72   72)
      (dr2      drift   18  18   1   ny    49   68)
      (dr       drift   18  18   1   ny    69   72)
      (dr2      drift   9   17   1   ny    68   68)
```

```
(dr2     drift   9    9   1   ny   69   71)
(dr      drift   9    9   1   ny   72   72)
(dr2     drift   1    8   1   ny   71   71)
(dr      drift   28   49  1   ny   49   60)
(dr1     drift   50   50  1   ny   49   60)
(dr      drift   28   45  1   ny   61   61)
(dr1     drift   46   50  1   ny   61   61)
(dr      drift   28   44  1   ny   62   69)
(dr1     drift   45   45  1   ny   62   69)
(at      atm     46   52  1   ny   62   70)
(dr      drift   28   38  1   ny   70   70)
(dr1     drift   39   45  1   ny   70   70)
(dr      drift   28   37  1   ny   71   72)
(dr1     drift   38   38  1   ny   71   72)
(at      atm     39   52  1   ny   71   72)
(in      invert  1    38  1   ny   73   77)
(at      atm     39   52  1   ny   73   77)
(in      invert  1    26  1   ny   78   82)
(at      atm     27   52  1   ny   78   82)
(at      atm     1    nx  1   ny   83   84)

    )

  (include  "results29")

)  ;; end of genmsh

) ;; end of model input
```

```
;; File 2Ddst4.rad
radiating_block 1 17 1 1 49 49 0 0 -1 0.5 0.98
connections     1 29 1 1  3  3 0 0  1

 ıdiating_block 1 17 1 1 49 49 0 0 -1 0.5 0.98
connections    30 42 1 1  9  9 0 0  1
c
radiating_block 1 17 1 1 49 49 0 0 -1 0.5 0.98
connections    43 50 1 1 19 19 0 0  1
c
radiating_block 1 17 1 1 49 49 1 0  0 0.5 0.98
connections    30 30 1 1  4  9 -1 0 0
c
radiating_block 1 17 1 1 49 49 1 0  0 0.5 0.98
connections    43 43 1 1 10 19 -1 0 0
c
radiating_block 1 17 1 1 49 49 1 0  0 0.5 0.98
connections    51 51 1 1 20 48 -1 0 0
c
radiating_block 17 17 1 1 49 67 0 0 -1 0.5 0.98
connections     30 42 1 1  9  9 0 0  1
c
radiating_block 17 17 1 1 49 67 0 0 -1 0.5 0.98
connections     43 50 1 1 19 19 0 0  1
c
radiating_block 17 17 1 1 49 67 1 0 0 0.5 0.98
connections     43 43 1 1 10 19 -1 0 0
c
radiating_block 17 17 1 1 49 67 1 0 0 0.5 0.98
 ›nnections     51 51 1 1 20 61 -1 0 0
c
radiating_block 17 17 1 1 49 67 1 0 0 0.5 0.98
connections     46 46 1 1 62 70 -1 0 0
c
radiating_block 17 17 1 1 49 67 0 0 1 0.5 0.98
connections     39 45 1 1 71 71 0 0 -1
c
radiating_block 17 17 1 1 49 67 0 0 1 0.5 0.98
connections     28 38 1 1 73 73 0 0 -1
c
radiating_block  9 17 1 1 67 67 0 0 1 0.5 0.98
connections      9 38 1 1 73 73 0 0 -1
c
radiating_block  9 17 1 1 67 67 0 0 1 0.5 0.98
connections     39 45 1 1 71 71 0 0 -1
c
radiating_block  9 17 1 1 67 67 1 0 0 0.5 0.98
connections     26 26 1 1 68 72 -1 0 0
c
radiating_block  8  8 1 1 68 70 1 0 0 0.5 0.98
connections     46 46 1 1 68 70 -1 0 0
c
radiating_block  8  8 1 1 68 70 0 0 1 0.5 0.98
connections      9 38 1 1 73 73 0 0 -1

 ıdiating_block  1  8 1 1 70 70 0 0 1 0.5 0.98
connections      1 38 1 1 73 73 0 0 -1
c
```

```
(usnt
(title " 2-D T-H Model w. drip shield for 1/4  scale test-fixed temp.@Bound."
(modelname usnt)
(include-pkg "vtough.pkg")
(tstop   1.1533e+06)
(time 0)
(stepmax 1000000)
(dtmax  1.1533e+06)
(dt 1e3)


;; ymp2Ddst01
;; Central heater fixed @ 80 C and canister wall (outer heater) @ 60 C

;; drift air K = 1E-6   , Tcond = 0.026

(output
   (field (format tabular) (variables  Vmag.gas P.gas T )
        (file-ext ".var")
        (outtimes 0.2d 0.5d 1d 1.5d 2d 3d 5d 10d 13d))

;; Compute fluxes

     (flux-history
      (variable Qrad)
      ( crange ("ht*" "sh*"))
      (file-ext ".rad")
     )

     (flux-history
      (variable Qrad)
      (crange ("ht*" "in*"))
      (file-ext ".ra1")
     )

  ;; (flux-history
   ;; (variable Qrad)
   ;; (crange ("sh*" "dr1*"))
   ;; ( file-ext ".ra1")
   ;;)



    (flux-history
     (variable Qd.energy)
     (crange ("ht*" "dr2*"))
     (file-ext ".con")
    )

   (flux-history
    (variable Qd.energy)
    (crange ("ht*" "in*"))
    (file-ext ".co1")
   )

   (flux-history
    (variable Qcond)
    (crange ("ht*" "dr2*"))
    (file-ext  ".co2")
   )
```

```
    (flux-history
     (variable Qcond)
     (crange ("ht*" "in*"))
     (file-ext ".co3")
    )

     (flux-history
      (variable Qa.energy)
      (crange ("dr2*" "dr3*"))
      (file-ext ".toq")
     )
     (flux-history
      (variable Q.energy)
      (crange ("ht*" "in*"))
      (file-ext ".to1")
     )


  ;;    (flux-history
  ;;     (variable Qad.energy)
  ;;     (crange ("dr2*" "dr*"))
  ;;     (file-ext ".adv")
  ;;     )

      (flux-history
       (variable Qa.air)
       (crange ("dr2*" "dr*"))
       (file-ext ".ad1")
      )

      (flux-history
       (variable Qa.air)
       (crange  ("dr2*" "dr3*"))
       (file-ext ".ad2")
      )


      (flux-field
       (file-ext ".vel")
       (format list)
       (variables V.gas)
       (crange ("dr2*" "dr*"))
       (outtimes 0.2d 0.5d 0.7d  1d 3d 5d 13d ))

        (extool (variables T RH S.liquid X.air.gas P qrad qcond V.liquid V.gas )
                (file-ext ".ext")(range "*")
(outtimes 0 0.2d 0.5d 1d 1.5d 2d 3d 5d 10d 13d
        )
  ))

  (rocktab
    (heatr
      (porosity 0.010) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 4.8886e+02) (solid-density 8.1892e+03)
      (tcond tcondLin (solid  14.420000)(liquid  14.420000)(gas  14.420000))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
      (tort (gas 0.000e+00) (liquid 0.0))
      (kr (gas 1.0)
```

```
          (liquid 1.0))
        (pc (liquid 0.0))
    )

    (drift
        (porosity 0.999) (Kd (air 0.0)(water 0.0))
        (KdFactor (water 0.0) (air 0.0))
        (Cp 1.007e+03) (solid-density 1.1614)
        (tcond tcondLin (solid 0.026000)(liquid 0.026000)(gas 0.026000))
        (K0 1.000e-06) (K1 1.000e-06) (K2 1.000e-06)
;; JJN     (tort (gas 0.000e+00) (liquid 0.0))
        (tort (gas 1.000e+00) (liquid 0.0))
        (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
            (liquid krPower (power 4) (Smax 1.000e+00)(Sr 0.000e+00)))
        (pc (liquid 0.0))
    )

    (invert
        (porosity 0.545) (Kd (air 0.0) (water 0.0))
        (KdFactor (water 0.0) ( air 0.0))
        (Cp 948.0) (solid-density 2.530e+03)
        (tcond tcondLin (solid 0.66) (liquid 0.66) (gas 0.66))
        (Kx 6.150e-10) (Ky 6.15e-10) (Kz 6.15e-10)
        (tort (gas 0.700) (liquid 0.0))
        (kr (gas krgEffCont) (liquid krlEffCont))
        (pc (liquid pcEffCont (alpham 1.2232E-03) (alphaf 1.22320E-03)
        (betam 2.7) (betaf 2.7)
        (Km 6.15E-10) (Kf 0.0)
        (phim 0.545) (phif 0.0)
        (Sresm 0.0920) (Sresf 0.0)
         ))
    )

    (shield
        (porosity 0.010) (Kd (air 0.0) (water 0.0))
        (KdFactor (water 0.0) (air 0.0))
        (Cp 5.5132e+2) (solid-density 7.900e+03)
        (tcond tcondLin (solid 20.55) (liquid 20.55) (gas 20.55))
        (K0 0.000) (K1 0.000) (K2 0.000)
        (tort (gas 0.000) (liquid 0.000))
        (kr  (gas 1.0)
             (liquid 1.0))
        (pc  (liquid 0.0))
    )

    (atm
        (porosity 0.990) (Kd (air 0.0)(water 0.0))
        (KdFactor (water 0.0) (air 0.0))
        (Cp 1.000e+08) (solid-density 1.000e+00)
        (tcond tcondLin (solid 0.026300)(liquid 0.026300)(gas 0.026300))
        (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
;;JJN     (tort (gas 0.000e+00) (liquid 0.0))
        (tort (gas 1.000e+00) (liquid 0.0))
        (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
            (liquid krlLinear (Smax 1.000e+00)(Sr 0.000e+00)))
        (pc (liquid 0.0))
    )
  )
```

```
;; Set Boundary Conditions

 (bctab
   (atmos
       (range "at*") (clamped)
   )
   (Heater
       (range "ht*") (clamped)
   )
 )

;; Define Initial Conditions

   (state
      (P by-key ("*" 1.e5))

      (S.liquid by-key ("at*" 0.0)
                       ("dr1*" 0.0)
                       ("dr*" 0.0)
                       ("sh*" 0.0)
                       ("ht*" 0.0)
                       ("in*" 0.1073)
                       ("dr2*" 0.0)
                       ("dr3*" 0.0)
      )

      (T by-key ("at*" 60.0)
                ("ht*" 80.0)
                ("dr*" 60.0)
                ("dr1*" 60.0)
                ("sh*" 60.0)
                ("in*" 60.0)
                ("dr2*" 60.0)
                ("dr3*" 60.0)
      )

      (X.air by-key ("*" -1.0)  ("at*" 0.999) ("dr*" 0.999) ("dr1*" 0.999)
                    ("ht*" 1.0) ("dr2*" 0.999) ("dr3*" 0.999) ("sh*" 1.0))

     ) ;; end state

  (input-mass-fraction on)

(linear-solver d4vband)
;;    (linear-solver pcg)
   (ilu-degree 1)
   (pcg-parameters (precond d4)(toler 1e-4)(itermax 100)(north 15))
```

```
(dr      drift   1   41   1   ny   11   19)
(dr1     drift   42  42   1   ny   11   19)
(dr      drift   1   42   1   ny   20   20)
(dr1     drift   43  50   1   ny   20   20)
(dr      drift   1   49   1   ny   21   35)
(dr1     drift   50  50   1   ny   21   35)
(at      atm     51  nx   1   ny   20   61)
(sh      shield  1   27   1   ny   36   37)
(dr      drift   28  49   1   ny   36   37)
(dr1     drift   50  50   1   ny   36   37)
(sh      shield  26  27   1   ny   38   72)
(dr      drift   1   24   1   ny   39   47)
(dr3     drift   25  25   1   ny   39   47)
(dr3     drift   1   25   1   ny   38   38)
(dr2     drift   1   18   1   ny   48   48)
(dr      drift   19  24   1   ny   48   48)
(dr3     drift   25  25   1   ny   48   48)
(dr      drift   28  49   1   ny   38   48)
(dr1     drift   50  50   1   ny   38   48)
(ht      heatr   1   17   1   ny   49   67)
(ht      heatr   1    8   1   ny   68   70)
(dr      drift   19  24   1   ny   49   71)
(dr3     drift   19  24   1   ny   72   72)
(dr3     drift   25  25   1   ny   49   72)
(dr      drift   10  17   1   ny   69   71)
(dr3     drift   10  17   1   ny   72   72)
(dr3     drift   1    8   1   ny   72   72)
(dr2     drift   18  18   1   ny   49   68)
(dr      drift   18  18   1   ny   69   71)
(dr3     drift   18  18   1   ny   72   72)
(dr2     drift    9  17   1   ny   68   68)
(dr2     drift    9   9   1   ny   69   71)
(dr3     drift    9   9   1   ny   72   72)
(dr2     drift    1   8   1   ny   71   71)
(dr      drift   28  49   1   ny   49   60)
(dr1     drift   50  50   1   ny   49   60)
(dr      drift   28  45   1   ny   61   61)
(dr1     drift   46  50   1   ny   61   61)
(dr      drift   28  44   1   ny   62   69)
(dr1     drift   45  45   1   ny   62   69)
(at      atm     46  52   1   ny   62   70)
(dr      drift   28  38   1   ny   70   70)
(dr1     drift   39  45   1   ny   70   70)
(dr      drift   28  37   1   ny   71   72)
(dr1     drift   38  38   1   ny   71   72)
(at      atm     39  52   1   ny   71   72)
(in      invert  1   38   1   ny   73   77)
(at      atm     39  52   1   ny   73   77)
(in      invert  1   26   1   ny   78   82)
(at      atm     27  52   1   ny   78   82)
(at      atm     1   nx   1   ny   83   84)

    )

  (include  "results28")

)  ;; end of genmsh
```

```
) ;; end of model input
```

```
;;
  (usnt
  (title " 2-D T-H Model w. drip shield for 1/4  scale test-fixed
temp.@Bound.")
  (modelname usnt)
  (include-pkg "vtough.pkg")
  (tstop   1.1533e+06)
  (time 0)
  (stepmax 1000000)
  (dtmax  1.1533e+06)
  (dt 1e3)


  (output
     (field (format tabular) (variables Vmag.gas P.gas T )
          (file-ext ".var")
          (outtimes 0.2d 0.5d 1d 1.5d 2d 3d 5d 10d 13d))

 ;; Compute fluxes

      (flux-history
       (variable Qrad)
       ( crange ("ht*" "sh*"))
       (file-ext ".rad")
      )

    ;; (flux-history
     ;; (variable Qrad)
     ;; (crange ("sh*" "dr1*"))
     ;; ( file-ext ".ra1")
     ;;)



      (flux-history
       (variable Qd.energy)
       (crange ("ht*" "dr2*"))
       (file-ext ".con")
      )



       (flux-history
        (variable Qa.energy)
        (crange ("dr2*" "dr*"))
        (file-ext ".adv")
        )


       (flux-field
        (file-ext ".vel")
        (format list)
        (variables V.gas)
        (crange ("dr2*" "dr*"))
        (outtimes 0.2d 0.5d 0.7d  1d 3d 5d 13d ))
```

```
      (extool (variables T RH S.liquid X.air.gas P Qrad Qcond Qd.energy
V.liquid V.gas )
              (file-ext ".ext")(range "*")
(outtimes 0 0.2d 0.5d 1d 1.5d 2d 3d 5d 10d 13d
        )
  ))

  (rocktab
    (heatr
      (porosity 0.010) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 4.340e+02) (solid-density 7.854e+03)
      (tcond tcondLin (solid  60.500000)(liquid  60.500000)(gas
60.500000))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
      (tort (gas 0.000e+00) (liquid 0.0))
      (kr (gas 1.0)
          (liquid 1.0))
      (pc (liquid 0.0))
    )

    (drift
      (porosity 0.999) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.007e+03) (solid-density 1.1614)
      (tcond tcondLin (solid 0.026300)(liquid 0.026300)(gas 0.026300))
      (K0 1.000e-06) (K1 1.000e-06) (K2 1.000e-06)
;; JJN     (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krPower (power 4) (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
    )

    (invert
      (porosity 0.545) (Kd (air 0.0) (water 0.0))
      (KdFactor (water 0.0) ( air 0.0))
      (Cp 939.0) (solid-density 1.150e+03)
      (tcond tcondLin (solid 0.66) (liquid 0.66) (gas 0.66))
      (Kx 1.000e-10) (Ky 1.00e-10) (Kz 1.00e-10)
      (tort (gas 0.700) (liquid 0.0))
      (kr (gas krgEffCont) (liquid krlEffCont))
      (pc (liquid pcEffCont (alpham 8.0E-08) (alphaf 1.0E-02)
      (betam 1.4) (betaf 1.4)
      (Km 1.0E-20) (Kf 1.0E-07)
      (phim 1.0E-01) (phif 1.0E-03)
      (Sresm 0.1073) (Sresf 0.0)
      (Smaxm 0.7)))
    )

    (shield
      (porosity 0.010) (Kd (air 0.0) (water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 4.7700e+2) (solid-density 7.900e+03)
      (tcond tcondLin (solid 14.90) (liquid 14.90) (gas 14.90))
      (K0 0.000) (K1 0.000) (K2 0.000)
      (tort (gas 0.000) (liquid 0.000))
```

```
      (kr   (gas 1.0)
            (liquid 1.0))
      (pc   (liquid 0.0))
    )

    (atm
      (porosity 0.990) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.000e+08) (solid-density 1.000e+00)
      (tcond tcondLin (solid 0.170000)(liquid 0.170000)(gas 0.170000))
      (K0 1.000e-08) (K1 0.000e+00) (K2 0.000e+00)
;;JJN      (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krlLinear (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
    )
  )


  ;; Set Boundary Conditions


   (bctab
     (atmos
         (range "at*") (clamped)
     )
     (Heater
         (range "ht*") (clamped)
     )
   )


  ;; Define Initial Conditions


     (state
        (P by-key ("*" 1.e5))

        (S.liquid by-key ("at*" 0.0)
                         ("dr1*" 0.0)
                         ("dr*" 0.0)
                         ("sh*" 0.0)
                         ("ht*" 0.0)
                         ("in*" 0.1073)
                         ("dr2*" 0.0)
        )

        (T by-key ("at*" 60.0)
                  ("ht*" 80.0)
                  ("dr*" 60.0)
                  ("dr1*" 60.0)
                  ("sh*" 60.0)
                  ("in*" 60.0)
                  ("dr2*" 60.0)
        )
```

```
        (X.air by-key ("*" -1.0)  ("at*" 0.999) ("dr*" 0.999) ("dr1*"
0.999)
                        ("ht*" 1.0) ("dr2*" 0.999) ("sh*" 1.0))

       ) ;; end state


   (input-mass-fraction on)


(linear-solver d4vband)
;;   (linear-solver pcg)
   (ilu-degree 1)
   (pcg-parameters (precond d4)(toler 1e-4)(itermax 100)(north 15))




   ;;(srctab
   ;;  (compflux
   ;;  (comp energy)
   ;;  (name REPO)
   ;;  (range "ht*")
   ;;  (allocate-by-element ("*" 0.5))
   ;;  (table
   ;;     0.0000e+00  6.00e+02  6.3072e+07  5.80e+02  1.2614e+08
5.55e+02
   ;;     1.8922e+08  5.34e+02  2.5229e+08  5.14e+02  3.1536e+08
4.97e+02
   ;;     9.4608e+08  3.60e+02  1.5768e+09  2.75e+02  2.2075e+09
2.19e+02
   ;;     2.8382e+09  1.82e+02  4.7304e+09  1.26e+02  7.8840e+09
9.29e+01
   ;;     1.1038e+10  7.64e+01  1.4191e+10  6.59e+01  1.7345e+10
5.76e+01
   ;;     2.0498e+10  5.12e+01  2.3652e+10  4.57e+01  2.6806e+10
4.12e+01
   ;;     2.9959e+10  3.77e+01  6.3072e+10  1.95e+01  1.2614e+11
1.36e+01
   ;;     1.8922e+11  1.18e+01  2.5229e+11  1.03e+01  3.1536e+11
9.29e+00

   ;;    ) ;; end table
   ;;   (allocate-by-volume)
   ;;  ) ;; end compflux


    ;; (compflux
    ;; (comp water)
    ;; (name infil)
    ;; (range "*#*:1:2")
    ;; (mult-by-area z)
    ;; (table
```

```
;;      0.0                 1.5847e-07 ;; 5.0 mm/yr
;;      1.0e30              1.5847e-07
;;     )  ;; end table

;;  (enthalpy   0.0   6.84E+04   1E+30   6.84E+04  ) ;; 16.3 C

;;     )  ;;  end compflux
;;  ) ;;  end srctab


(genmsh
   (down 0. 0. 1.0)
   (coord rect)

   (dx          32*0.01  20*0.02  )


   (dy               1)


   (dz
                28*0.02   24*0.01  32*0.02        )

   (mat
      (at       atm      1   nx   1   ny    1    3)
      (dr1      drift    1   29   1   ny    4    4)
      (dr       drift    1   28   1   ny    5    9)
      (dr1      drift    29  29   1   ny    5    9)
      (at       atm      30  nx   1   ny    4    9)
      (at       atm      43  nx   1   ny   10   19)
      (dr       drift    1   29   1   ny   10   10)
      (dr1      drift    30  42   1   ny   10   10)
      (dr       drift    1   41   1   ny   11   19)
      (dr1      drift    42  42   1   ny   11   19)
      (dr       drift    1   42   1   ny   20   20)
      (dr1      drift    43  50   1   ny   20   20)
      (dr       drift    1   49   1   ny   21   35)
      (dr1      drift    50  50   1   ny   21   35)
      (at       atm      51  nx   1   ny   20   61)
      (sh       shield   1   27   1   ny   36   37)
      (dr       drift    28  49   1   ny   36   37)
      (dr1      drift    50  50   1   ny   36   37)
      (sh       shield   26  27   1   ny   38   72)
      (dr       drift    1   25   1   ny   38   47)
      (dr2      drift    1   18   1   ny   48   48)
      (dr       drift    19  25   1   ny   48   48)
      (dr       drift    28  49   1   ny   38   48)
      (dr1      drift    50  50   1   ny   38   48)
      (ht       heatr    1   17   1   ny   49   67)
      (ht       heatr    1    8   1   ny   68   70)
      (dr       drift    19  25   1   ny   49   72)
      (dr       drift    10  17   1   ny   69   72)
      (dr       drift    1    8   1   ny   72   72)
      (dr2      drift    18  18   1   ny   49   68)
      (dr       drift    18  18   1   ny   69   72)
      (dr2      drift     9  17   1   ny   68   68)
```

```
(dr2     drift    9   9   1   ny   69   71)
(dr      drift    9   9   1   ny   72   72)
(dr2     drift    1   8   1   ny   71   71)
(dr      drift   28  49   1   ny   49   60)
(dr1     drift   50  50   1   ny   49   60)
(dr      drift   28  45   1   ny   61   61)
(dr1     drift   46  50   1   ny   61   61)
(dr      drift   28  44   1   ny   62   69)
(dr1     drift   45  45   1   ny   62   69)
(at      atm     46  52   1   ny   62   70)
(dr      drift   28  38   1   ny   70   70)
(dr1     drift   39  45   1   ny   70   70)
(dr      drift   28  37   1   ny   71   72)
(dr1     drift   38  38   1   ny   71   72)
(at      atm     39  52   1   ny   71   72)
(in      invert  1   38   1   ny   73   77)
(at      atm     39  52   1   ny   73   77)
(in      invert  1   26   1   ny   78   82)
(at      atm     27  52   1   ny   78   82)
(at      atm     1   nx   1   ny   83   84)

    )

  (include  "results28")

)  ;; end of genmsh

) ;; end of model input
```

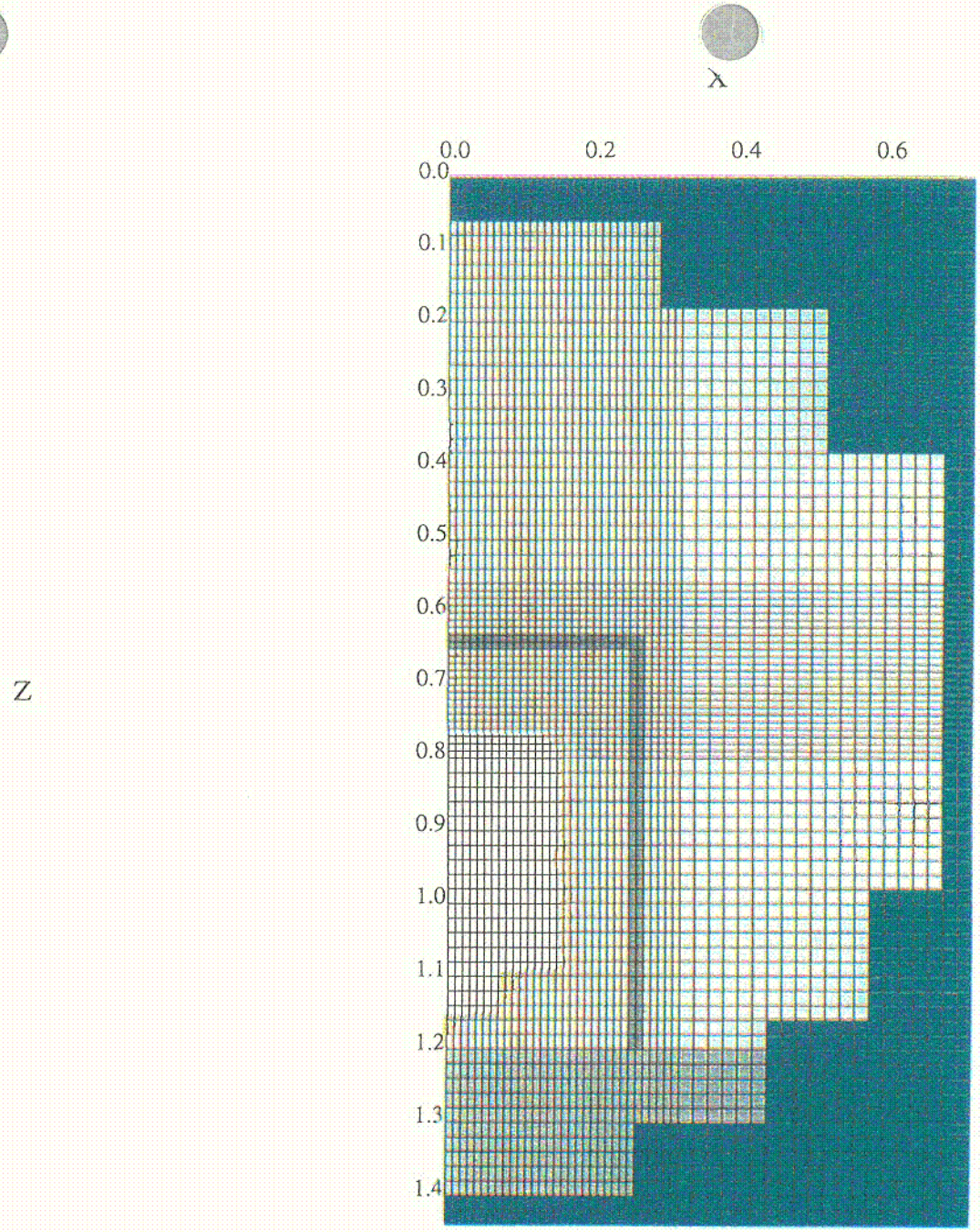
```
;; File 2Ddst0.rad
radiating_block 1  17  1  1  49  49  0  0  -1 0.5  0.98
connections     1  25  1  1  37  37  0  0   1

 adiating_block 1  17  1  1  49  49  1  0   0 0.5  0.98
connections    26  26  1  1  38  48 -1  0   0
c
radiating_block 17 17  1  1  49  67  0  0  -1 0.5  0.98
connections    18  25  1  1  37  37  0  0   1
c
radiating_block 17 17  1  1  49  67  1  0   0 0.5  0.98
connections    26  26  1  1  38  72 -1  0   0
c
radiating_block 17 17  1  1  49  67  0  0   1 0.5  0.98
connections    18  25  1  1  73  73  0  0  -1
c
radiating_block  9 17  1  1  67  67  0  0   1 0.5  0.98
connections     9  25  1  1  73  73  0  0  -1
c
radiating_block  9 17  1  1  67  67  1  0   0 0.5  0.98
connections    26  26  1  1  68  72 -1  0   0
c
radiating_block  8  8  1  1  68  70  1  0   0 0.5  0.98
connections    26  26  1  1  68  72 -1  0   0
c
radiating_block  8  8  1  1  68  70  0  0   1 0.5  0.98
connections     9  25  1  1  73  73  0  0  -1
c
radiating_block  1  8  1  1  70  70  0  0   1 0.5  0.98
 onnections     1  25  1  1  73  73  0  0  -1
c
radiating_block  1 27  1  1  36  36  0  0  -1 0.5  0.39
connections     1  29  1  1   3   3  0  0   1
c
radiating_block  1 27  1  1  36  36  0  0  -1 0.5  0.39
connections    30  42  1  1   9   9  0  0   1
c
radiating_block  1 27  1  1  36  36  0  0  -1 0.5  0.39
connections    43  50  1  1  19  19  0  0   1
c
radiating_block  1 27  1  1  36  36  1  0   0 0.5  0.39
connections    30  30  1  1   4   9 -1  0   0
c
radiating_block  1 27  1  1  36  36  1  0   0 0.5  0.39
connections    43  43  1  1  10  19 -1  0   0
c
radiating_block  1 27  1  1  36  36  1  0   0 0.5  0.39
connections    51  51  1  1  20  35 -1  0   0
c
radiating_block 27 27  1  1  36  72  0  0  -1 0.5  0.39
connections    30  42  1  1   9   9  0  0   1
c
radiating_block 27 27  1  1  36  72  0  0  -1 0.5  0.39
connections    43  50  1  1  19  19  0  0   1

 adiating_block 27 27  1  1  36  72  0  0   1 0.5  0.39
connections    39  45  1  1  71  71  0  0  -1
c
radiating_block 27 27  1  1  36  72  0  0   1 0.5  0.39
connections    28  38  1  1  73  73  0  0  -1
```

```
c
radiating_block 27 27  1  1  36  72  1  0   0 0.5  0.39
connections     43 43  1  1  10  19 -1  0   0

 ıdiating_block 27 27  1  1  36  72  1  0   0 0.5  0.39
connections     51 51  1  1  20  61 -1  0   0
c
radiating_block 27 27  1  1  36  72  1  0   0 0.5  0.39
connections     46 46  1  1  62  70 -1  0   0
c
```



Input file: radymp2Ddst0
Connection file: 2Ddst0.rad

```
  (usnt
  (title "2D T-H Model/drip shield/water appl.for pilot test-fixed
temp.@Bound")
  (modelname usnt)
  (include-pkg "vtough.pkg")
  (tstop   4.3200e+06)
  (time 0)
  (stepmax 1000000)
  (dtmax  4.3200e+06)
  (dt 1e3)

  ;; Run ymp2Ddstw8R

  ;; fix invert mat saturation at 0.8 and temp. @ 70 C.
  ;; Wicks set at   0 cm suction  & and no outflow

  (output
     (field (format tabular) (variables Vmag.gas P.gas T S.liquid P )
          (file-ext ".var")
          (outtimes 0.2d 0.5d 1d 1.5d 2d 3d 5d 10d 13d 21d 35d 49d))


 ;; compute fluxes across invert surface
    (flux-history
     (variable Q.water)
     (crange ("in*" "dr*"))
     (file-ext ".fl1")
     )

    (flux-history
     (variable Q.water)
     (index-crange (28 1 73 28 1 72) (29 1 73 29 1 72) (30 1 73 30 1
72)
                   (31 1 73 31 1 72) (32 1 73 32 1 72) (33 1 73 33 1
72)
                   (34 1 73 34 1 72) (35 1 73 35 1 72) (36 1 73 36 1
72)
                   (37 1 73 37 1 72) (38 1 73 38 1 72) )
        (file-ext ".fl3")
     )

 ;; compute fluxes across approx. water-vapor interface

    (flux-history
     (variable Q.water)
     (index-crange (29 1 77 29 1 76) (30 1 77 30 1 76) (31 1 77 31 1
76)
                   (32 1 77 32 1 76) (33 1 77 33 1 76) (34 1 77 34 1
76)
                   (35 1 77 35 1 76) (36 1 77 36 1 76) (37 1 77 37 1
76)
                   (38 1 77 38 1 76) )
       (file-ext ".fl2")
     )

 ;; Compute thermal fluxes
```

```
(flux-history
 (variable Qrad)
 ( crange ("ht*" "sh*"))
 (file-ext ".rad")
)

;; (flux-history
 ;; (variable Qrad)
 ;; (crange ("sh*" "dr1*"))
 ;; ( file-ext ".ra1")
 ;;)


(flux-history
 (variable Qd.energy)
 (crange ("ht*" "dr2*"))
 (file-ext ".con")
)


(flux-history
 (variable Qa.energy)
 (crange ("dr2*" "dr*"))
 (file-ext ".adv")
 )


(flux-field
 (file-ext ".vel")
 (format list)
 (variables V.gas)
 (crange ("dr2*" "dr*"))
 (outtimes 0.2d 0.5d 0.7d  1d 3d 5d 13d ))


;;  Compute mass flux of water in all phases into wick
   ;;  Wick #1

 (flux-history
 (variable Q.water)
 (index-crange (26 1 77 27 1 77))
 (file-ext ".ss1")
 )

 (flux-history
 (variable Q.water)
 (index-crange (27 1 76 27 1 77))
 (file-ext ".ss2")
 )

 (flux-history
 (variable Q.water)
 (index-crange (28 1 77 27 1 77))
 (file-ext ".ss3")
```

```
      )

     ;; Wick # 2

      (flux-history
      (variable Q.water)
      (index-crange (1 1 81 1 1 82))
      (file-ext ".ss4")
      )

      (flux-history
      (variable Q.water)
      (index-crange (2 1 82 1 1 82))
      (file-ext ".ss5")
      )



      (extool (variables T RH X.air.gas X.water.gas C.water.gas
C.air.gas q.water P V.liquid V.gas S.liquid P.liquid)
              (file-ext ".ext")(range "*")
(outtimes 0 0.0002d .0005d 0.005d .01d 0.1d 0.2d 0.5d 1d 1.5d 2d 3d 5d
10d 13d 21d 35d 49d
        )
  ))

  (rocktab
    (heatr
      (porosity 0.010) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 4.340e+02) (solid-density 7.854e+03)
      (tcond tcondLin (solid  60.500000)(liquid  60.500000)(gas
60.500000))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
      (tort (gas 0.000e+00) (liquid 0.0))
      (kr (gas 1.0)
          (liquid 1.0))
      (pc (liquid 0.0))
    )

    (drift
      (porosity 0.999) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.007e+03) (solid-density 1.1614)
      (tcond tcondLin (solid 0.026300)(liquid 0.026300)(gas 0.026300))
      (K0 1.000e-06) (K1 1.000e-06) (K2 1.000e-06)
;; JJN     (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krPower (power 4) (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
    )

    (invert
      (porosity 0.632) (Kd (air 0.0) (water 0.0))
      (KdFactor (water 0.0) ( air 0.0))
      (Cp 939.0) (solid-density 1.150e+03)
```

```
      (tcond tcondLin (solid 0.66) (liquid 0.66) (gas 0.66))
      (Kx 6.160e-10) (Ky 6.16e-10) (Kz 6.16e-10)
      (tort (gas 0.700) (liquid 0.0))
      (kr (gas krgEffCont) (liquid krlEffCont))
      (pc (liquid pcEffCont (alpham 1.18E-03) (alphaf 1.18E-03)
      (betam 2.744) (betaf 2.744)
      (Km 6.16e-10) (Kf  0.0)
      (phim  0.632) (phif  0.0)
      (Sresm 0.0500) (Sresf 0.0)
       ))
    )

    (shield
      (porosity 0.010) (Kd (air 0.0) (water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 4.7700e+2) (solid-density 7.900e+03)
      (tcond tcondLin (solid 14.90) (liquid 14.90) (gas 14.90))
      (K0 0.000) (K1 0.000) (K2 0.000)
      (tort (gas 0.000) (liquid 0.000))
      (kr  (gas 1.0)
           (liquid 1.0))
      (pc  (liquid 0.0))
    )

    (wick
     (porosity 0.990) (Kd (contam 0.0) (air 0.0) (water 0.0))
     (KdFactor (water 0.0) (air 0.0))
     (Cp 939.0) (solid-density 1.150e+03)
     (tcond tcondLin (solid 0.66) (liquid 0.66) (gas 0.66))
     (K0 0.00e+00) (K1 0.00e+00) (K2 0.00e+00)
     (tort (liquid 0.0) (gas 1.00e+00))
     (kr (gas krLinear (Sr 0.0)) (liquid 1.0))
     (pc (liquid 0.0))
    )

    (atm
      (porosity 0.990) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.000e+08) (solid-density 1.000e+00)
      (tcond tcondLin (solid 0.026300)(liquid 0.026300)(gas 0.026300))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
;;JJN       (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krlLinear (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
    )
  )


  ;; Set Boundary Conditions


    (bctab
      (atmos
          (range "at*" ) (clamped)
      )
```

```
    (heater
        (range  "ht*") (clamped)
    )
    (wick
        (range "wi*") (clamped)
    )
    (invert
        (range "in*") (clamped)
    )
    (invert
        (range "src2*") (clamped)
    )
    (invert
        (range "src3*") (clamped)
    )
  )


;; Define Initial Conditions


    (state
       (P by-key ("*" 1.e5)  )

       (S.liquid by-key ("at*" 0.0)
                        ("dr1*" 0.0)
                        ("dr*" 0.0)
                        ("sh*" 0.0)
                        ("ht*" 0.0)
                        ("in*" 0.8000 )
                        ("dr2*" 0.0)
                ;;        ("src1*" 0.0)
                        ("src2*" 0.8)
                        ("src3*" 0.8)
                        ("wi*" 0.0)
       )

       (T by-key ("at*" 60.0)
                 ("ht*" 80.0)
                 ("dr*" 60.0)
                 ("dr1*" 60.0)
                 ("sh*" 60.0)
                 ("in*" 70.0)
                 ("dr2*" 60.0)
              ;;   ("src1*" 60.0)
                 ("src2*" 70.0)
                 ("src3*" 70.0)
                 ("wi*" 20.0)
       )


       (X.air by-key ("*" -1.0)  ("at*" 0.990) ("dr*" 0.990) ("dr1*"
0.990)
                     ("ht*" 1.0) ("dr2*" 0.990) ("sh*" 1.0) ("wi*"
0.990)
                     )
```

```
      ) ;; end state

   (input-mass-fraction on)

(linear-solver d4vband)
;;   (linear-solver pcg)
   (ilu-degree 2)
   (pcg-parameters (precond d4)(toler 1e-2)(itermax 200)(north 25))

     (srctab
   ;;  (compflux
   ;;  (comp energy)
   ;;  (name REPO)
   ;;  (range "ht*")
   ;;  (allocate-by-element ("*" 0.5))
   ;;  (table
   ;;     0.0000e+00  6.00e+02  6.3072e+07  5.80e+02  1.2614e+08
5.55e+02
   ;;     1.8922e+08  5.34e+02  2.5229e+08  5.14e+02  3.1536e+08
4.97e+02
   ;;     9.4608e+08  3.60e+02  1.5768e+09  2.75e+02  2.2075e+09
2.19e+02
   ;;     2.8382e+09  1.82e+02  4.7304e+09  1.26e+02  7.8840e+09
9.29e+01
   ;;     1.1038e+10  7.64e+01  1.4191e+10  6.59e+01  1.7345e+10
5.76e+01
   ;;     2.0498e+10  5.12e+01  2.3652e+10  4.57e+01  2.6806e+10
4.12e+01
   ;;     2.9959e+10  3.77e+01  6.3072e+10  1.95e+01  1.2614e+11
1.36e+01
   ;;     1.8922e+11  1.18e+01  2.5229e+11  1.03e+01  3.1536e+11
9.29e+00

   ;;    ) ;; end table
   ;;   (allocate-by-volume)
   ;;  ) ;; end compflux

    ;;   (compflux
    ;;   (comp water)
    ;;   (name infil)
    ;;   (range "src1*")
    ;;   (mult-by-area z)
    ;;   (table
    ;;       0.0              1.1567e-05 ;; kg/s
    ;;       4.3200e+06       1.1567e-05
    ;;      )  ;; end table

    ;;    (enthalpy   0.0   6.84E+04   1E+30   6.84E+04   ) ;; 16.3 C
```

```
;;        )  ;;  end compflux

;;       (compflux
;;       (comp water)
;;       (name infil)
;;     (range "src2*")
;;     (table
;;         0.0              1.1566e-05 ;; kg/s
;;         4.3200e+06       1.1566e-05
;;       )  ;; end table

;;      (enthalpy   0.0   6.84E+04   4.3200E+06   6.84E+04)

;;       )  ;; end compflux

;;     (compflux
;;     (comp water)
;;     (name infil)
;;     (range "src3*")
;;     (table
;;        0.0               2.3132e-05 ;; kg/s
;;        4.3200e+06        2.3132e-05
;;     )
;; (enthalpy   0.0   6.84E+04   4.3200E+06  6.84E+04)

;;     ) ;; end compflux

   ) ;;  end srctab


(genmsh
   (down 0. 0. 1.0)
   (coord rect)

   (dx          32*0.01  20*0.02  )


   (dy               1)


   (dz
                28*0.02   24*0.01  32*0.02        )

   (mat
      (at       atm      1   nx   1   ny     1    3)
      (dr1      drift    1    1   1   ny     4    4) ;; src1
      (dr1      drift    2   27   1   ny     4    4)
      (dr1      drift   29   29   1   ny     4    4)
      (dr1      drift   28   28   1   ny     4    4) ;; src3
      (dr       drift    1   28   1   ny     5    9)
      (dr1      drift   29   29   1   ny     5    9)
      (at       atm     30   nx   1   ny     4    9)
      (at       atm     43   nx   1   ny    10   19)
      (dr       drift    1   29   1   ny    10   10)
      (dr1      drift   30   34   1   ny    10   10)
```

```
(dr1     drift   35  35  1  ny  10  10)  ;; src2
(dr1     drift   36  42  1  ny  10  10)
(dr      drift   1   41  1  ny  11  19)
(dr1     drift   42  42  1  ny  11  19)
(dr      drift   1   42  1  ny  20  20)
(dr1     drift   43  50  1  ny  20  20)
(dr      drift   1   49  1  ny  21  35)
(dr1     drift   50  50  1  ny  21  35)
(at      atm     51  nx  1  ny  20  61)
(sh      shield  1   27  1  ny  36  37)
(dr      drift   28  49  1  ny  36  37)
(dr1     drift   50  50  1  ny  36  37)
(sh      shield  26  27  1  ny  38  72)
(dr      drift   1   25  1  ny  38  47)
(dr2     drift   1   18  1  ny  48  48)
(dr      drift   19  25  1  ny  48  48)
(dr      drift   28  49  1  ny  38  48)
(dr1     drift   50  50  1  ny  38  48)
(ht      heatr   1   17  1  ny  49  67)
(ht      heatr   1    8  1  ny  68  70)
(dr      drift   19  25  1  ny  49  72)
(dr      drift   10  17  1  ny  69  72)
(dr      drift   1    8  1  ny  72  72)
(dr2     drift   18  18  1  ny  49  68)
(dr      drift   18  18  1  ny  69  72)
(dr2     drift    9  17  1  ny  68  68)
(dr2     drift    9   9  1  ny  69  71)
(dr      drift    9   9  1  ny  72  72)
(dr2     drift    1   8  1  ny  71  71)
(dr      drift   28  49  1  ny  49  60)
(dr1     drift   50  50  1  ny  49  60)
(dr      drift   28  45  1  ny  61  61)
(dr1     drift   46  50  1  ny  61  61)
(dr      drift   28  44  1  ny  62  69)
(dr1     drift   45  45  1  ny  62  69)
(at      atm     46  52  1  ny  62  70)
(dr      drift   28  38  1  ny  70  70)
(dr1     drift   39  45  1  ny  70  70)
(dr      drift   28  37  1  ny  71  72)
(dr1     drift   38  38  1  ny  71  72)
(at      atm     39  52  1  ny  71  72)
(in      invert  1   27  1  ny  73  73)
(src3    invert  28  28  1  ny  73  73)
(in      invert  29  34  1  ny  73  73)
(src2    invert  35  35  1  ny  73  73)
(in      invert  36  38  1  ny  73  73)
(in      invert  1   38  1  ny  74  76)
(in      invert  1   26  1  ny  77  77)
(wi      wick    27  27  1  ny  77  77)
(in      invert  28  38  1  ny  77  77)
(at      atm     39  52  1  ny  73  77)
(in      invert  1   26  1  ny  78  81)
(wi      wick    1    1  1  ny  82  82)
(in      invert  2   26  1  ny  82  82)
(at      atm     27  52  1  ny  78  82)
(at      atm     1   nx  1  ny  83  84)
)  (include  "results28"))  ;; end of genmsh) ;; end of model input
```

```
(usnt
(title "2D T-H Model/drip shield/water appl.for pilot test-fixed
temp.@Bound")
(modelname usnt)
(include-pkg "vtough.pkg")
(tstop   4.3200e+06)
(time 0)
(stepmax 1000000)
(dtmax  4.3200e+06)
(dt 1e3)

;; Run ymp2Ddstw9R

;; Wicks set at   0 cm suction  & and no outflow

;; set invert mat. at .8 sat. and 60 C

(output
   (field (format tabular) (variables Vmag.gas P.gas T S.liquid P )
        (file-ext ".var")
        (outtimes 0.2d 0.5d 1d 1.5d 2d 3d 5d 10d 13d 21d 35d 49d))


;; compute fluxes across invert surface
   (flux-history
    (variable Q.water)
    (crange ("in*" "dr*"))
    (file-ext ".fl1")
    )

   (flux-history
    (variable Q.water)
    (index-crange (28 1 73 28 1 72) (29 1 73 29 1 72) (30 1 73 30 1
72)
                  (31 1 73 31 1 72) (32 1 73 32 1 72) (33 1 73 33 1
72)
                  (34 1 73 34 1 72) (35 1 73 35 1 72) (36 1 73 36 1
72)
                  (37 1 73 37 1 72) (38 1 73 38 1 72) )
       (file-ext ".fl3")
    )

;; compute fluxes across approx. water-vapor interface

   (flux-history
    (variable Q.water)
    (index-crange (29 1 77 29 1 76) (30 1 77 30 1 76) (31 1 77 31 1
76)
                  (32 1 77 32 1 76) (33 1 77 33 1 76) (34 1 77 34 1
76)
                  (35 1 77 35 1 76) (36 1 77 36 1 76) (37 1 77 37 1
76)
                  (38 1 77 38 1 76) )
      (file-ext ".fl2")
    )

;; Compute thermal fluxes
```

```
(flux-history
 (variable Qrad)
 ( crange ("ht*" "sh*"))
 (file-ext ".rad")
)

;; (flux-history
 ;; (variable Qrad)
 ;; (crange ("sh*" "dr1*"))
 ;; ( file-ext ".ra1")
 ;;)


(flux-history
 (variable Qd.energy)
 (crange ("ht*" "dr2*"))
 (file-ext ".con")
)


(flux-history
 (variable Qa.energy)
 (crange ("dr2*" "dr*"))
 (file-ext ".adv")
 )


(flux-field
 (file-ext ".vel")
 (format list)
 (variables V.gas)
 (crange ("dr2*" "dr*"))
 (outtimes 0.2d 0.5d 0.7d  1d 3d 5d 13d ))


;;  Compute mass flux of water in all phases into wick
   ;;  Wick #1

 (flux-history
 (variable Q.water)
 (index-crange (26 1 77 27 1 77))
 (file-ext ".ss1")
 )

 (flux-history
 (variable Q.water)
 (index-crange (27 1 76 27 1 77))
 (file-ext ".ss2")
 )

 (flux-history
 (variable Q.water)
 (index-crange (28 1 77 27 1 77))
```

```
      (file-ext ".ss3")
      )

     ;; Wick # 2

      (flux-history
      (variable Q.water)
      (index-crange (1 1 81 1 1 82))
      (file-ext ".ss4")
      )

      (flux-history
      (variable Q.water)
      (index-crange (2 1 82 1 1 82))
      (file-ext ".ss5")
      )



      (extool (variables T RH X.air.gas X.water.gas C.water.gas
C.air.gas q.water P V.liquid V.gas S.liquid P.liquid)
              (file-ext ".ext")(range "*")
(outtimes 0 0.0002d .0005d 0.005d .01d 0.1d 0.2d 0.5d 1d 1.5d 2d 3d 5d
10d 13d 21d 35d 49d
        )
  ))

  (rocktab
    (heatr
      (porosity 0.010) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 4.340e+02) (solid-density 7.854e+03)
      (tcond tcondLin (solid  60.500000)(liquid  60.500000)(gas
60.500000))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
      (tort (gas 0.000e+00) (liquid 0.0))
      (kr (gas 1.0)
          (liquid 1.0))
      (pc (liquid 0.0))
    )

    (drift
      (porosity 0.999) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.007e+03) (solid-density 1.1614)
      (tcond tcondLin (solid 0.026300)(liquid 0.026300)(gas 0.026300))
      (K0 1.000e-06) (K1 1.000e-06) (K2 1.000e-06)
;; JJN     (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krPower (power 4) (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
    )

    (invert
      (porosity 0.632) (Kd (air 0.0) (water 0.0))
      (KdFactor (water 0.0) ( air 0.0))
```

```
      (Cp 939.0) (solid-density 1.150e+03)
      (tcond tcondLin (solid 0.66) (liquid 0.66) (gas 0.66))
      (Kx 6.160e-10) (Ky 6.16e-10) (Kz 6.16e-10)
      (tort (gas 0.700) (liquid 0.0))
      (kr (gas krgEffCont) (liquid krlEffCont))
      (pc (liquid pcEffCont (alpham 1.18E-03) (alphaf 1.18E-03)
      (betam 2.744) (betaf 2.744)
      (Km 6.16e-10) (Kf  0.0)
      (phim  0.632) (phif  0.0)
      (Sresm 0.0500) (Sresf 0.0)
       ))
    )

    (shield
      (porosity 0.010) (Kd (air 0.0) (water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 4.7700e+2) (solid-density 7.900e+03)
      (tcond tcondLin (solid 14.90) (liquid 14.90) (gas 14.90))
      (K0 0.000) (K1 0.000) (K2 0.000)
      (tort (gas 0.000) (liquid 0.000))
      (kr  (gas 1.0)
           (liquid 1.0))
      (pc  (liquid 0.0))
    )

    (wick
     (porosity 0.990) (Kd (contam 0.0) (air 0.0) (water 0.0))
     (KdFactor (water 0.0) (air 0.0))
     (Cp 939.0) (solid-density 1.150e+03)
     (tcond tcondLin (solid 0.66) (liquid 0.66) (gas 0.66))
     (K0 0.00e+00) (K1 0.00e+00) (K2 0.00e+00)
     (tort (liquid 0.0) (gas 1.00e+00))
     (kr (gas krLinear (Sr 0.0)) (liquid 1.0))
     (pc (liquid 0.0))
    )

    (atm
      (porosity 0.990) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.000e+08) (solid-density 1.000e+00)
      (tcond tcondLin (solid 0.026300)(liquid 0.026300)(gas 0.026300))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
;;JJN      (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krlLinear (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
    )
  )


  ;; Set Boundary Conditions


    (bctab
      (atmos
          (range "at*" ) (clamped)
```

```
    )
    (heater
        (range  "ht*") (clamped)
    )
    (wick
        (range "wi*") (clamped)
    )
    (invert
        (range "in*") (clamped)
    )
    (invert
        (range "src2*") (clamped)
    )
    (invert
        (range "src3*") (clamped)
    )
  )


;; Define Initial Conditions


    (state
       (P by-key ("*" 1.e5)  )

       (S.liquid by-key ("at*" 0.0)
                        ("dr1*" 0.0)
                        ("dr*" 0.0)
                        ("sh*" 0.0)
                        ("ht*" 0.0)
                        ("in*" 0.8000 )
                        ("dr2*" 0.0)
                  ;;      ("src1*" 0.0)
                        ("src2*" 0.8)
                        ("src3*" 0.8)
                        ("wi*" 0.0)
       )

       (T by-key ("at*" 60.0)
                 ("ht*" 80.0)
                 ("dr*" 60.0)
                 ("dr1*" 60.0)
                 ("sh*" 60.0)
                 ("in*" 60.0)
                 ("dr2*" 60.0)
              ;;   ("src1*" 60.0)
                 ("src2*" 60.0)
                 ("src3*" 60.0)
                 ("wi*" 20.0)
       )


       (X.air by-key ("*" -1.0)  ("at*" 0.990) ("dr*" 0.990) ("dr1*"
0.990)
                     ("ht*" 1.0) ("dr2*" 0.990) ("sh*" 1.0) ("wi*"
0.990)
                     )
```

```
      ) ;; end state

   (input-mass-fraction on)

(linear-solver d4vband)
;;    (linear-solver pcg)
   (ilu-degree 2)
   (pcg-parameters (precond d4)(toler 1e-2)(itermax 200)(north 25))

     (srctab
   ;;  (compflux
   ;;  (comp energy)
   ;;  (name REPO)
   ;;  (range "ht*")
   ;;  (allocate-by-element ("*" 0.5))
   ;;  (table
   ;;     0.0000e+00  6.00e+02  6.3072e+07  5.80e+02  1.2614e+08
5.55e+02
   ;;     1.8922e+08  5.34e+02  2.5229e+08  5.14e+02  3.1536e+08
4.97e+02
   ;;     9.4608e+08  3.60e+02  1.5768e+09  2.75e+02  2.2075e+09
2.19e+02
   ;;     2.8382e+09  1.82e+02  4.7304e+09  1.26e+02  7.8840e+09
9.29e+01
   ;;     1.1038e+10  7.64e+01  1.4191e+10  6.59e+01  1.7345e+10
5.76e+01
   ;;     2.0498e+10  5.12e+01  2.3652e+10  4.57e+01  2.6806e+10
4.12e+01
   ;;     2.9959e+10  3.77e+01  6.3072e+10  1.95e+01  1.2614e+11
1.36e+01
   ;;     1.8922e+11  1.18e+01  2.5229e+11  1.03e+01  3.1536e+11
9.29e+00

   ;;    ) ;; end table
   ;;   (allocate-by-volume)
   ;;  ) ;; end compflux

    ;;   (compflux
    ;;   (comp water)
    ;;   (name infil)
    ;;   (range "src1*")
    ;;   (mult-by-area z)
    ;;   (table
    ;;       0.0              1.1567e-05 ;; kg/s
    ;;       4.3200e+06       1.1567e-05
    ;;      )  ;; end table
```

```
;;     (enthalpy   0.0    6.84E+04    1E+30    6.84E+04   ) ;; 16.3 C

;;       )  ;;  end compflux

;;      (compflux
;;      (comp water)
;;      (name infil)
;;    (range "src2*")
;;    (table
;;        0.0                1.1566e-05 ;; kg/s
;;        4.3200e+06         1.1566e-05
;;      )  ;; end table

;;     (enthalpy   0.0    6.84E+04    4.3200E+06    6.84E+04)

;;      )  ;; end compflux

;;    (compflux
;;    (comp water)
;;    (name infil)
;;    (range "src3*")
;;    (table
;;       0.0                2.3132e-05 ;; kg/s
;;       4.3200e+06         2.3132e-05
;;    )
;; (enthalpy   0.0    6.84E+04    4.3200E+06   6.84E+04)

;;    ) ;; end compflux

  ) ;;  end srctab


(genmsh
   (down 0. 0. 1.0)
   (coord rect)

   (dx          32*0.01   20*0.02   )


   (dy                1)


   (dz
                28*0.02    24*0.01   32*0.02        )

   (mat
      (at       atm      1    nx    1    ny      1     3)
      (dr1      drift    1     1    1    ny      4     4) ;; src1
      (dr1      drift    2    27    1    ny      4     4)
      (dr1      drift    29   29    1    ny      4     4)
      (dr1      drift    28   28    1    ny      4     4) ;; src3
      (dr       drift    1    28    1    ny      5     9)
      (dr1      drift    29   29    1    ny      5     9)
      (at       atm      30   nx    1    ny      4     9)
      (at       atm      43   nx    1    ny     10    19)
      (dr       drift    1    29    1    ny     10    10)
```

```
(dr1     drift   30  34  1  ny   10  10)
(dr1     drift   35  35  1  ny   10  10)  ;; src2
(dr1     drift   36  42  1  ny   10  10)
(dr      drift   1   41  1  ny   11  19)
(dr1     drift   42  42  1  ny   11  19)
(dr      drift   1   42  1  ny   20  20)
(dr1     drift   43  50  1  ny   20  20)
(dr      drift   1   49  1  ny   21  35)
(dr1     drift   50  50  1  ny   21  35)
(at      atm     51  nx  1  ny   20  61)
(sh      shield  1   27  1  ny   36  37)
(dr      drift   28  49  1  ny   36  37)
(dr1     drift   50  50  1  ny   36  37)
(sh      shield  26  27  1  ny   38  72)
(dr      drift   1   25  1  ny   38  47)
(dr2     drift   1   18  1  ny   48  48)
(dr      drift   19  25  1  ny   48  48)
(dr      drift   28  49  1  ny   38  48)
(dr1     drift   50  50  1  ny   38  48)
(ht      heatr   1   17  1  ny   49  67)
(ht      heatr   1    8  1  ny   68  70)
(dr      drift   19  25  1  ny   49  72)
(dr      drift   10  17  1  ny   69  72)
(dr      drift   1    8  1  ny   72  72)
(dr2     drift   18  18  1  ny   49  68)
(dr      drift   18  18  1  ny   69  72)
(dr2     drift    9  17  1  ny   68  68)
(dr2     drift    9   9  1  ny   69  71)
(dr      drift    9   9  1  ny   72  72)
(dr2     drift    1   8  1  ny   71  71)
(dr      drift   28  49  1  ny   49  60)
(dr1     drift   50  50  1  ny   49  60)
(dr      drift   28  45  1  ny   61  61)
(dr1     drift   46  50  1  ny   61  61)
(dr      drift   28  44  1  ny   62  69)
(dr1     drift   45  45  1  ny   62  69)
(at      atm     46  52  1  ny   62  70)
(dr      drift   28  38  1  ny   70  70)
(dr1     drift   39  45  1  ny   70  70)
(dr      drift   28  37  1  ny   71  72)
(dr1     drift   38  38  1  ny   71  72)
(at      atm     39  52  1  ny   71  72)
(in      invert  1   27  1  ny   73  73)
(src3    invert  28  28  1  ny   73  73)
(in      invert  29  34  1  ny   73  73)
(src2    invert  35  35  1  ny   73  73)
(in      invert  36  38  1  ny   73  73)
(in      invert  1   38  1  ny   74  76)
(in      invert  1   26  1  ny   77  77)
(wi      wick    27  27  1  ny   77  77)
(in      invert  28  38  1  ny   77  77)
(at      atm     39  52  1  ny   73  77)
(in      invert  1   26  1  ny   78  81)
(wi      wick    1    1  1  ny   82  82)
(in      invert  2   26  1  ny   82  82)(at      atm     27
52   1   ny    78   82)(at      atm     1   nx   1   ny    83   84) )
(include  "results28"))  ;; end of genmsh) ;; end of model input
```

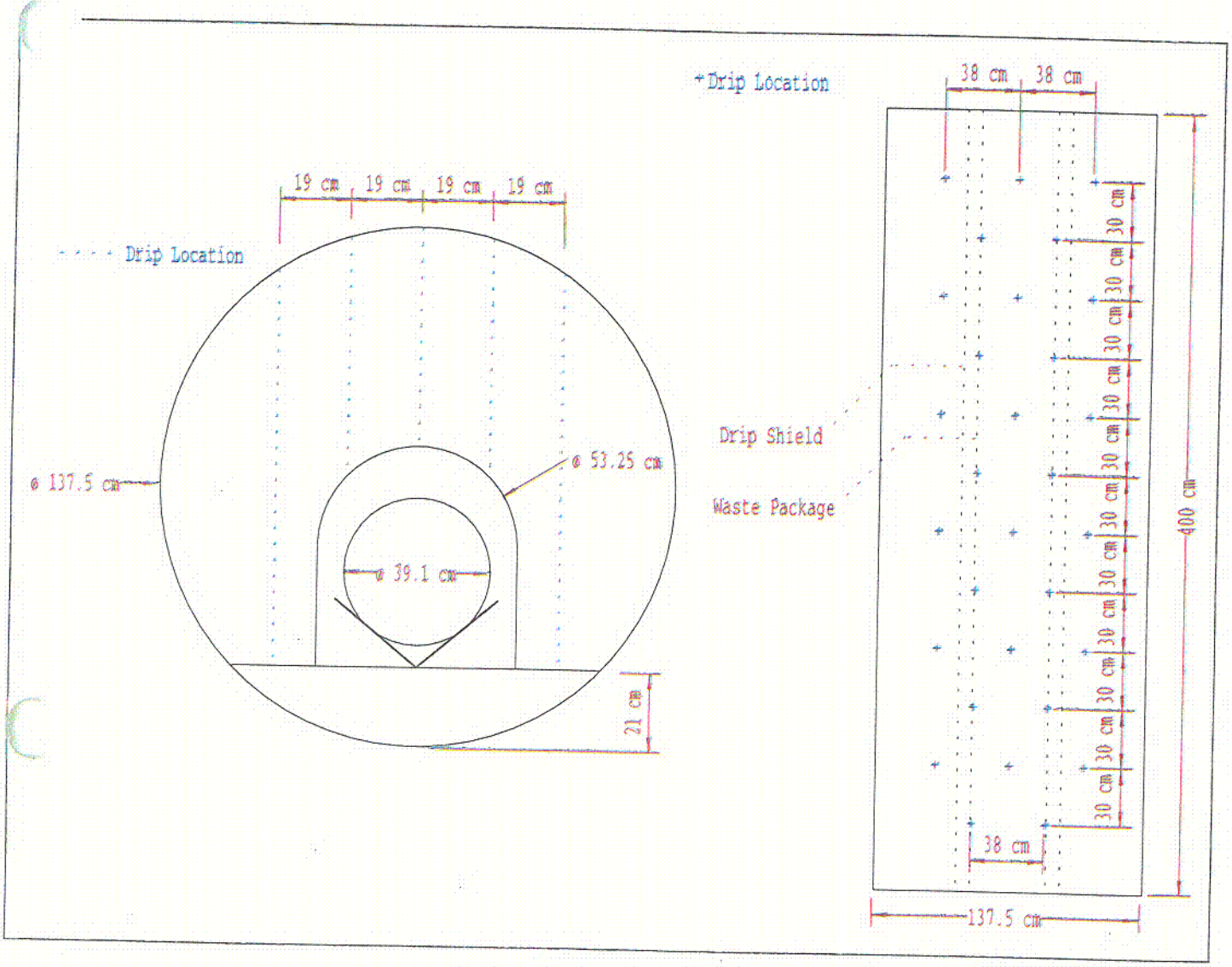


Figure 1. Quarter Scale Test Configuration

C12

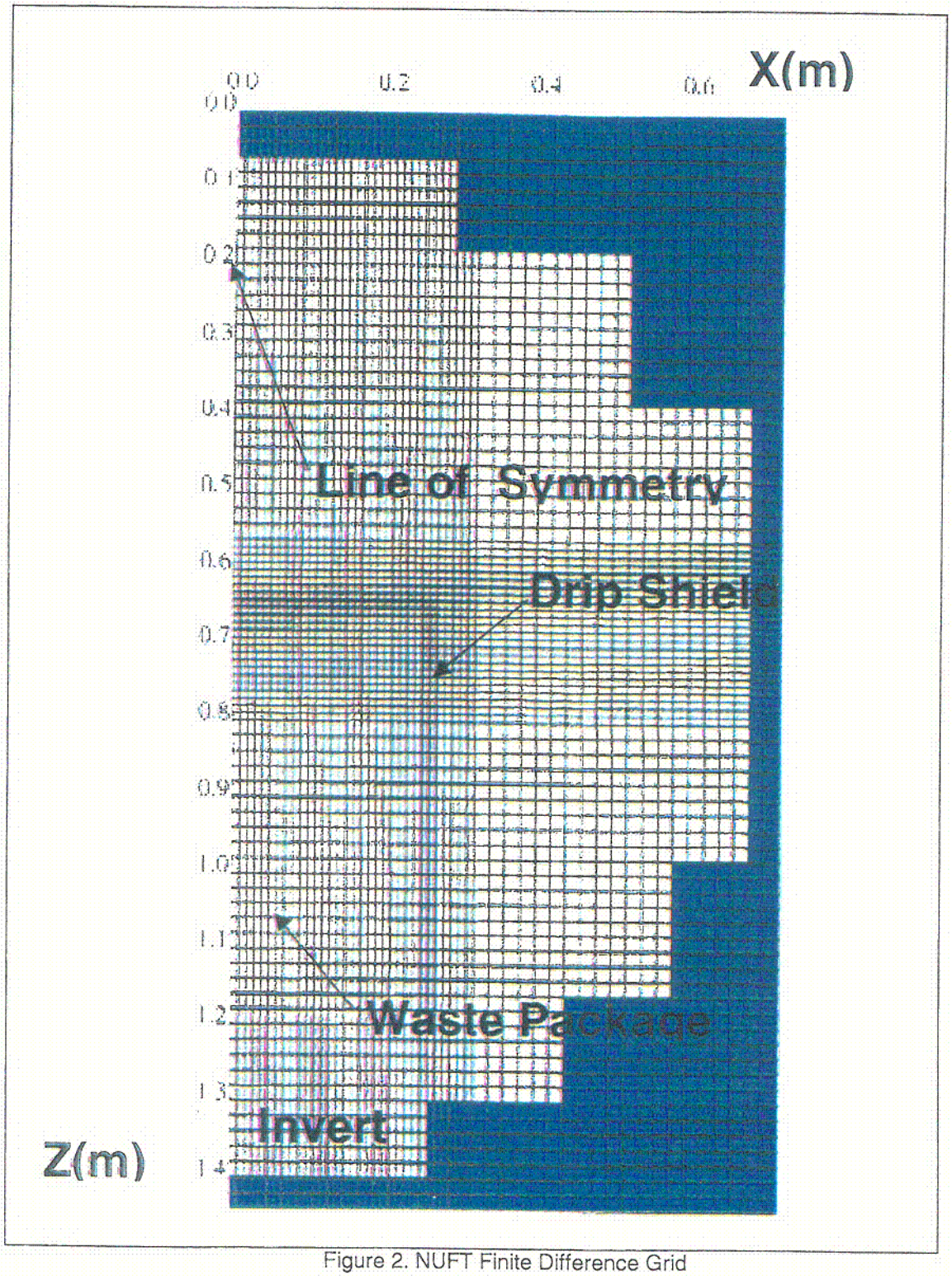


Figure 2. NUFT Finite Difference Grid

C13

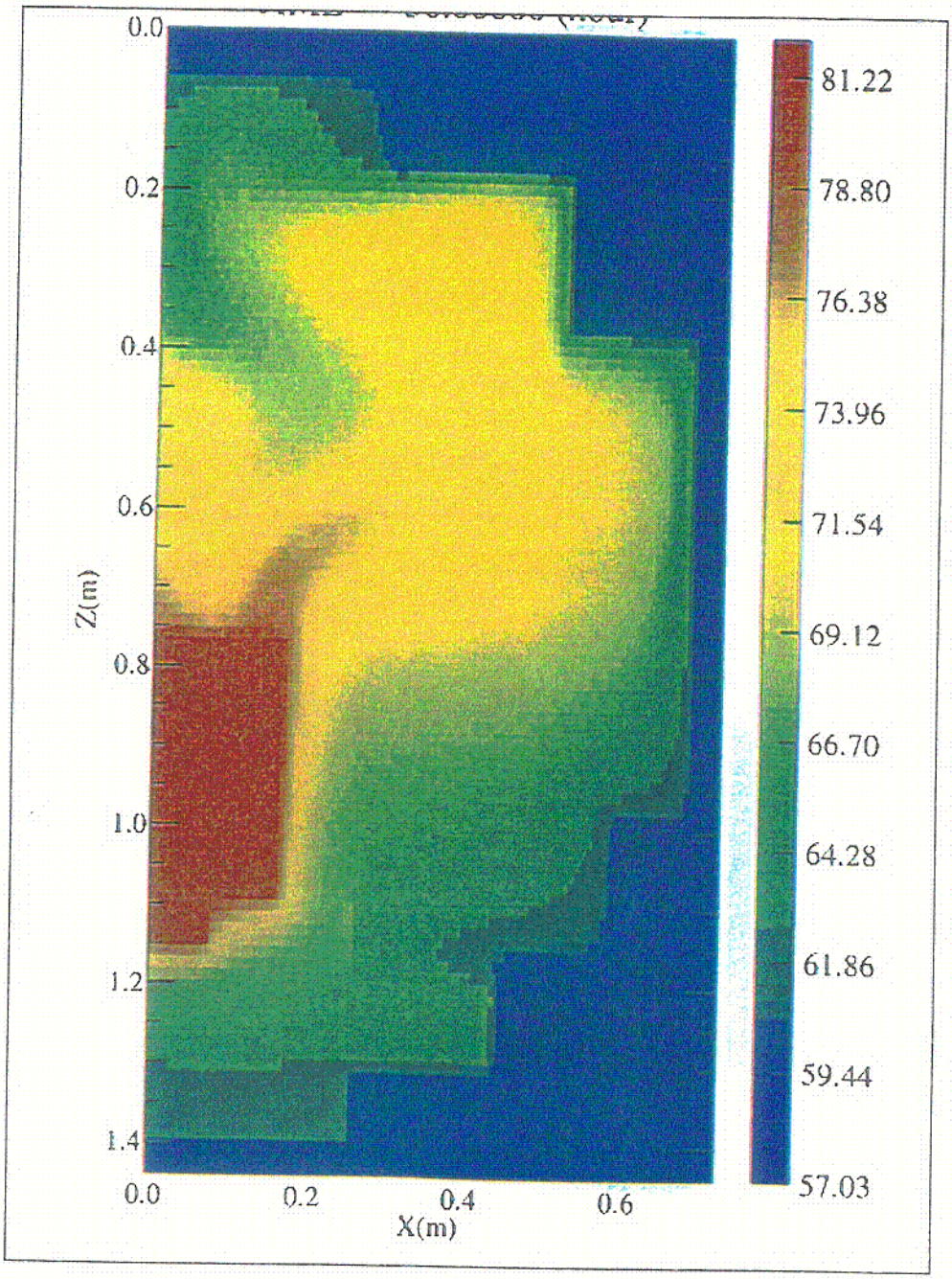


Figure 3 T-H NUFT Analysis for the Case of No Drip Shield After 36 Hours

C14

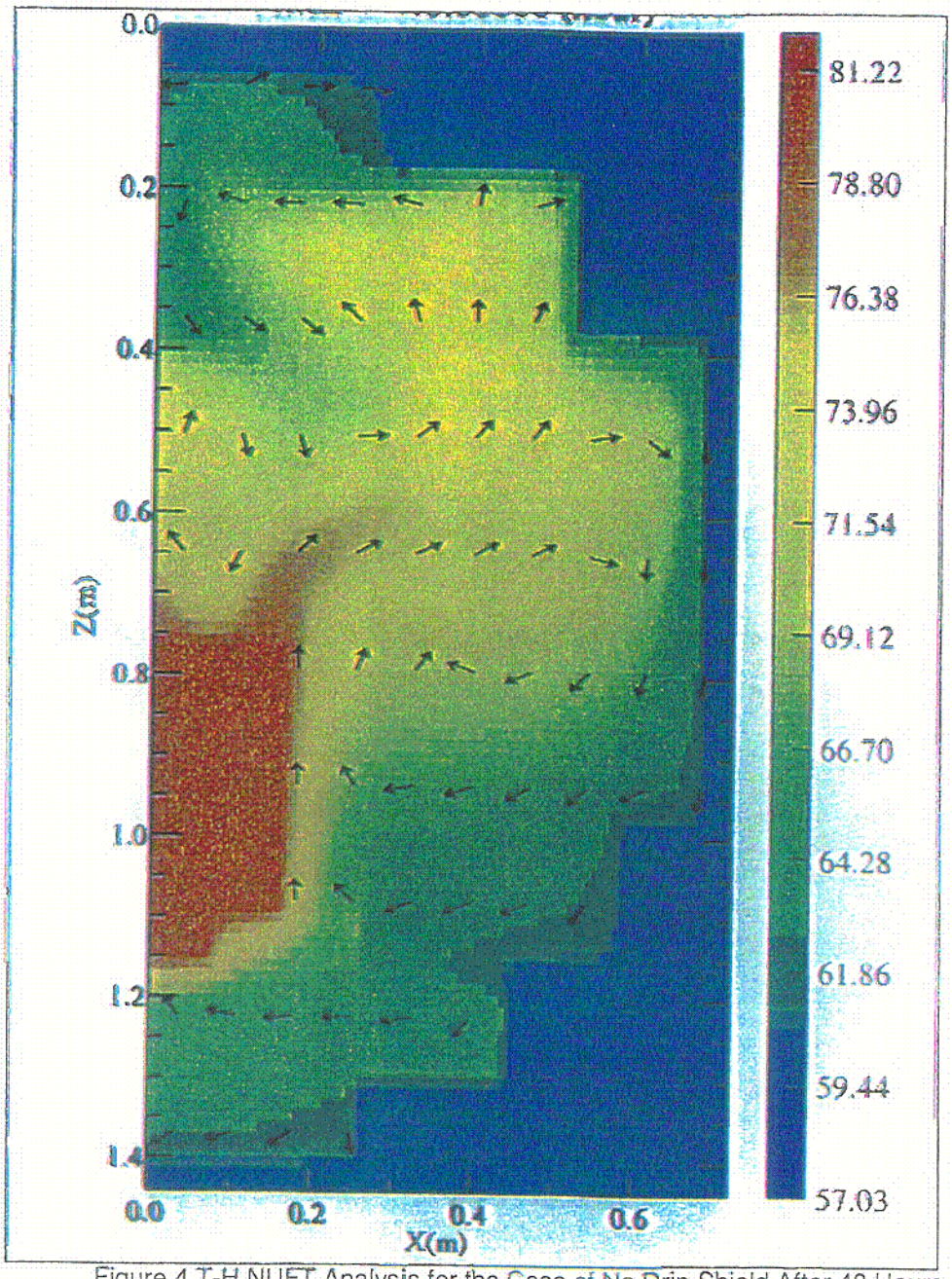


Figure 4 T-H NUFT Analysis for the Case of No Drip Shield After 48 Hours

C15

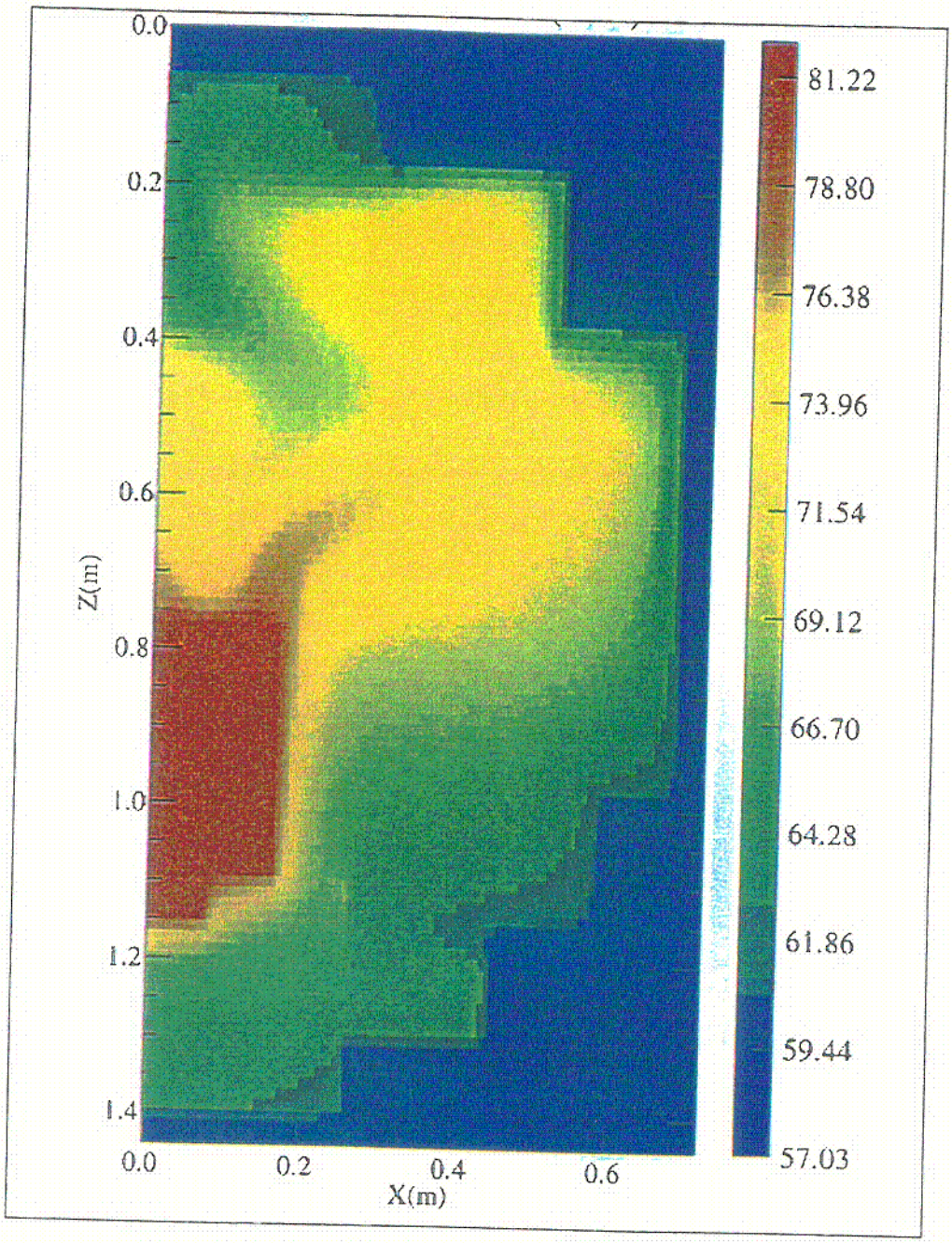


Figure 5 T-H NUFT Analysis for the Case of No Drip Shield After 72 Hours

C16

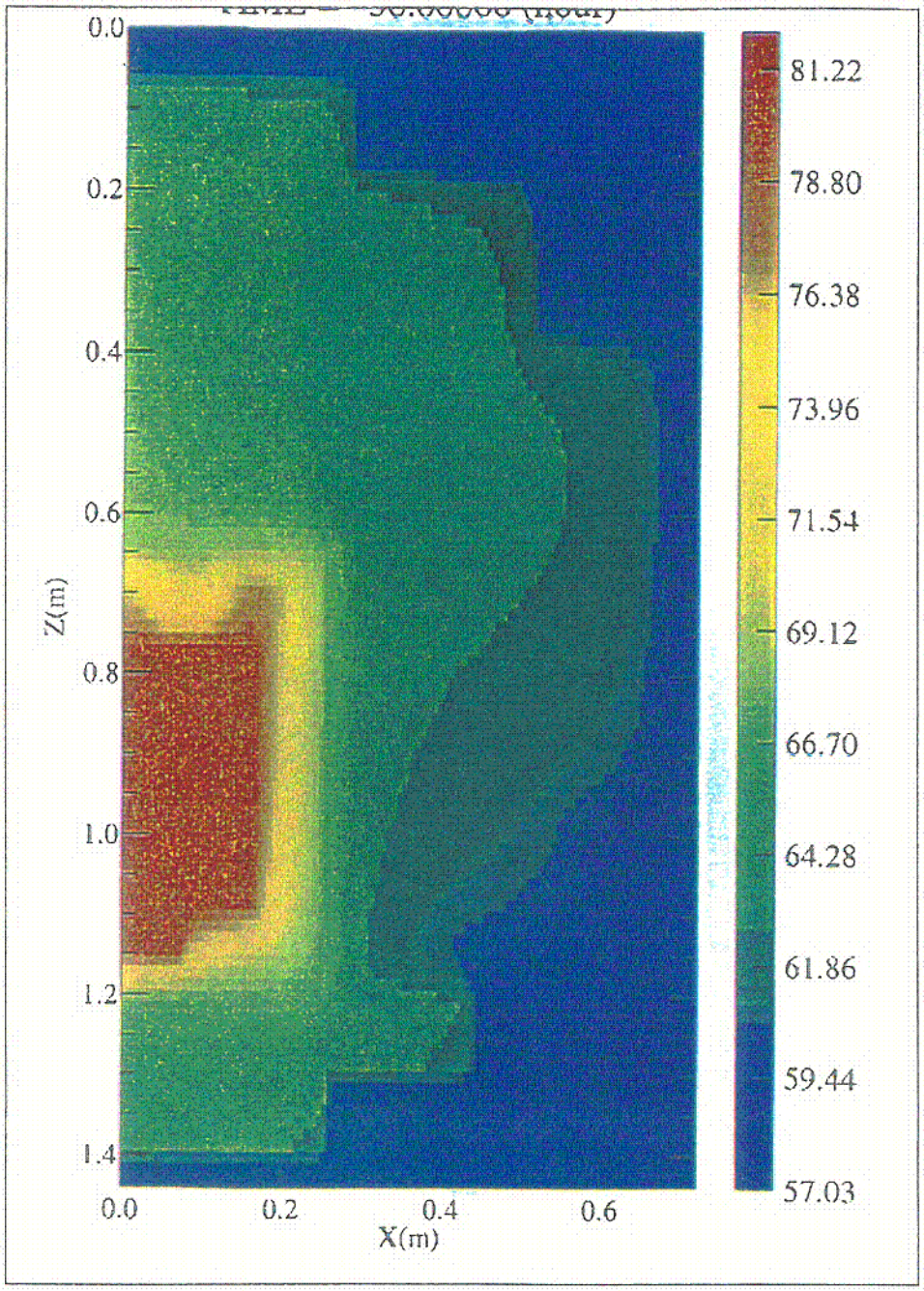


Figure 6 T-H NUFT Analysis for the Case of a Drip Shield After 36 Hours

C17

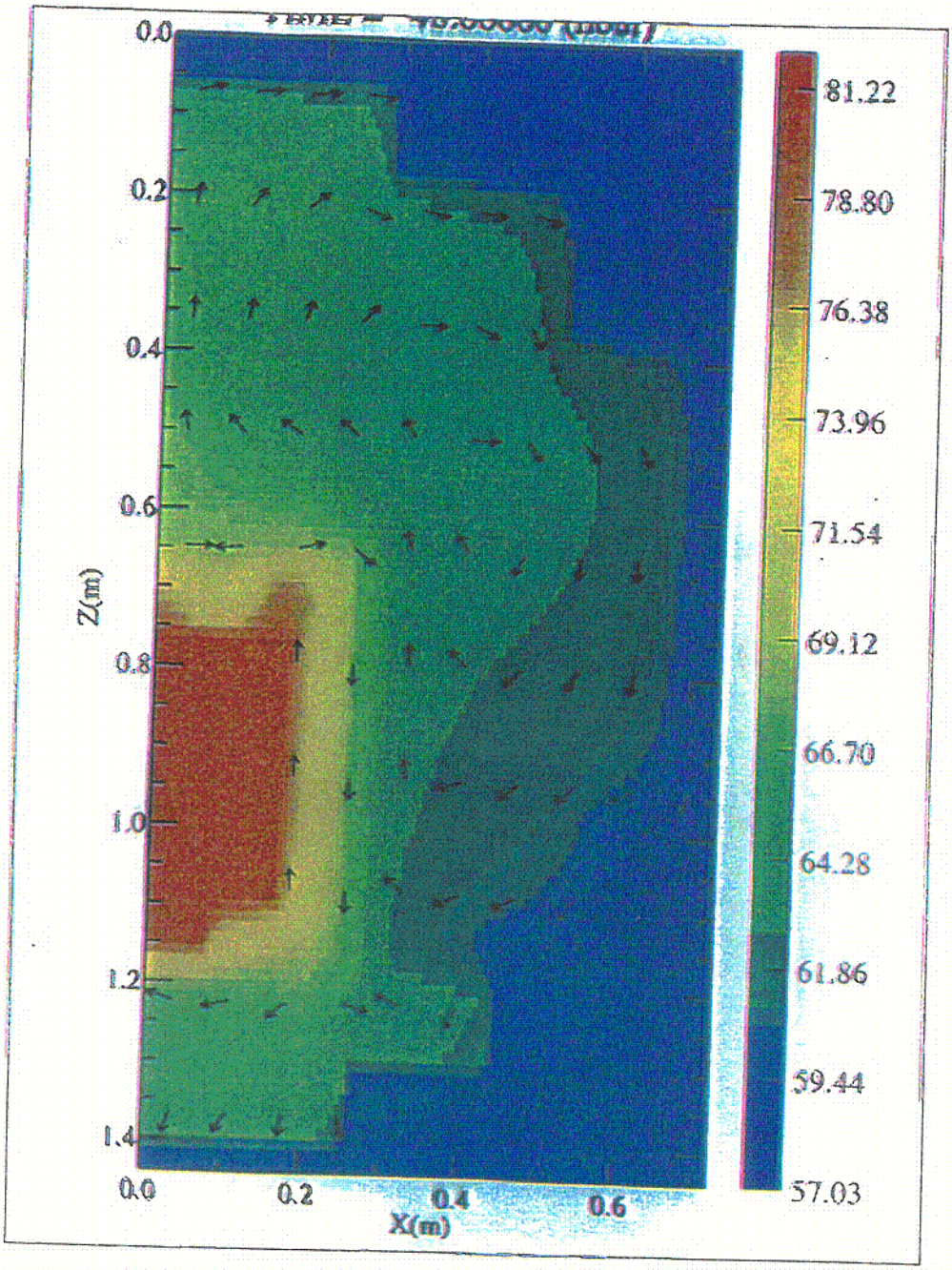


Figure 7 T-H NUFT Analysis for the Case of a Drip Shield After 48 Hours

C18

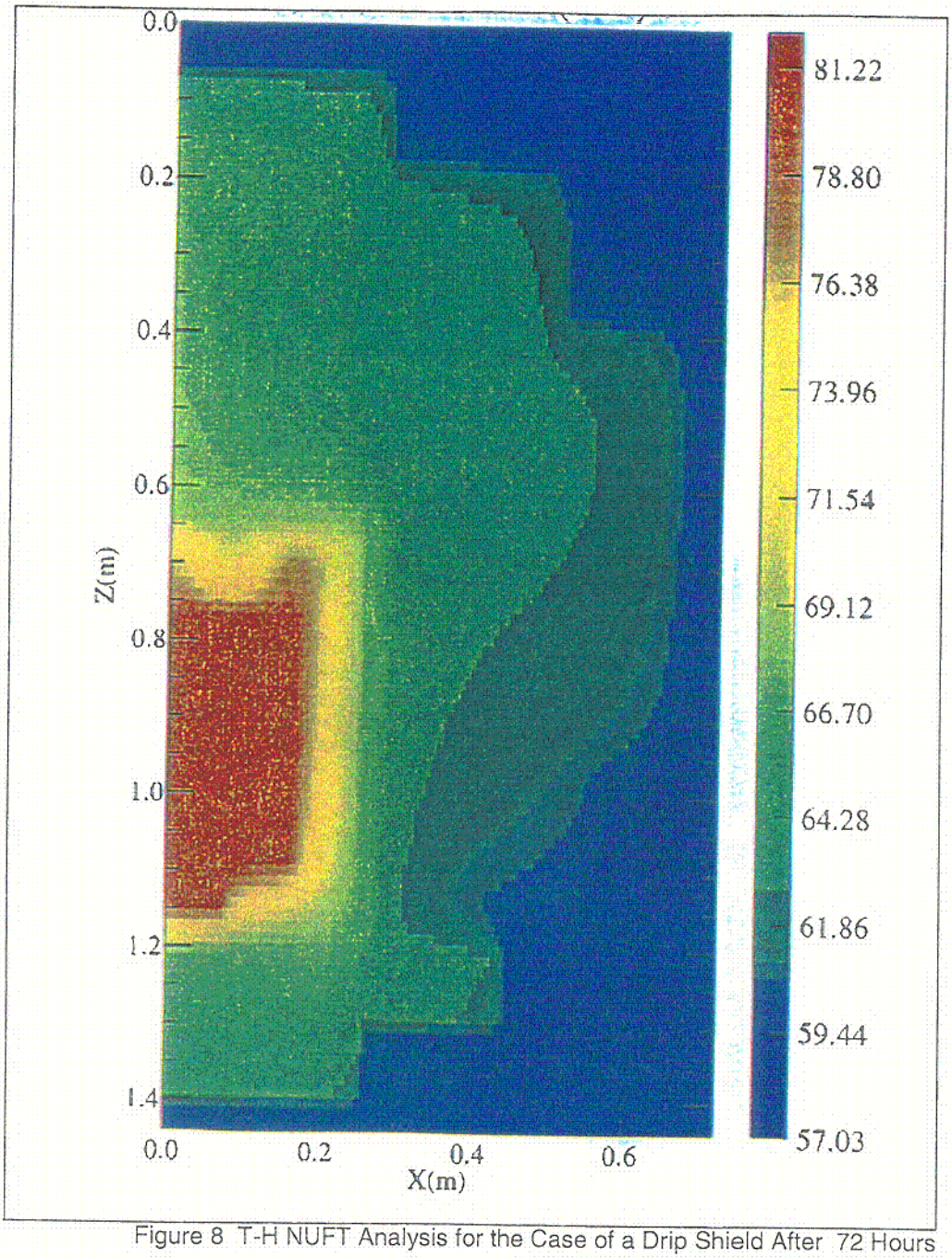


Figure 8 T-H NUFT Analysis for the Case of a Drip Shield After 72 Hours

C19

Cliff Howard
09/13/99 01:54 PM

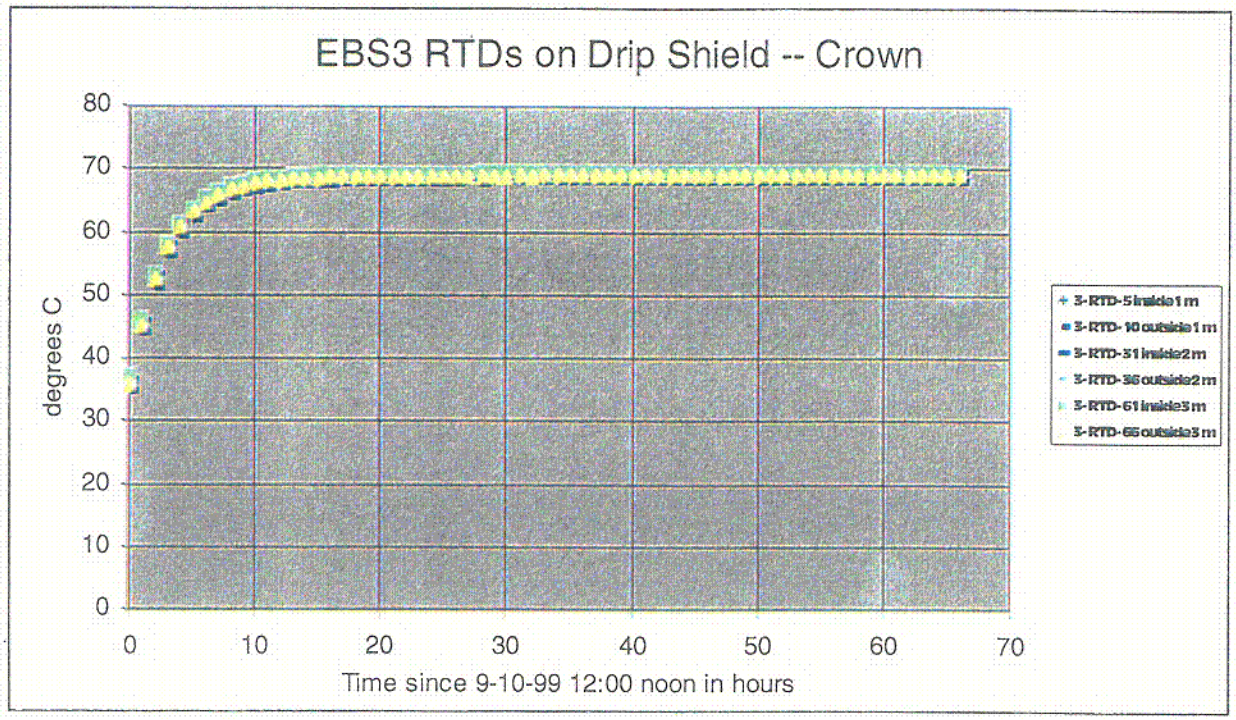
To: Jim Kam/YM/RWDOE@CRWMS, John Case/YM/RWDOE@CRWMS, swwebb@sandia.gov, Randolph Schreiner/YM/RWDOE@CRWMS, Dwayne Chestnut/YM/RWDOE@CRWMS

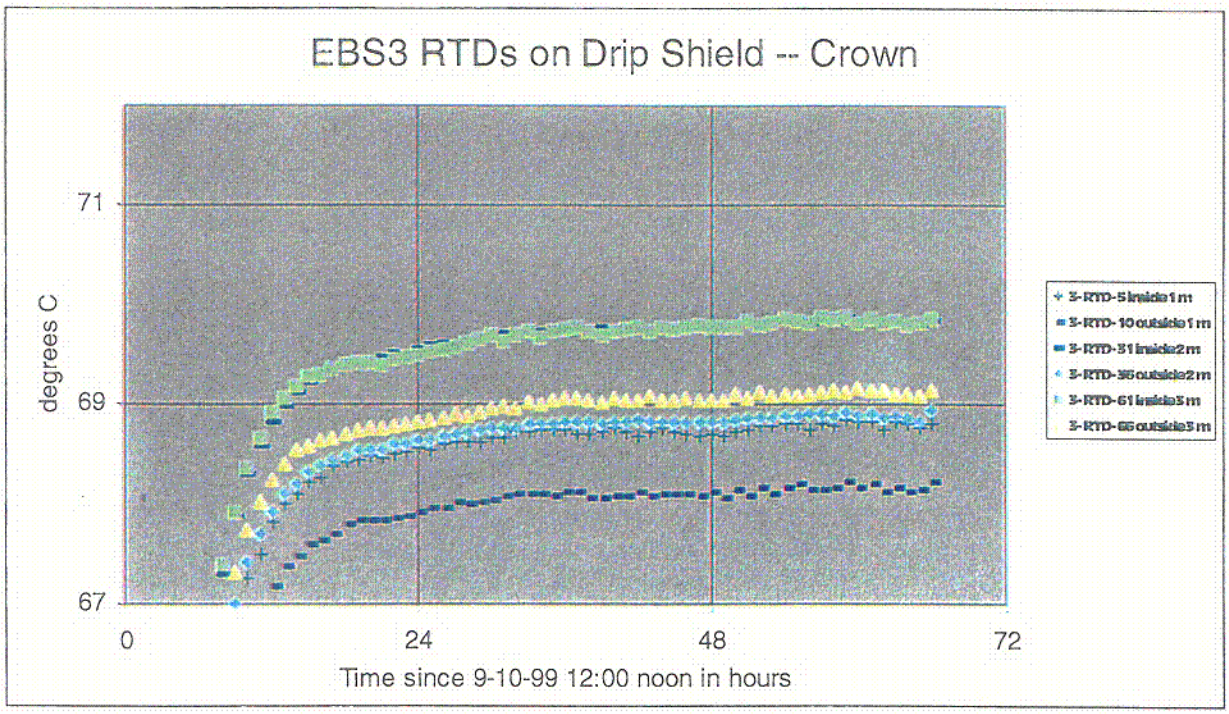
cc: John Pye/YM/RWDOE@CRWMS, Hemendra Kalia/YM/RWDOE@CRWMS, REFINLE@SANDIA.GOV, Fred Homuth/YM/RWDOE@CRWMS, Douglas Weaver/YM/RWDOE@CRWMS, David Kessel/YM/RWDOE@CRWMS, Ron Taylor/YM/RWDOE@CRWMS, William Lowry/YM/RWDOE@CRWMS, jtgeorg@sandia.gov, Roy Johnston/YM/RWDOE@CRWMS, Troy Williams/YM/RWDOE@CRWMS, Tom Kostalek/YM/RWDOE@CRWMS, David Hudson/YM/RWDOE@CRWMS

Subject: 60 degree and 80 degree data - Water Turn-on Set for Tomorrow

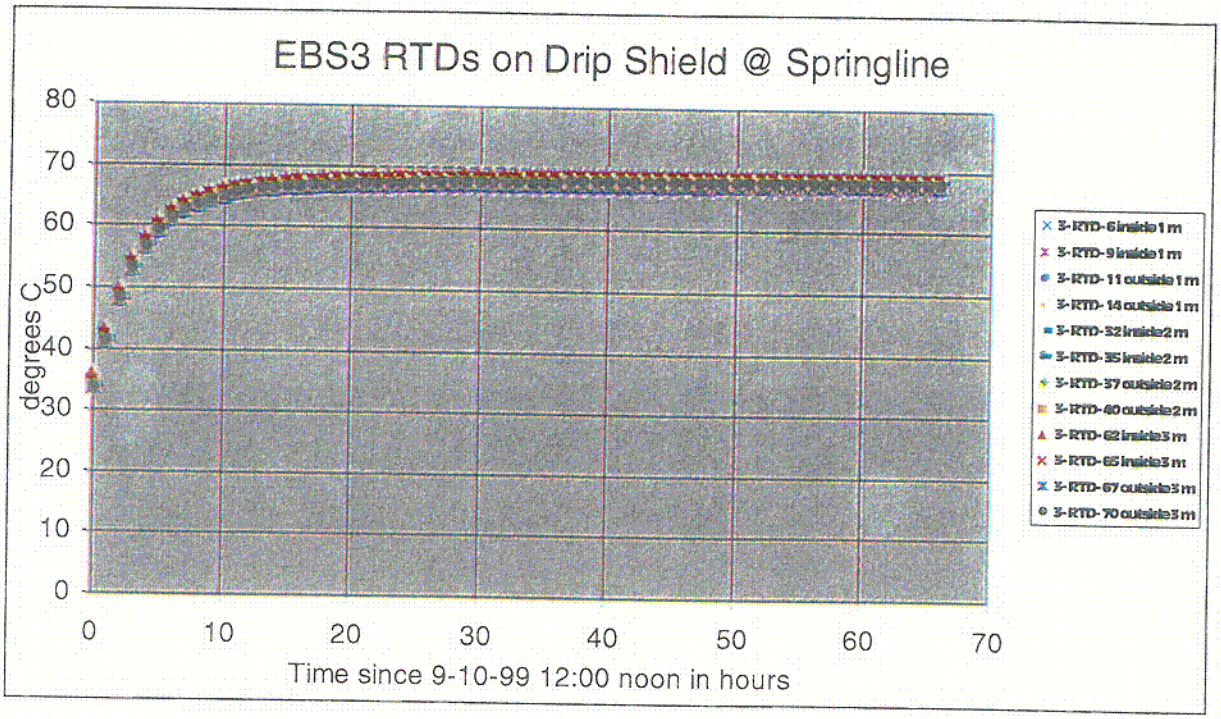
Gentlemen,
In my previous E-mail, I did not include data from the test that showed the 60 degree and 80 degree set points. This is because this data is driven by the power control circuit and I thought the other data would provide the more definitive evidence of steady state heat flow and distribution. Anyway, the attached file shows this data which comes from RTDs at the top of the waste package (80 degrees) and test cell (60 degrees). These set points were reached between 5 and 10 hours after starting the test. Unless I hear otherwise, dripping will begin about mid-day tomorrow to give us another 24 hours of data without water.
Cliff

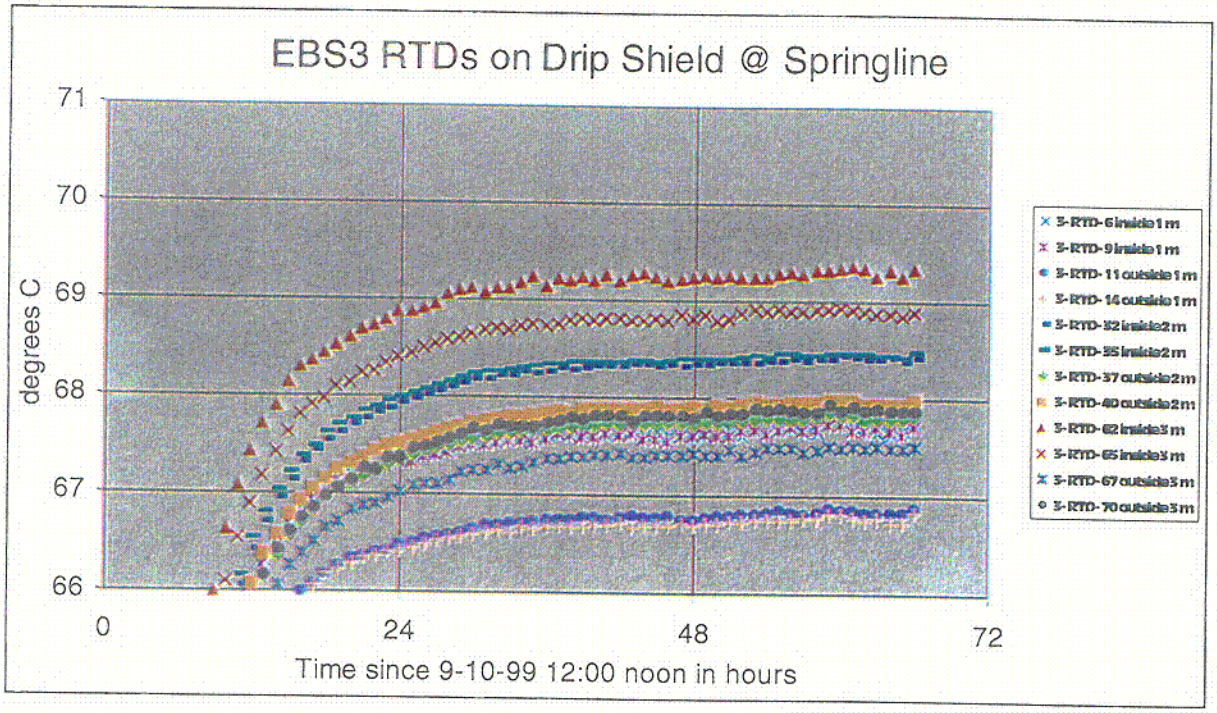
DripShieldTurnOn.do



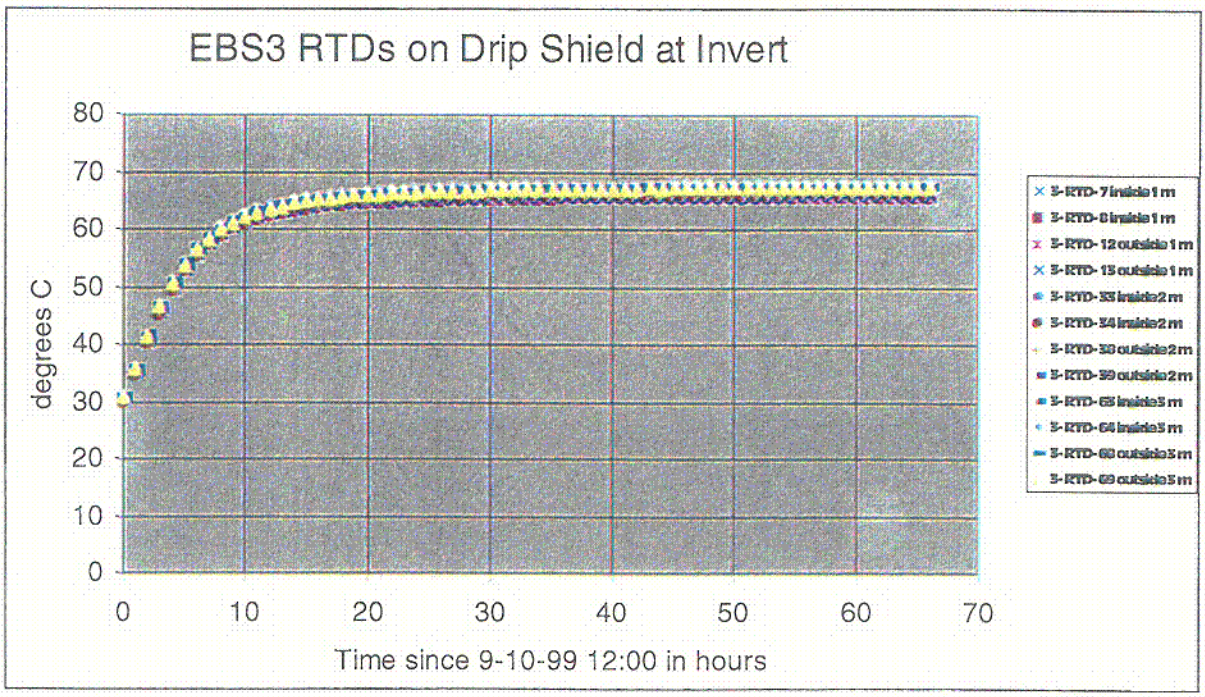


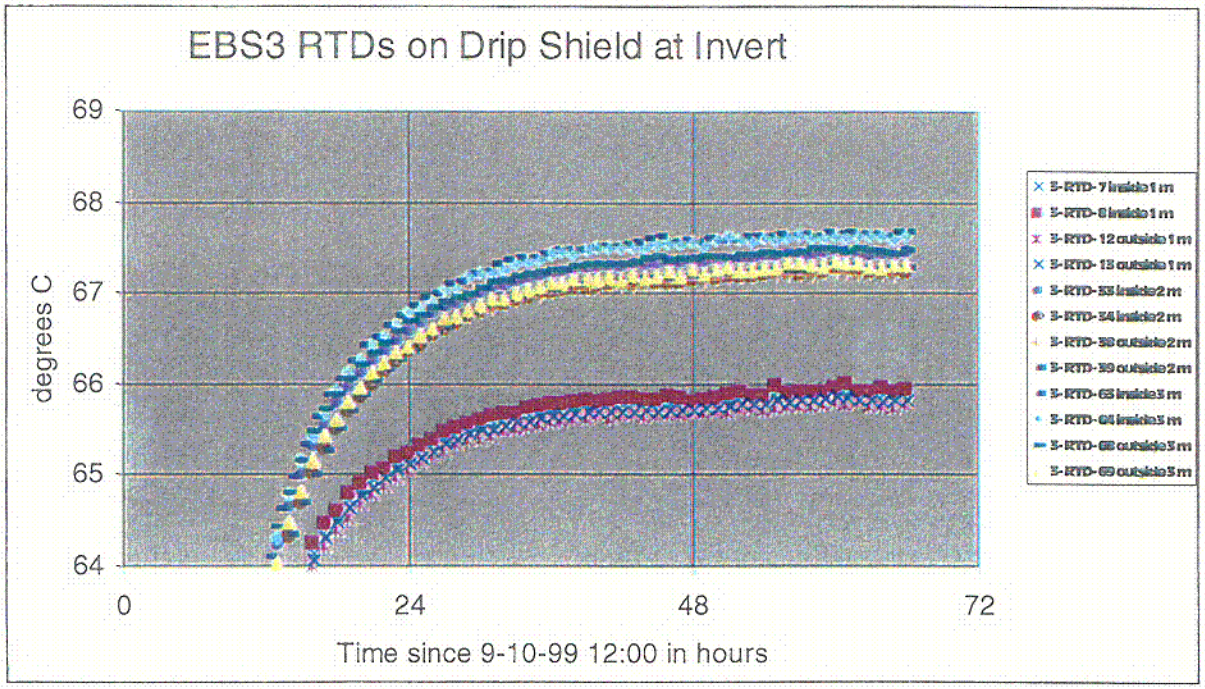
Preliminary Data – Not yet qualified to project standards – approximate conversions used from raw data
Power turned on about 11:30 am on 9-10-99



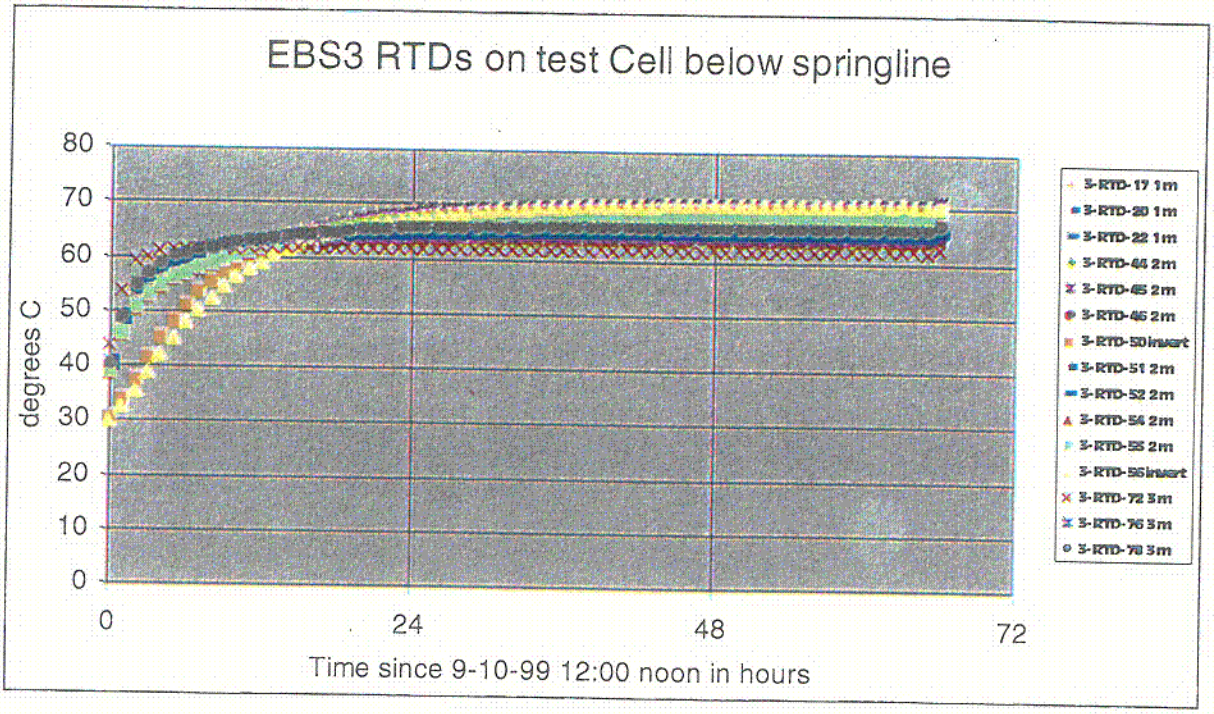


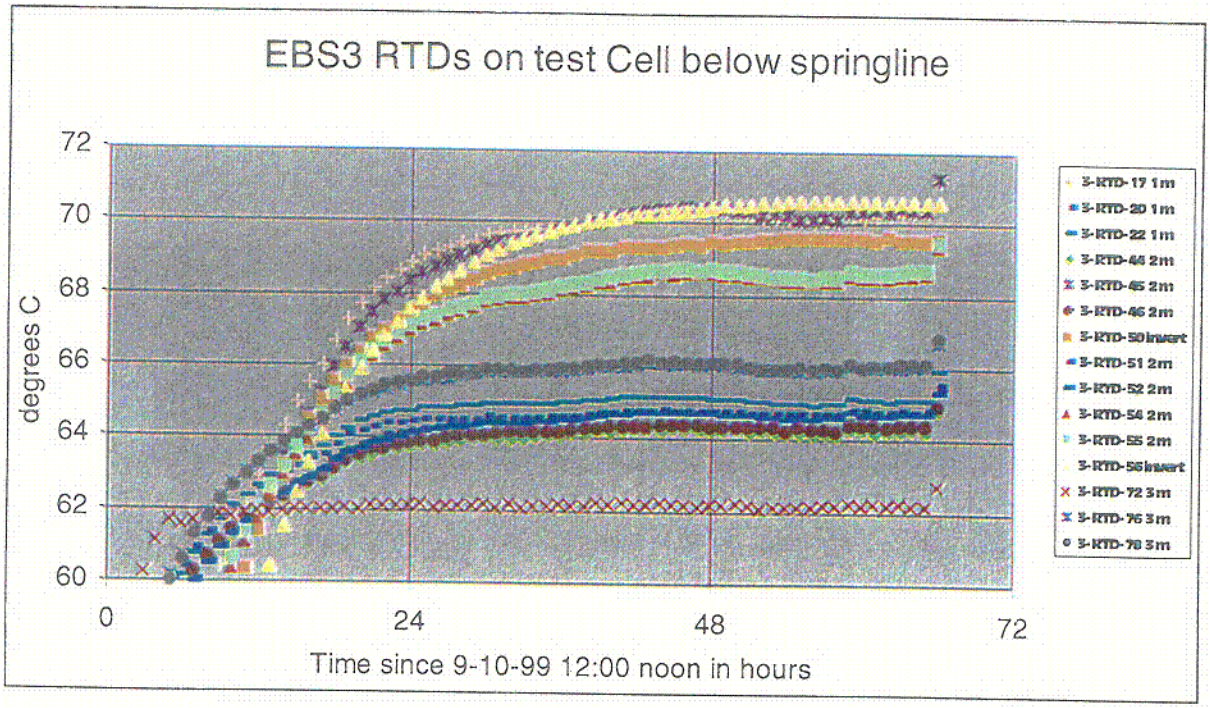
Preliminary Data – Not yet qualified to project standards – approximate conversions used from raw data
Power turned on about 11:30 am on 9-10-99



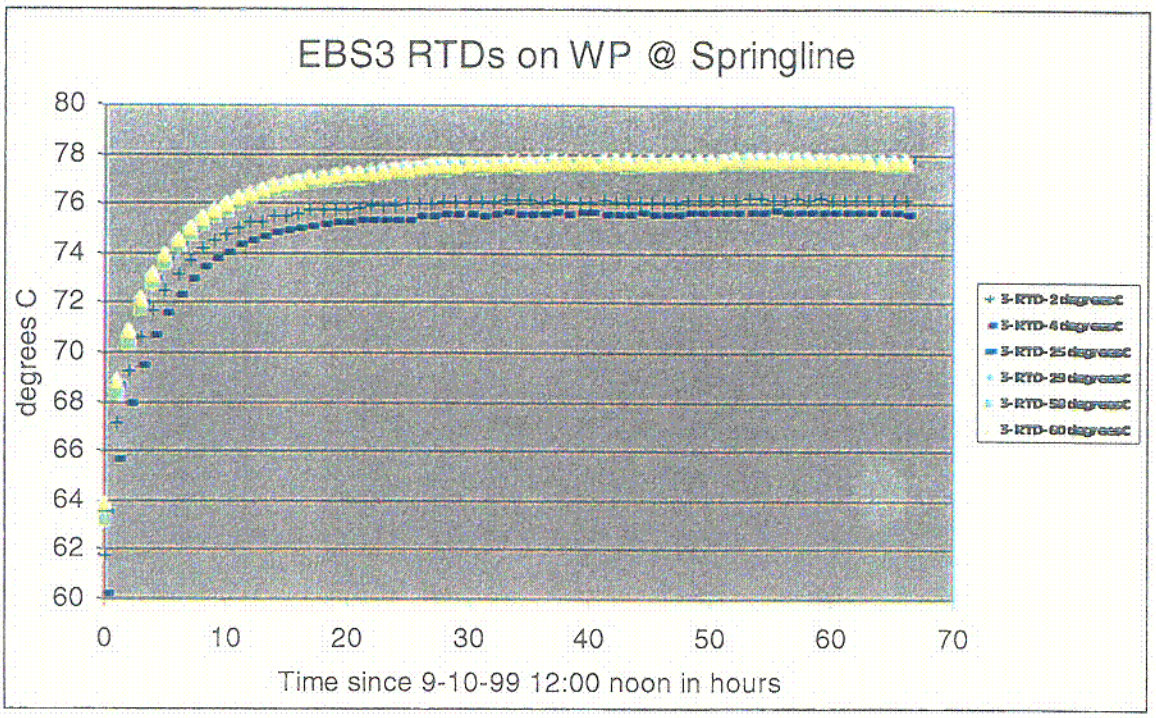


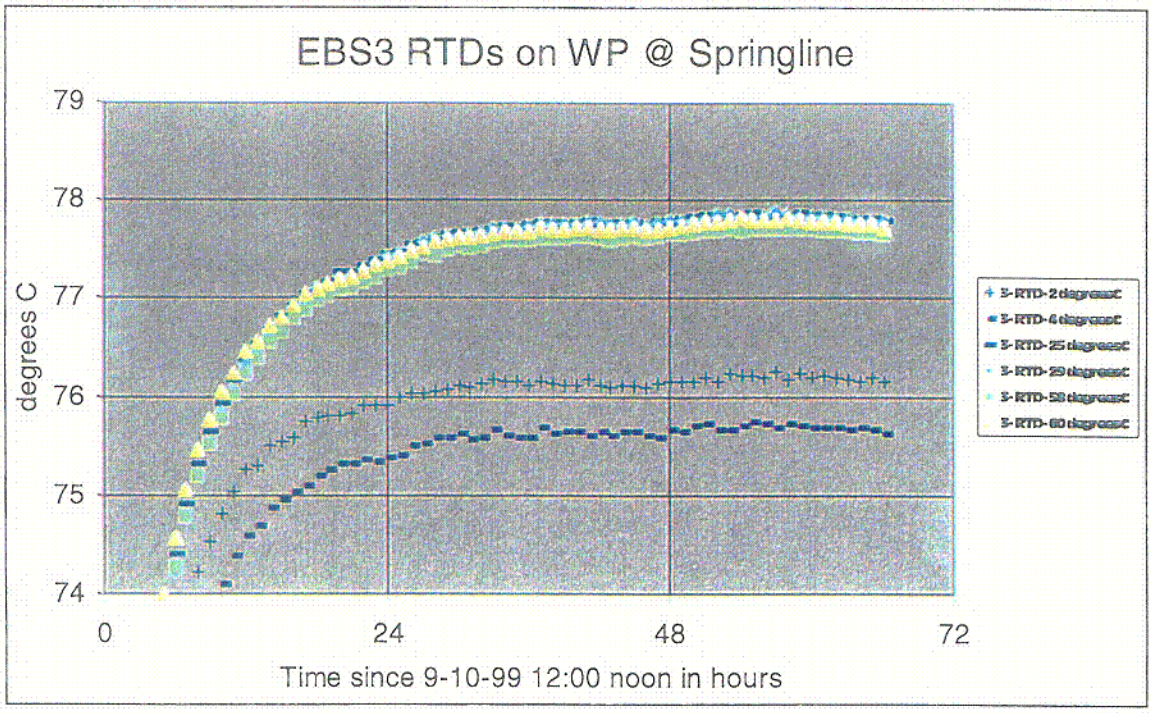
Preliminary Data – Not yet qualified to project standards – approximate conversions used from raw data
Power turned on about 11:30 am on 9-10-99



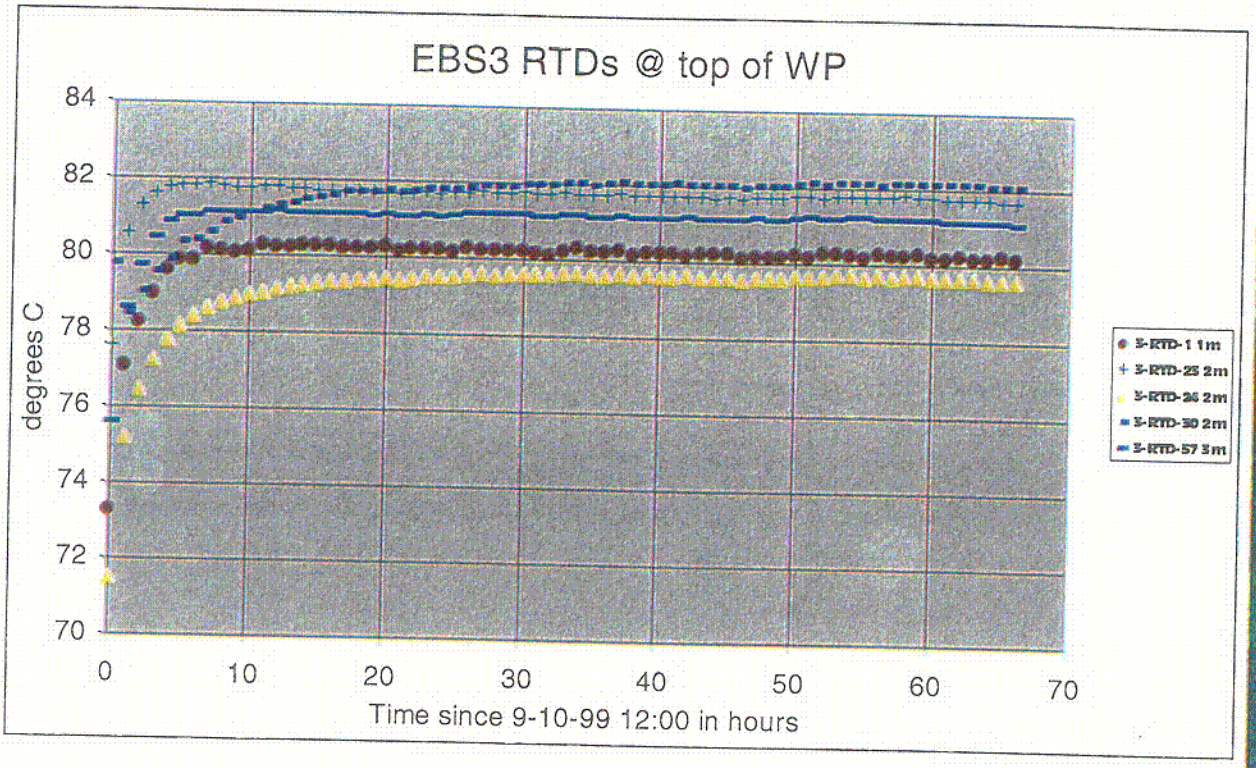


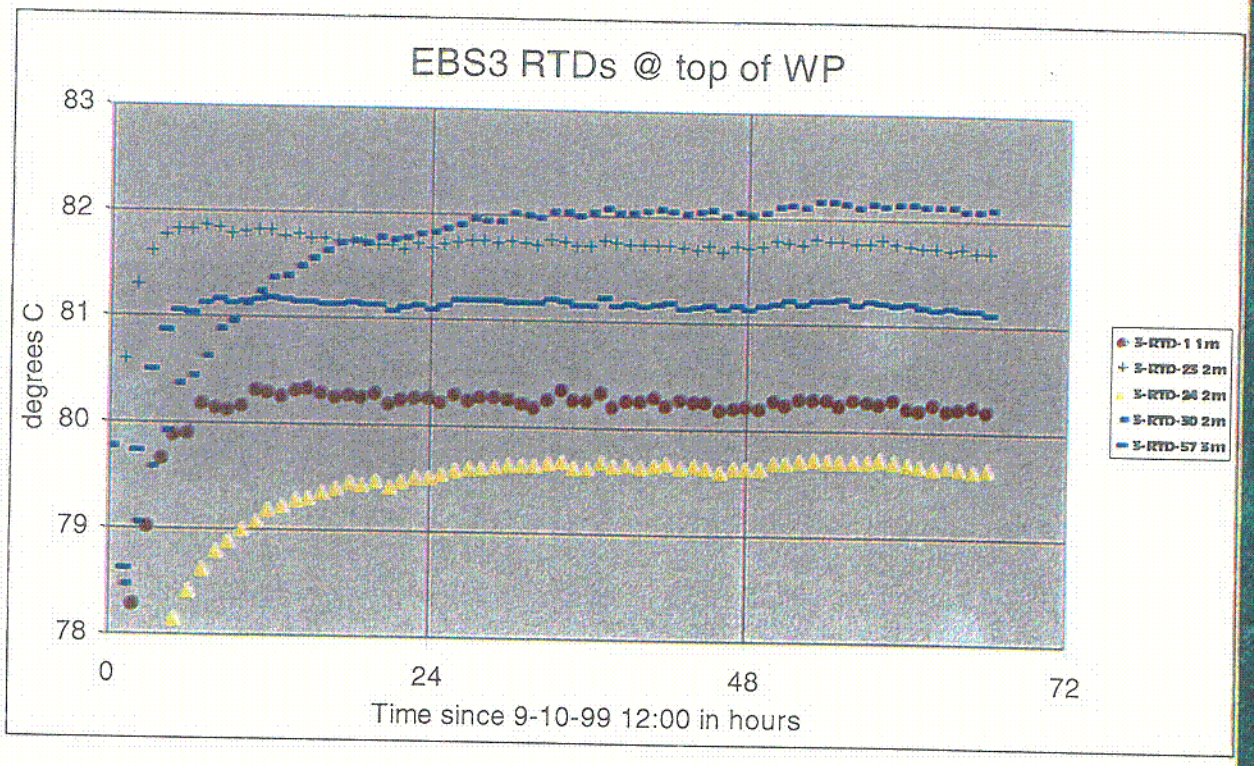
Preliminary Data – Not yet qualified to project standards – approximate conversions used from raw data
Power turned on about 11:30 am on 9-10-99



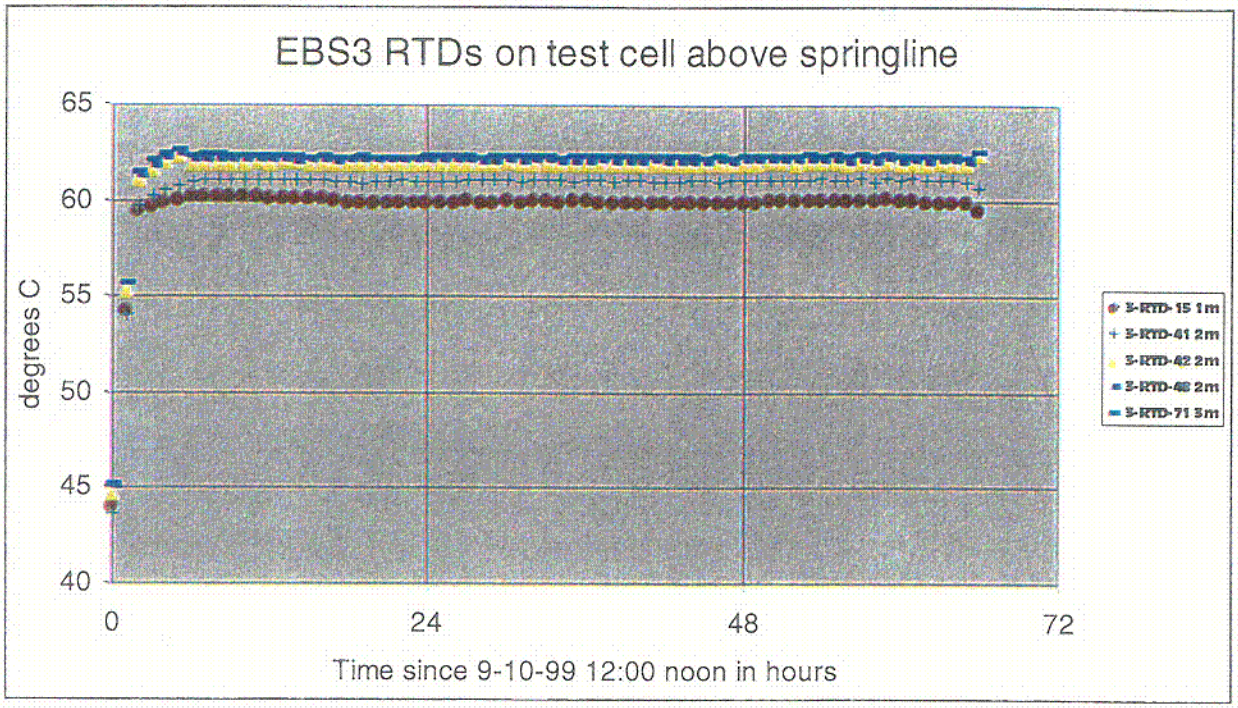


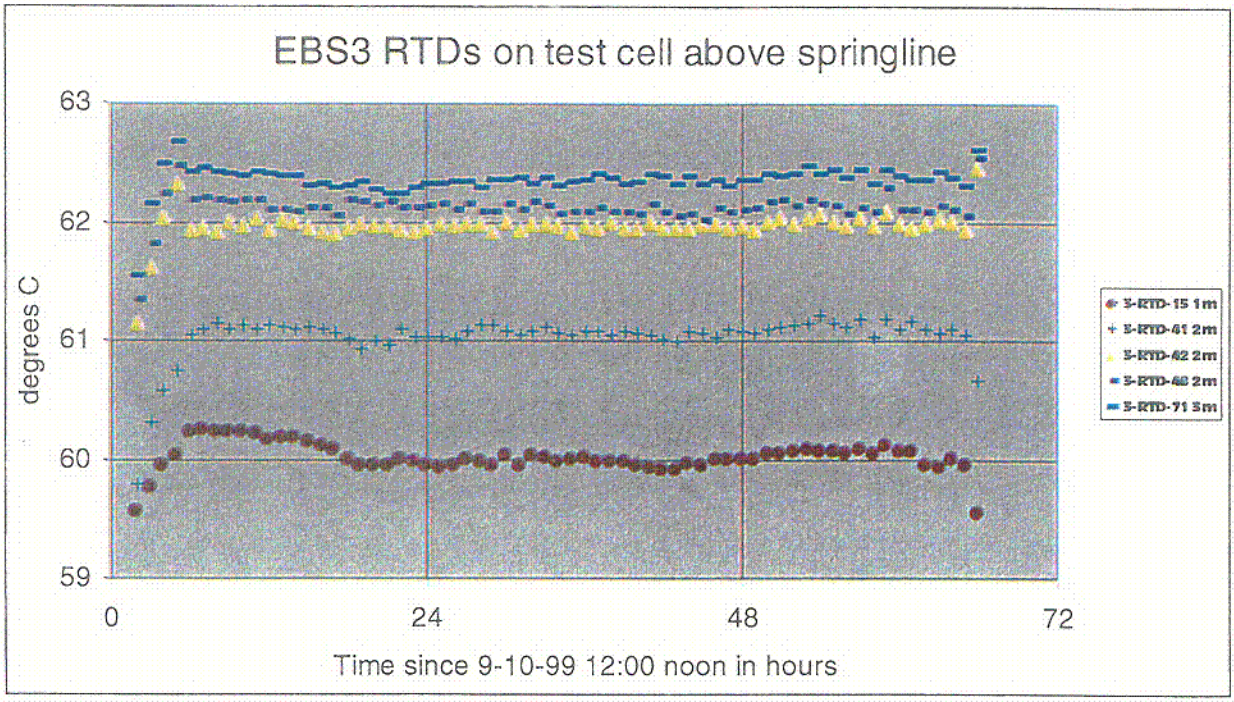
Preliminary Data – Not yet qualified to project standards – approximate conversions used from raw data
Power turned on about 11:30 am on 9-10-99



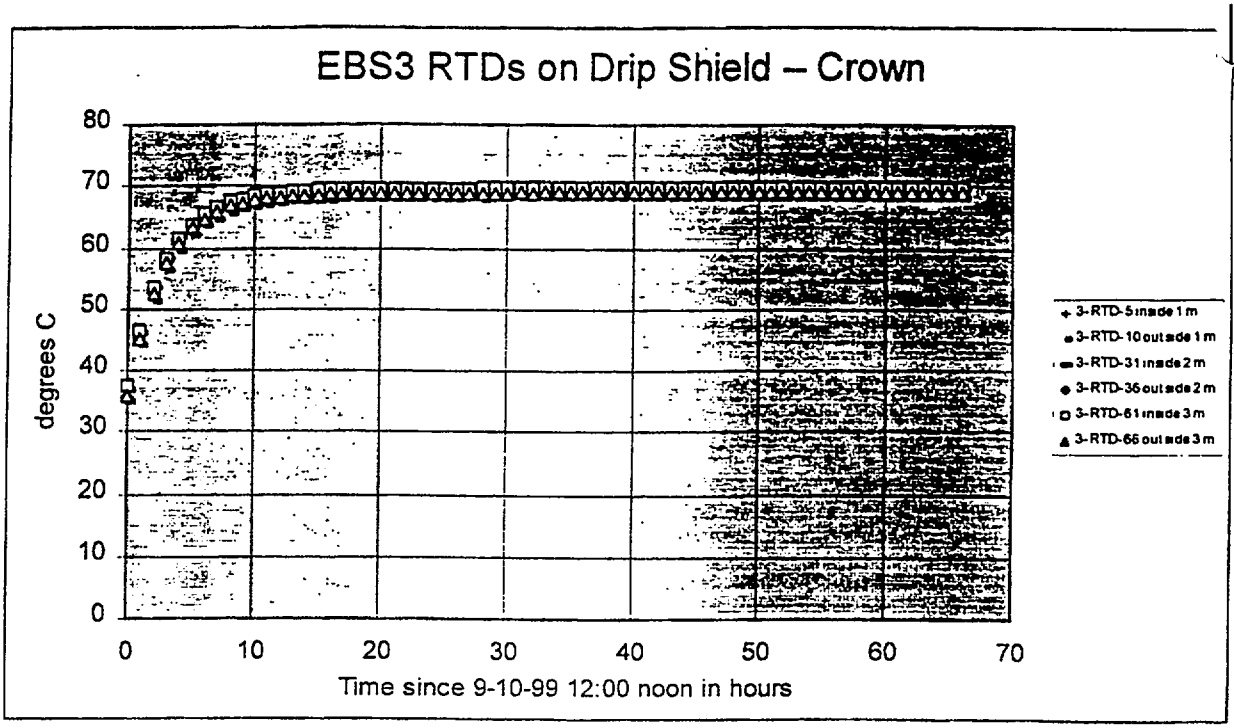


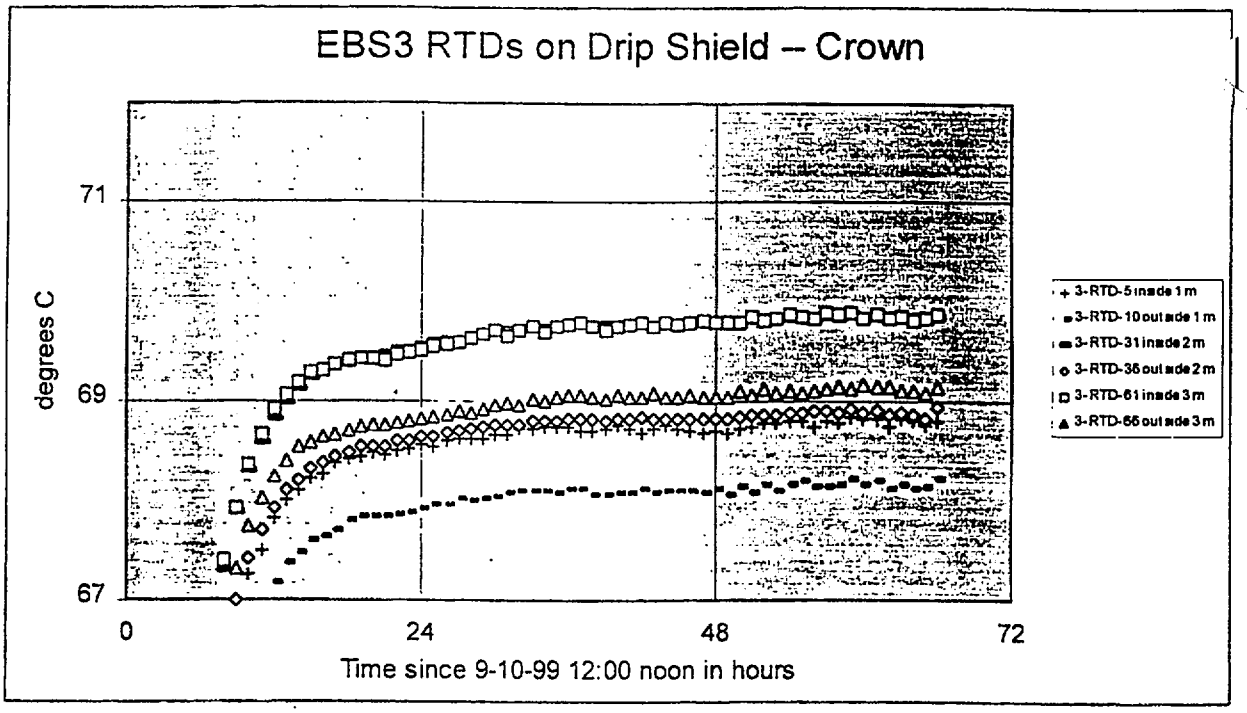
Preliminary Data – Not yet qualified to project standards – approximate conversions used from raw data
Power turned on about 11:30 am on 9-10-99



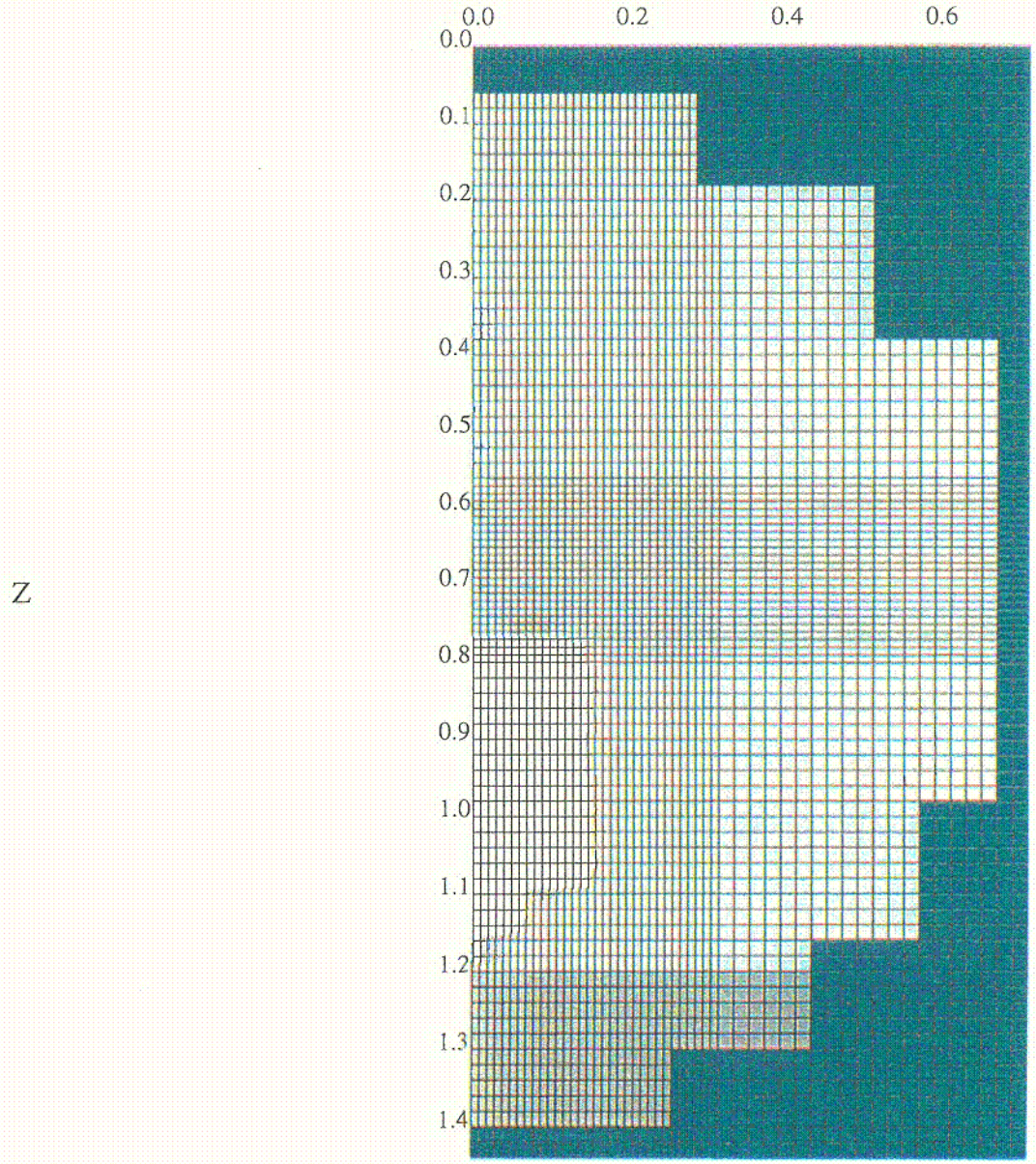


Preliminary Data – Not yet qualified to project standards – approximate conversions used from raw data
Power turned on about 11:30 am on 9-10-99





Preliminary Data – Not yet qualified to project standards – approximate conversions used from raw data
Power turned on about 11:30 am on 9-10-99



Input file: radymp2Ddst2
Connection file: 2Ddst4.rad

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EVALUATION OF THE NUFT CODE TO SIMULATE NATURAL CONVECTION

NUFT is basically developed for simulating flow and heat transport in porous and fractured media and, therefore, has limitations in modeling natural convection in air space, such as that underneath the drip shield. Recognizing these limitations, the code has to be used with cautions to predict the average temperature and heat transfer rate below the drip shield. This may be accomplished by adjusting the pseudo-porous medium properties of air so that the average model results would match an analytical solution.

A heat transfer problem for concentric cylinders with analytical solution is selected for validating NUFT. Accordingly, a NUFT model has been constructed to approximate the concentric cylinders with rectangular cylinders using the drip shield and the heater (simulated waste package) as the outer and inner cylinders, respectively. The bottom of the outer cylinder is represented by invert material. The model dimensions correspond approximately to the repository scale model. The purpose of this calculation is to adjust the thermal conductivity in the air space between the heater and the drip shield such that the model results would be consistent with an accepted, analytical solution to a natural convection problem for concentric cylinders. Since this NUFT model is designed for simulating natural convection only, radiation has been eliminated altogether.

This calculation describes three cases with different thermal loading conditions resulting in a variation of temperature between the heater and the drip shield. A simulation grid, thermal loading curves and input listings for these cases are included in this attachment. For each case, the temperature difference between the drip shield and the heater has, in general, stabilized after 70 days of simulation, with a rise of temperature difference of less than 0.5 degree C in 10 days. On day 70, there is a variation of temperature on the surface of the drip shield while the heater temperature is practically stable throughout its surface. As a result, the temperature difference between the heater and the drip shield changes along the surface of the drip shield for a given time. Therefore, to match the analytical solution which assumes a constant temperature difference between the drip shield and the heater, an average temperature difference from the model is used in the analysis.

It was found that by using a thermal conductivity of 0.0263 W/(m-K) for air as input to NUFT, the average model results are consistent with the closed-form solution. Below is a calculation to substantiate this finding.

Following the approach and using the equations with the same notations in Example 9.5 (Incropera & Dewitt, "Introduction to Heat Transfer" pg. 477, or "Fundamentals of Heat and Mass Transfer" pg. 513) for heat transfer in concentric cylinders, the NUFT problem is defined as follows:

Rectangular area enclosed by heater = 2.72 sq. m.
Diameter of cylinder with equivalent area = 1.86 m.

Rectangular area enclosed by drip shield = 6.96 sq. m.
Diameter of cylinder with equivalent area = 2.98 m.

Therefore,
D_0 = 2.98 m
D_i = 1.86 m.
L = 0.56 m.

Case 1. Thermal loading stabilized at 43 W/m

At 70 days of simulation, T_i = 82.41 C

66% of the outer cylinder is in 74.65 – 75.19 C range -> average T = 74.92 C = 347.92 K
T_0 = 74.92 C
$\Delta T = T_i - T_0$ = 7.49 C

Air properties at 347.92 K,

k = 0.0298W/m.K
β = 0.00287 K^{-1}
ν = 2.070E-5 m^2/s
α = 2.960E-5 m^2/s

$Pr = \nu / \alpha = 0.70$

$$Ra_L = g\beta (T_i - T_0) L^3 / (\nu\alpha) = 6.030E+7$$

$$Ra_c^* = [\ln(D_0/D_i)]^4 \, Ra_L / [L^3 (D_i^{-3/5} + D_0^{-3/5})^5] = 6.576E+6$$

$$k_{eff} = 0.386 [Pr / (0.861 + Pr)]^{1/4} (Ra_c^*)^{1/4} k = 0.477$$

$$q' = 2\pi \cdot \Delta T \cdot k_{eff} / [\ln(D_0 / D_i)] = 48.0 \text{ W/m (vs. 43.0 W/m from NUFT input)}$$

33% of outer cylinder (represented by the invert material) is in the 62.40 – 73.59 C range
-> Average T = 68.0 C = 341.0 K.
ΔT = 14.41 C

Air properties at 341.0 K, k = 0.0293 W/m-K
β = 0.00293 K^{-1}
ν = 2.001E-5 m^2/s

$\alpha = 2.856E\text{-}5\ m^2/s$
$Pr = 0.7$

$Ra_L = 1.271E+8$
$Ra_C^* = 1.389E+7$
$K_{eff} = 0.565$

$q' = 108.7 W/m$

Note that the higher rate q' for the 33% portion is mainly due to the extraordinarily low temperature of the 2 invert elements at the bottom of the outer cylinder, thus increases tremendously ΔT for the that portion of the cylinder. In the production simulations with a repository model, the air gap for this 33% portion will be filled with invert material and there will not be huge ΔT at that location. As mentioned previously, the model results show after approximately 70 days, the temperature difference between the heater and the drip shield stays fairly constant within 1 degree, although there is a slight rising trend in temperature for both of them.

Case 2. Thermal loading stabilized at 25 W/m

Run model with lower thermal loading than Case 1 so a smaller temperature difference will result.

At 70 days of simulation, $T_i = 72.94$ C

66% of the outer cylinder is in the 68.43 – 68.74 C range -> Average T = 68.59 C (341.59K)

$T_0 = 68.59$ C
therefore, $\Delta T = 4.35$ C

At 341.59 K, the air properties are:

$k = 0.0294 W/m.K$
$\beta = 0.00293\ K^{-1}$
$\nu = 2.007E\text{-}5\ m^2/s$
$\alpha = 2.866E\text{-}5\ m^2/s$
$Pr = 0.70$

$Ra_L = 3.812E+7$
$Ra_c^* = 4.166E+6$

$k_{eff} = 0.4194$

$q' = 24.3$ W/m (vs. 25.0 W/m from NUFT input)

33% of the outer cylinder (represented by the invert material) is in the 61.39 – 67.81 C range -> Average T = 64.60 C = 337.60 K.

$\Delta T = 8.34$ C

Air properties at 337.6 K,

$k = 0.0291$ W/m.K
$\beta = 0.00296$ K^{-1}
$\nu = 1.967E\text{-}5$ m^2/s
$\alpha = 2.806E\text{-}5$ m^2/s
$Pr = 0.70$

$Ra_L = 7.695E+7$
$Ra_c^* = 8.392E+6$
$K_{eff} = 0.4945$

$q' = 55.1$ W/m

Case 3. Thermal loading stabilized at 10 W/m

At 70 days of simulation, $T_i = 65.21$ C

66% of the outer cylinder is in the 63.39 – 63.52 C range -> Average T = 63.46 C = 336.46 K.

$\Delta T = 1.75$ C

For T = 336.46 K, $k = 0.0290$ W/m.K
$\beta = 0.0029$ K^{-1}
$\nu = 1.956E\text{-}5$ m^2/s
$\alpha = 2.789E\text{-}5$ m^2/s
$Pr = 0.70$

$Ra_L = 1.649E+7$
$Ra_c^* = 1.798E+6$
$k_{eff} = 0.335$

$q' = 7.93$ W/m (vs. 10.0 W/m from NUFT input)

33% of outer cylinder (representd by the invert material) is in the 60.56 – 63.14 C range ->Average T = 61.85 C = 334.85 K

$\Delta T = 3.36$ C

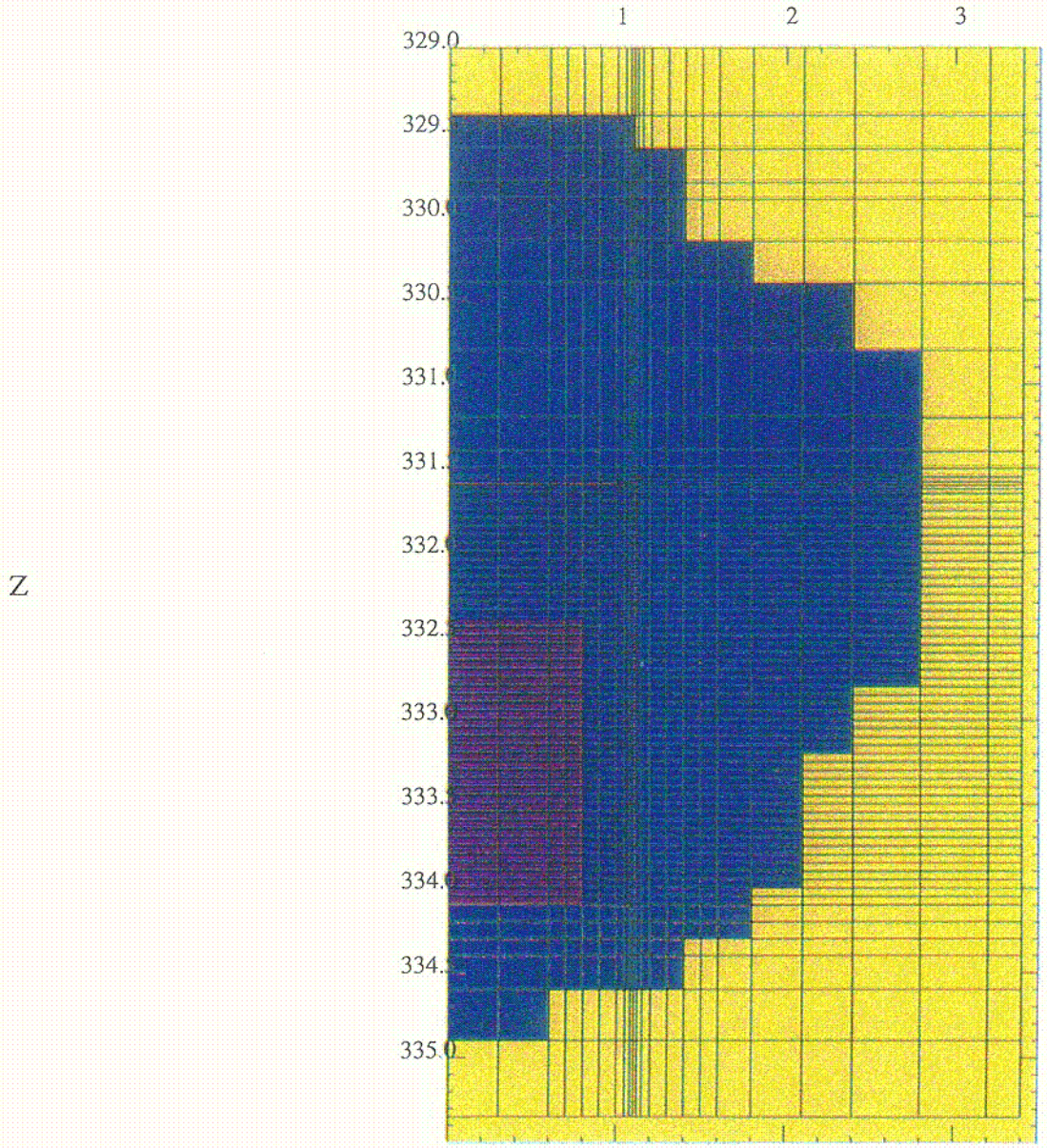
At 334.85 K, air properties are:

$k = 0.0289$ W/m.K
$\beta = 0.00299$ K^{-1}
$\nu = 1.940E\text{-}5$ m^2/s
$\alpha = 2.766E\text{-}5$ m^2/s

$Pr = 0.70$

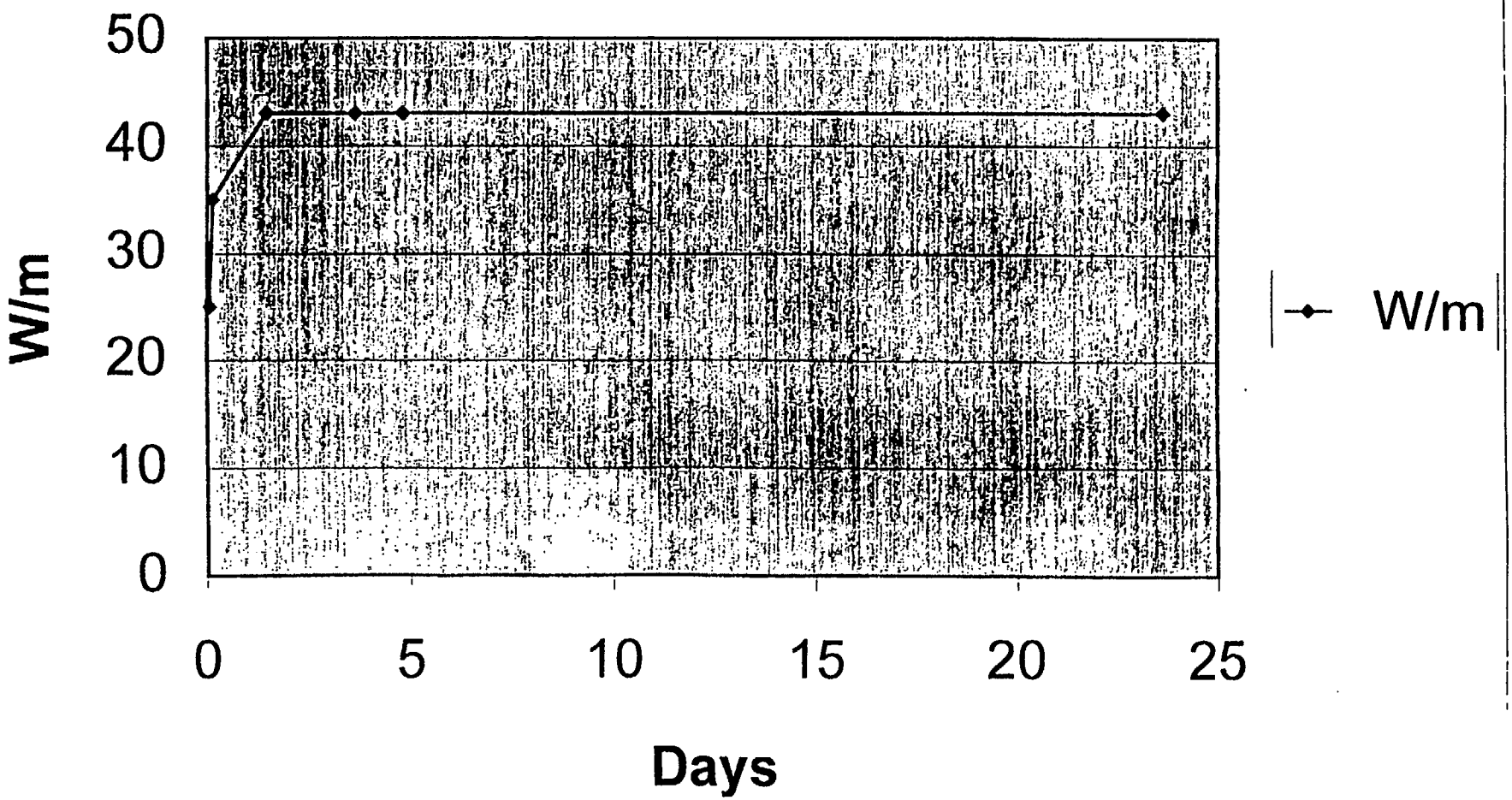
$Ra_L = 3.222E+7$
$Ra_c^* = 3.514E+6$
$k_{eff} = 0.395$

$q' = 17.8$ W/m

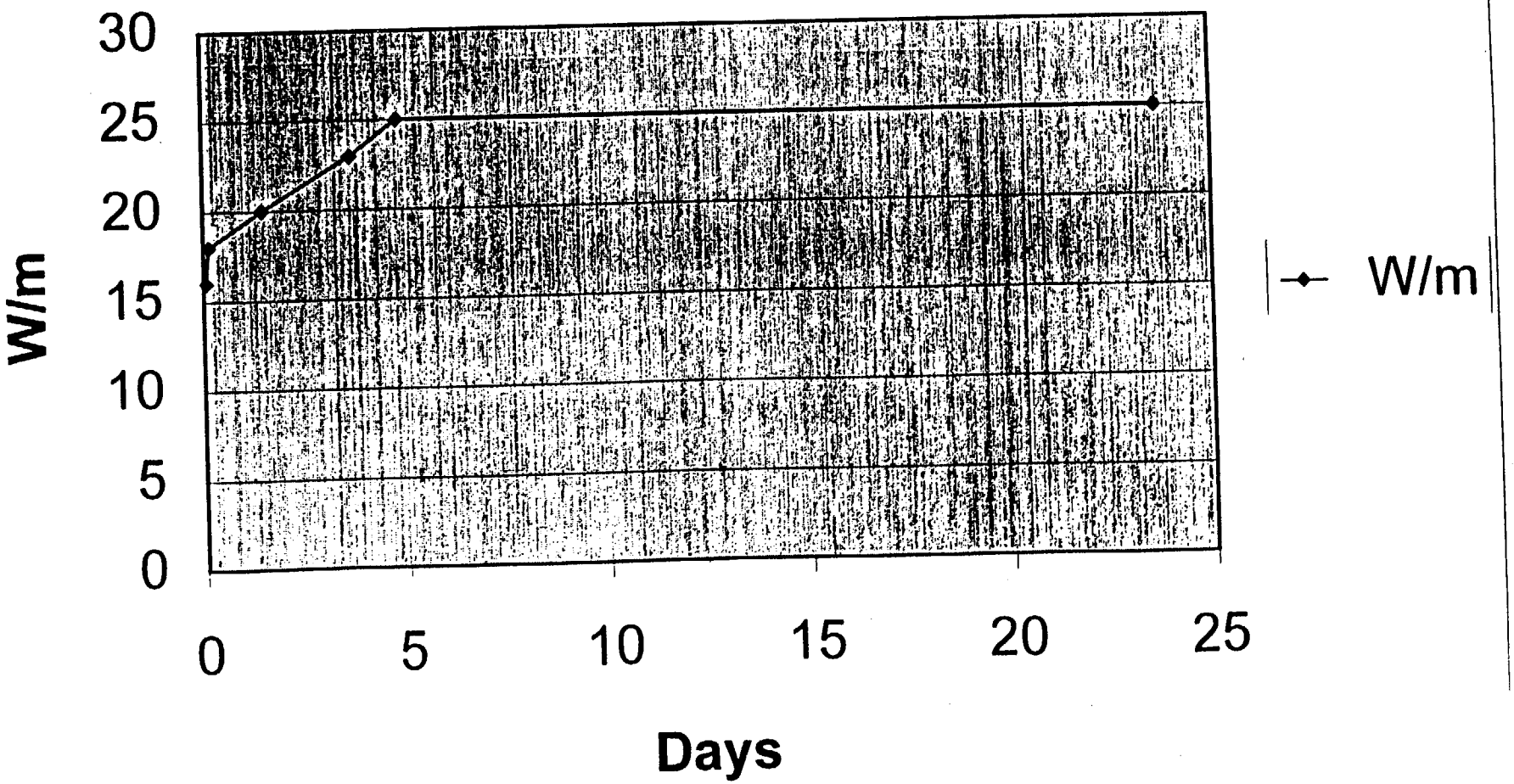


Input file: radymp
Connection file: 2Ddst0.rad

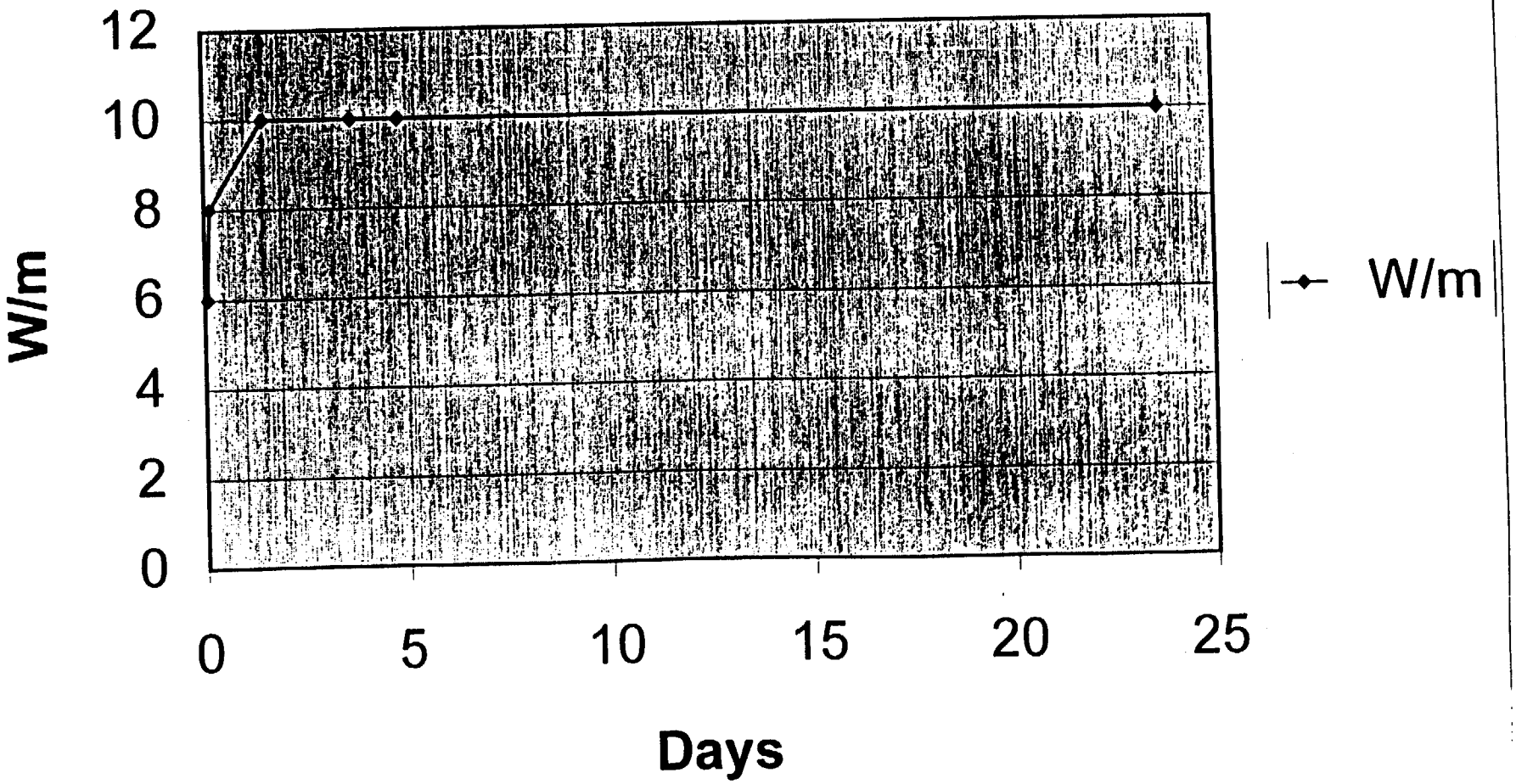
Case 1. Thermal Loading vs. Time



Case 2. Thermal Loading vs. Time



Case 3. Thermal Loading vs. Time



OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

NOTICE:

SPECIAL HANDLING INSTRUCTIONS

QA: QA

Document Identifier: ANL-EBS-MD-000026

Document Title: Water Diversion Model

Document Revision/Change: 00

Document Date: 02/01/2000

This document requires special handling in accordance with AP-6.1Q.

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```
  (usnt
  (title " Yucca Mountain Project 2-D T-H Model w. drip shield")
  (modelname usnt)
  (vapor-pressure-lowering off)
  (include-pkg "vtough.pkg")
  (tstop   8.0380e+06)
  (time 0)
  (stepmax 1000000)
  (dtmax  8.0380e+06)
  (dt 1e3)


;; Run ymp2DdstR4

;; Using a thickness of  2 cm for the drip shield
;; Use drift air K = 1E-08 and Tcond = 0.0263

;; calibrate model drift air K & Tcond for repository model
;; no radiation

;; Peak thermal loading @ 43 W/m


  (output


      (extool (variables T RH S.liquid X.air.gas P Qrad Qcond Qd.energy
V.liquid V.gas )
              (file-ext ".ext")(range "**")
(outtimes 0 0.2d 0.5d 1d 1.5d 2d 3d 5d 7d 8d 10d 12d 15d 18d 20d 22d
30d 40d 45d 60d 70d 80d)
  ))

  (rocktab
    (heatr
      (porosity 0.010) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 4.8886e+02) (solid-density 8.1892e+03)
      (tcond tcondLin (solid  14.420000)(liquid  14.420000)(gas
14.420000))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
      (tort (gas 0.000e+00) (liquid 0.0))
      (kr (gas 1.0)
          (liquid 1.0))
      (pc (liquid 0.0))
    )
    (drift
      (porosity 0.999) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.007e+03) (solid-density 1.1614 )
      (tcond tcondLin (solid 0.026300)(liquid 0.026300)(gas 0.026300))
      (K0 1.000e-08) (K1 1.000e-08) (K2 1.000e-08)
;; JJN     (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krPower (power 4) (Smax 1.000e+00)(Sr 0.000e+00)))
```

```
      (pc (liquid 0.0))
    )
    (shield
      (porosity 0.010) (Kd (air 0.0) (water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 5.5132e+2) (solid-density 7.900e+03)
      (tcond tcondLin (solid 20.55) (liquid 20.55) (gas 20.55))
      (K0 0.000) (K1 0.000) (K2 0.000)
      (tort (gas 0.000) (liquid 0.000))
      (kr  (gas 1.0)
           (liquid 1.0))
      (pc  (liquid 0.0))
    )
    (invert
    (porosity 0.545) (Kd (air 0.0) (water 0.0))
    (KdFactor (water 0.0) (air 0.0))
    (Cp 948.0) (solid-density 2.530e+03)
    (tcond tcondLin (solid 0.66) (liquid 0.66) (gas 0.66))
    (K0 6.150e-10) (K1 6.150e-10) (K2 6.150e-10)
    (tort (gas 0.700) (liquid 0.0))
    (kr  (gas 1.0)
         (liquid 1.0))
    (pc  (liquid 0.0))
    )
    (atm
      (porosity 0.990) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.000e+08) (solid-density 1.0000)
      (tcond tcondLin (solid 0.000000)(liquid 0.000000)(gas 0.000000))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
;;JJN      (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krlLinear (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
    )
    (insul
      (porosity 0.990) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 0.7) (solid-density 2.40e+01)
      (tcond tcondLin (solid 0.000000)(liquid 0.000000)(gas 0.000000))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
;;JJN      (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krlLinear (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
    )
  )

(state
    (P by-key ("*" 1.e5))

    (S.liquid by-key
                      ("sh*" 0.0)
                      ("dr*" 0.0)
                      ("ht*" 0.0)
```

```
                    ("ins*" 0.0)
                    ("in*" 0.0)
 )

   (T by-key ("*" 60.0)
   )

(X.air by-key ("*" -1.0)  ("dr*" 0.999) ("ht*" 1.0)
              ("sh*" 1.0) ("ins*" 0.999) ("in*" 0.999))

) ;; end state


 (input-mass-fraction on)


 (linear-solver d4vband)
;;  (linear-solver pcg)
  (ilu-degree 1)
  (pcg-parameters (precond d4)(toler 1e-4)(itermax 100)(north 15))

  (adaptive-ilu ON)



  (srctab
    (compflux
    (comp energy)
    (name REPO)
    (range "ht*")
    (allocate-by-element ("*" 0.5))
    (table
       0.00          10.       2.00e+01    1.50e+01    2.000e+02  1.80e+01
       6.3072e+03  2.50e+01 1.2614e+04  3.50e+01    1.260e+05  4.30e+01
       3.1533e+05  4.30e+01 4.1533e+05  4.30e+01    1.038e+06  4.30e+01
       2.0380e+06  4.30e+01 4.0380e+06  4.30e+01    8.0380e+06 4.30e+01
      ) ;; end table
     (allocate-by-volume)
    ) ;; end compflux

    ) ;;  end srctab



(genmsh
   (down 0. 0. 1.0)
   (coord rect)

   (dx
                2*0.3   4*.1 .05 .03 2*.02 .03 .05  4*.1  0.2
2*0.3
                2*0.4         2*0.2            0.4           0.5
0.8
                  1.1           1.6            3.0           3.9
5.1
                  5.3           6.6            8.6           )
```

```
(dy          1)

(dz
          0.40      2*0.20          0.10      2*0.25
        2*0.40   0.20   0.1 .05 .03 2*.02 .03 .05  6*0.05  8*0.05
4*0.05
        30*0.05  3*0.1  0.2  0.3  0.45
      )

(mat

    (ins     insul   1     nx     1    ny    1    1)
    (sh      shield  1      9     1    ny   13   13)
    (sh      shield  10    10     1    ny   13   64)
    (in      invert  10    10     1    ny   65   68)
    (dr      drift   11    12     1    ny   47   64)
    (dr      drift   1      9     1    ny   14   30)
    (dr      drift   5      9     1    ny   31   64)
    (ht      heatr   1      4     1    ny   31   64)
    (dr      drift   1      9     1    ny    2    4)
    (dr      drift   10    14     1    ny    3    4)
    (ins     insul   10    nx     1    ny    2    2)
    (ins     insul   15    nx     1    ny    3    4)
    (dr      drift   1     14     1    ny    5    5)
    (ins     insul   15    nx     1    ny    5    5)
    (dr      drift   1     17     1    ny    6    6)
    (ins     insul   18    nx     1    ny    6    6)
    (dr      drift   1     19     1    ny    7    7)
    (ins     insul   20    nx     1    ny    7    7)
    (dr      drift   1     20     1    ny    8   10)
    (ins     insul   21    nx     1    ny    8   10)
    (dr      drift   1     20     1    ny   11   12)
    (dr      drift   11    20     1    ny   13   38)
    (ins     insul   21    nx     1    ny   11   38)
    (dr      drift   11    19     1    ny   39   46)
    (ins     insul   20    nx     1    ny   39   46)
    (dr      drift   13    18     1    ny   47   62)
    (ins     insul   19    nx     1    ny   47   62)
    (dr      drift   13    17     1    ny   63   64)
    (ins     insul   18    nx     1    ny   63   64)
    (dr      drift   1      9     1    ny   65   66)
    (dr      drift   11    17     1    ny   65   66)
    (ins     insul   18    nx     1    ny   65   66)
    (dr      drift   1      9     1    ny   67   68)
    (dr      drift   11    14     1    ny   67   68)
    (ins     insul   15    nx     1    ny   67   68)
    (dr      drift   1      2     1    ny   69   69)
    (in      invert  3     nx     1    ny   69   69)
    (in      invert  1     nx     1    ny   70   70)

    )
```

```
)   ;; end of genmsh

) ;; end of model input
```

```
  (usnt
  (title " Yucca Mountain Project 2-D T-H Model w. drip shield")
  (modelname usnt)
  (vapor-pressure-lowering off)
  (include-pkg "vtough.pkg")
  (tstop   8.0380e+06)
  (time 0)
  (stepmax 1000000)
  (dtmax  8.0380e+06)
  (dt 1e3)


;; Run ymp2DdstR3

;; Using a thickness of  2 cm for the drip shield
;; Use drift air K = 1E-08 and Tcond = 0.0263

;; calibrate model drift air K & Tcond for repository model
;; no radiation

;; Peak thermal loading @ 25 W/m


  (output


      (extool (variables T RH S.liquid X.air.gas P Qrad Qcond Qd.energy
V.liquid V.gas )
              (file-ext ".ext")(range "*")
(outtimes 0 0.2d 0.5d 1d 1.5d 2d 3d 5d 7d 8d 10d 12d 15d 18d 20d 22d
30d 40d 45d 60d 70d 80d)
  ))

  (rocktab
    (heatr
      (porosity 0.010) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 4.8886e+02) (solid-density 8.1892e+03)
      (tcond tcondLin (solid  14.420000)(liquid  14.420000)(gas
14.420000))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
      (tort (gas 0.000e+00) (liquid 0.0))
      (kr (gas 1.0)
          (liquid 1.0))
      (pc (liquid 0.0))
    )
    (drift
      (porosity 0.999) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.007e+03) (solid-density 1.1614 )
      (tcond tcondLin (solid 0.026300)(liquid 0.026300)(gas 0.026300))
      (K0 1.000e-08) (K1 1.000e-08) (K2 1.000e-08)
;; JJN     (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krPower (power 4) (Smax 1.000e+00)(Sr 0.000e+00)))
```

```
      (pc (liquid 0.0))
    )
    (shield
      (porosity 0.010) (Kd (air 0.0) (water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 5.5132e+2) (solid-density 7.900e+03)
      (tcond tcondLin (solid 20.55) (liquid 20.55) (gas 20.55))
      (K0 0.000) (K1 0.000) (K2 0.000)
      (tort (gas 0.000) (liquid 0.000))
      (kr  (gas 1.0)
           (liquid 1.0))
      (pc  (liquid 0.0))
    )
    (invert
    (porosity 0.545) (Kd (air 0.0) (water 0.0))
    (KdFactor (water 0.0) (air 0.0))
    (Cp 948.0) (solid-density 2.530e+03)
    (tcond tcondLin (solid 0.66) (liquid 0.66) (gas 0.66))
    (K0 6.150e-10) (K1 6.150e-10) (K2 6.150e-10)
    (tort (gas 0.700) (liquid 0.0))
    (kr  (gas 1.0)
         (liquid 1.0))
    (pc  (liquid 0.0))
    )
    (atm
      (porosity 0.990) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.000e+08) (solid-density 1.0000)
      (tcond tcondLin (solid 0.000000)(liquid 0.000000)(gas 0.000000))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
;;JJN      (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krlLinear (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
    )
    (insul
      (porosity 0.990) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 0.7) (solid-density 2.40e+01)
      (tcond tcondLin (solid 0.000000)(liquid 0.000000)(gas 0.000000))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
;;JJN      (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krlLinear (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
    )
  )

(state
    (P by-key ("*" 1.e5))

    (S.liquid by-key
                      ("sh*" 0.0)
                      ("dr*" 0.0)
                      ("ht*" 0.0)
```

```
                    ("ins*" 0.0)
                    ("in*" 0.0)
  )

    (T by-key ("*" 60.0)
    )

 (X.air by-key ("*" -1.0)  ("dr*" 0.999) ("ht*" 1.0)
               ("sh*" 1.0) ("ins*" 0.999) ("in*" 0.999))

 ) ;; end state


  (input-mass-fraction on)


 (linear-solver d4vband)
;;  (linear-solver pcg)
  (ilu-degree 1)
  (pcg-parameters (precond d4)(toler 1e-4)(itermax 100)(north 15))

  (adaptive-ilu ON)



  (srctab
    (compflux
    (comp energy)
    (name REPO)
    (range "ht*")
    (allocate-by-element ("*" 0.5))
    (table
       0.00         10.       2.00e+01    1.20e+01    2.000e+02  1.40e+01
       6.3072e+03   1.60e+01 1.2614e+04  1.80e+01    1.260e+05  2.00e+01
       3.1533e+05   2.30e+01 4.1533e+05  2.50e+01    1.038e+06  2.50e+01
       2.0380e+06   2.50e+01 4.0380e+06  2.50e+01    8.0380e+06 2.50e+01
      ) ;; end table
     (allocate-by-volume)
    ) ;; end compflux

    ) ;;  end srctab


(genmsh
   (down 0. 0. 1.0)
   (coord rect)

   (dx
                2*0.3   4*.1 .05 .03 2*.02 .03 .05  4*.1  0.2
2*0.3
                2*0.4         2*0.2           0.4          0.5
0.8
                  1.1           1.6           3.0           3.9
5.1
                  5.3           6.6           8.6           )
```

```
(dy              1)

(dz
                0.40      2*0.20          0.10      2*0.25
              2*0.40   0.20   0.1  .05  .03 2*.02  .03  .05  6*0.05  8*0.05
4*0.05
              30*0.05  3*0.1  0.2  0.3  0.45
          )

(mat

        (ins     insul   1     nx     1    ny    1    1)
        (sh      shield  1      9     1    ny   13   13)
        (sh      shield  10    10     1    ny   13   64)
        (in      invert  10    10     1    ny   65   68)
        (dr      drift   11    12     1    ny   47   64)
        (dr      drift   1      9     1    ny   14   30)
        (dr      drift   5      9     1    ny   31   64)
        (ht      heatr   1      4     1    ny   31   64)
        (dr      drift   1      9     1    ny    2    4)
        (dr      drift   10    14     1    ny    3    4)
        (ins     insul   10    nx     1    ny    2    2)
        (ins     insul   15    nx     1    ny    3    4)
        (dr      drift   1     14     1    ny    5    5)
        (ins     insul   15    nx     1    ny    5    5)
        (dr      drift   1     17     1    ny    6    6)
        (ins     insul   18    nx     1    ny    6    6)
        (dr      drift   1     19     1    ny    7    7)
        (ins     insul   20    nx     1    ny    7    7)
        (dr      drift   1     20     1    ny    8   10)
        (ins     insul   21    nx     1    ny    8   10)
        (dr      drift   1     20     1    ny   11   12)
        (dr      drift   11    20     1    ny   13   38)
        (ins     insul   21    nx     1    ny   11   38)
        (dr      drift   11    19     1    ny   39   46)
        (ins     insul   20    nx     1    ny   39   46)
        (dr      drift   13    18     1    ny   47   62)
        (ins     insul   19    nx     1    ny   47   62)
        (dr      drift   13    17     1    ny   63   64)
        (ins     insul   18    nx     1    ny   63   64)
        (dr      drift   1      9     1    ny   65   66)
        (dr      drift   11    17     1    ny   65   66)
        (ins     insul   18    nx     1    ny   65   66)
        (dr      drift   1      9     1    ny   67   68)
        (dr      drift   11    14     1    ny   67   68)
        (ins     insul   15    nx     1    ny   67   68)
        (dr      drift   1      2     1    ny   69   69)
        (in      invert  3     nx     1    ny   69   69)
        (in      invert  1     nx     1    ny   70   70)

        )
```

```
)   ;; end of genmsh

) ;; end of model input
```

```
(usnt
(title " Yucca Mountain Project 2-D T-H Model w. drip shield")
(modelname usnt)
(vapor-pressure-lowering off)
(include-pkg "vtough.pkg")
(tstop   8.0380e+06)
(time 0)
(stepmax 1000000)
(dtmax  8.0380e+06)
(dt 1e3)


;; Run ymp2DdstR2

;; Using a thickness of  2 cm for the drip shield
;; Use drift air K = 1E-08 and Tcond = 0.0263

;; calibrate model drift air K & Tcond for repository model
;; no radiation

;; Peak thermal loading @ 10 W/m


  (output


      (extool (variables T RH S.liquid X.air.gas P Qrad Qcond Qd.energy
V.liquid V.gas )
              (file-ext ".ext")(range "*")
(outtimes 0 0.2d 0.5d 1d 1.5d 2d 3d 5d 7d 8d 10d 12d 15d 18d 20d 22d
30d 40d 45d 60d 70d 80d)
  ))

  (rocktab
    (heatr
      (porosity 0.010) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 4.8886e+02) (solid-density 8.1892e+03)
      (tcond tcondLin (solid  14.420000)(liquid  14.420000)(gas
14.420000))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
      (tort (gas 0.000e+00) (liquid 0.0))
      (kr (gas 1.0)
          (liquid 1.0))
      (pc (liquid 0.0))
    )
    (drift
      (porosity 0.999) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.007e+03) (solid-density 1.1614 )
      (tcond tcondLin (solid 0.026300)(liquid 0.026300)(gas 0.026300))
      (K0 1.000e-08) (K1 1.000e-08) (K2 1.000e-08)
 ;; JJN     (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krPower (power 4) (Smax 1.000e+00)(Sr 0.000e+00)))
```

```
      (pc (liquid 0.0))
    )
    (shield
      (porosity 0.010) (Kd (air 0.0) (water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 5.5132e+2) (solid-density 7.900e+03)
      (tcond tcondLin (solid 20.55) (liquid 20.55) (gas 20.55))
      (K0 0.000) (K1 0.000) (K2 0.000)
      (tort (gas 0.000) (liquid 0.000))
      (kr  (gas 1.0)
           (liquid 1.0))
      (pc  (liquid 0.0))
    )
    (invert
    (porosity 0.545) (Kd (air 0.0) (water 0.0))
    (KdFactor (water 0.0) (air 0.0))
    (Cp 948.0) (solid-density 2.530e+03)
    (tcond tcondLin (solid 0.66) (liquid 0.66) (gas 0.66))
    (K0 6.150e-10) (K1 6.150e-10) (K2 6.150e-10)
    (tort (gas 0.700) (liquid 0.0))
    (kr  (gas 1.0)
         (liquid 1.0))
    (pc  (liquid 0.0))
    )
    (atm
      (porosity 0.990) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 1.000e+08) (solid-density 1.0000)
      (tcond tcondLin (solid 0.000000)(liquid 0.000000)(gas 0.000000))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
;;JJN      (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krlLinear (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
    )
    (insul
      (porosity 0.990) (Kd (air 0.0)(water 0.0))
      (KdFactor (water 0.0) (air 0.0))
      (Cp 0.7) (solid-density 2.40e+01)
      (tcond tcondLin (solid 0.000000)(liquid 0.000000)(gas 0.000000))
      (K0 0.000e+00) (K1 0.000e+00) (K2 0.000e+00)
;;JJN      (tort (gas 0.000e+00) (liquid 0.0))
      (tort (gas 1.000e+00) (liquid 0.0))
      (kr (gas    krgLinear (Smax 1.000e+00)(Sr 0.000e+00))
          (liquid krlLinear (Smax 1.000e+00)(Sr 0.000e+00)))
      (pc (liquid 0.0))
    )
  )

(state
    (P by-key ("*" 1.e5))

    (S.liquid by-key
                      ("sh*" 0.0)
                      ("dr*" 0.0)
                      ("ht*" 0.0)
```

```
                    ("ins*" 0.0)
                    ("in*" 0.0)
  )

    (T by-key ("*" 60.0)
    )

 (X.air by-key ("*" -1.0)  ("dr*" 0.999) ("ht*" 1.0)
               ("sh*" 1.0) ("ins*" 0.999) ("in*" 0.999))

 ) ;; end state


  (input-mass-fraction on)


 (linear-solver d4vband)
;;  (linear-solver pcg)
  (ilu-degree 1)
  (pcg-parameters (precond d4)(toler 1e-4)(itermax 100)(north 15))

  (adaptive-ilu ON)



  (srctab
    (compflux
    (comp energy)
    (name REPO)
    (range "ht*")
    (allocate-by-element ("*" 0.5))
    (table
       0.00         1.0       2.00e+01    0.20e+01    2.000e+02  0.40e+01
       6.3072e+03   0.60e+01 1.2614e+04   0.80e+01    1.260e+05  1.00e+01
       3.1533e+05   1.00e+01 4.1533e+05   1.00e+01    1.038e+06  1.00e+01
       2.0380e+06   1.00e+01 4.0380e+06   1.00e+01    8.0380e+06 1.00e+01
      ) ;; end table
     (allocate-by-volume)
    ) ;; end compflux

    ) ;;  end srctab



(genmsh
   (down 0. 0. 1.0)
   (coord rect)

   (dx
                 2*0.3   4*.1 .05 .03 2*.02 .03 .05  4*.1  0.2
2*0.3
                 2*0.4         2*0.2            0.4           0.5
0.8
                   1.1           1.6            3.0            3.9
5.1
                   5.3           6.6            8.6            )
```

```
(dy              1)

(dz
            0.40      2*0.20          0.10      2*0.25
          2*0.40   0.20   0.1 .05 .03 2*.02 .03 .05  6*0.05  8*0.05
4*0.05
          30*0.05  3*0.1  0.2  0.3  0.45
       )

(mat

     (ins     insul   1     nx     1    ny    1    1)
     (sh      shield  1      9     1    ny   13   13)
     (sh      shield  10    10     1    ny   13   64)
     (in      invert  10    10     1    ny   65   68)
     (dr      drift   11    12     1    ny   47   64)
     (dr      drift   1      9     1    ny   14   30)
     (dr      drift   5      9     1    ny   31   64)
     (ht      heatr   1      4     1    ny   31   64)
     (dr      drift   1      9     1    ny    2    4)
     (dr      drift   10    14     1    ny    3    4)
     (ins     insul   10    nx     1    ny    2    2)
     (ins     insul   15    nx     1    ny    3    4)
     (dr      drift   1     14     1    ny    5    5)
     (ins     insul   15    nx     1    ny    5    5)
     (dr      drift   1     17     1    ny    6    6)
     (ins     insul   18    nx     1    ny    6    6)
     (dr      drift   1     19     1    ny    7    7)
     (ins     insul   20    nx     1    ny    7    7)
     (dr      drift   1     20     1    ny    8   10)
     (ins     insul   21    nx     1    ny    8   10)
     (dr      drift   1     20     1    ny   11   12)
     (dr      drift   11    20     1    ny   13   38)
     (ins     insul   21    nx     1    ny   11   38)
     (dr      drift   11    19     1    ny   39   46)
     (ins     insul   20    nx     1    ny   39   46)
     (dr      drift   13    18     1    ny   47   62)
     (ins     insul   19    nx     1    ny   47   62)
     (dr      drift   13    17     1    ny   63   64)
     (ins     insul   18    nx     1    ny   63   64)
     (dr      drift   1      9     1    ny   65   66)
     (dr      drift   11    17     1    ny   65   66)
     (ins     insul   18    nx     1    ny   65   66)
     (dr      drift   1      9     1    ny   67   68)
     (dr      drift   11    14     1    ny   67   68)
     (ins     insul   15    nx     1    ny   67   68)
     (dr      drift   1      2     1    ny   69   69)
     (in      invert  3     nx     1    ny   69   69)
     (in      invert  1     nx     1    ny   70   70)

    )
```

```
)  ;; end of genmsh

) ;; end of model input
```

ATTACHMENT V

THERMAL RADIATION CALCULATION

(See files in Directory Attachment 5 of CD-ROM)

THERMAL RADIATION CALCULATIONS
(Explanation of files in directory Attachment 5 of CD-ROM)

This attachment provides a list of computer files for the thermal radiation calculations for the full-scale repository analysis:

radymp – input file for simulation grid.

radymp.con – radiation connection file defining connection between radiating and reflecting surfaces; with emissivity of radiating surface = 0.87

radympc.con – radiation connection file defining connection between radiating and reflecting surfaces; with emissivity of radiating surface = 0.70

results9.9 (also named as results99) – output radiation file from radymp and radymp.con used as input to NUFT.

Results1.00 (also named as results100) – output radiation file from radymp and radympc.con used as input to NUFT.

ATTACHMENT VI

LISTING OF INPUT FILES

(See files in Directory Attachment 6 of CD-ROM)

LIST OF INPUT FILES
(Explanation of files in directory Attachment 6 of CD-ROM)

This attachment provides a list of the input files for the full-scale repository analysis.

File Name	File Description
rocktab1	Rock and material Properties
genmsh2	Simulation Grid for Initialization Run
genmsh3	Simulation Grid for Production Run - including radiation file with emissivity of radiating surface = 0.87
genmsh4	Simulation Grid for Production Run – including radiation file with emissivity of radiating surface = 0.70
ddymp2DdsR2 or ddsr2	Initialization Run with Infiltration Rate = 35 mm/yr
ddymp2DdsR2b or ddsr2b	Initialization Run with Infiltration Rate = 68 mm/yr
ymp2Dds2R22 or ds2r22	Production Run with Infiltration Rate = 35 mm/yr and 100% heat removal in the first 50 yr ; emissivity = 0.87
ymp2Dds2R23 or ds2r23	Production Run with Infiltration Rate = 35 mm/yr and 100% heat removal in the first 100 yr ; emissivity = 0.87
ymp2Dds2R23a or ds2r23a	Same as ymp2Dds2R23 or ds2r23 except in addition, outputs Vapor and Liquid Fluxes ; emissivity = 0.87
ymp2Dds2R23b or ds2r23b	Production Run with Infiltration Rate = 68 mm/yr and 100% heat removal in the first 100 yr ; emissivity = 0.87
ymp2Dds2R23c or ds2r23c	Same as ymp2Dds2R23a or ds2r23a except emissivity = 0.70
85-amb-pt-ctr-large-ix1.0walls.ics	Initial Temperature, saturation, and pressure distribution for NUFT run in another report
85-pt-ctr-large-ix1.0walls2.in	NUFT input file for another report.

ATTACHMENT VII

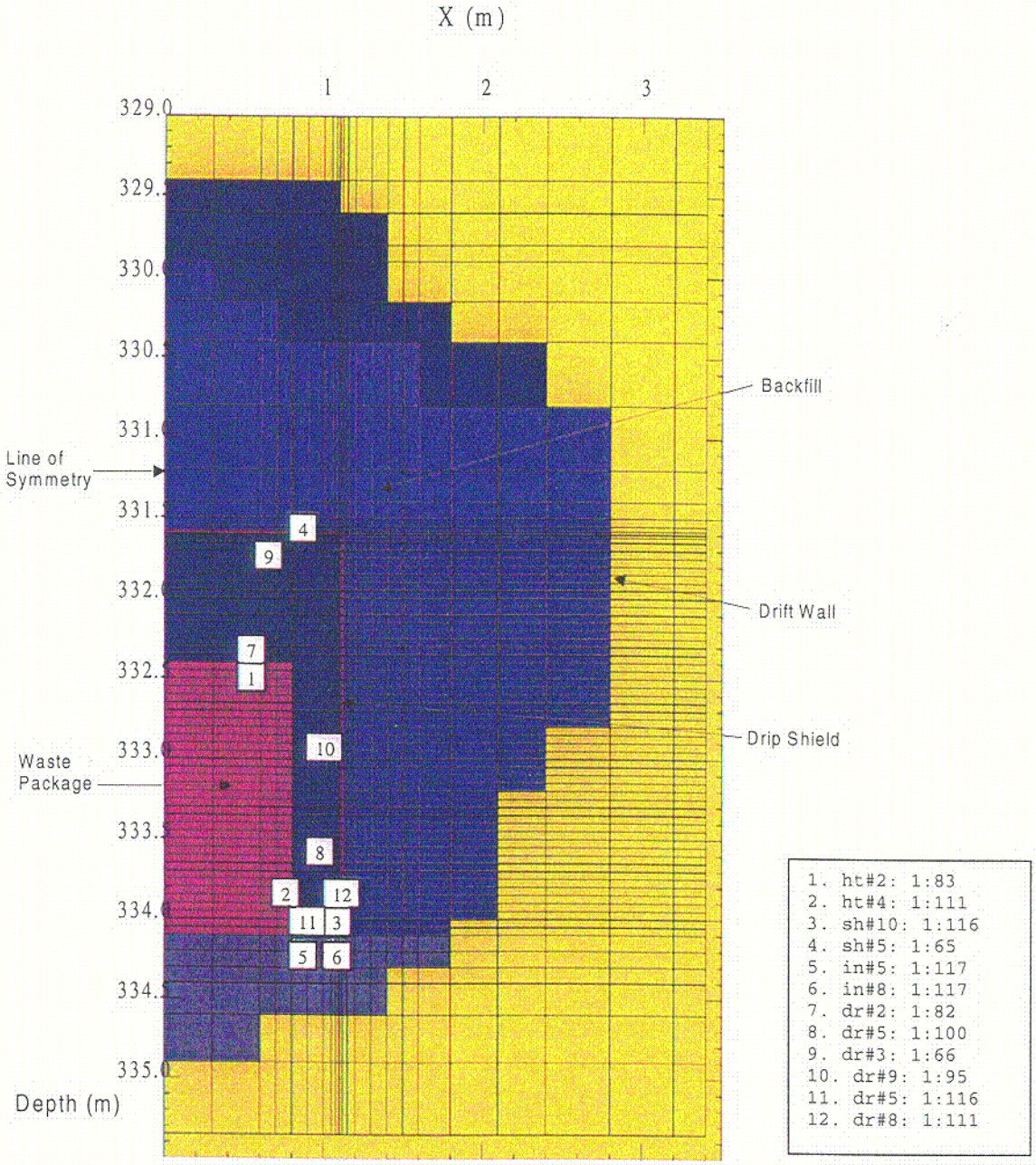
RESULTS OF ANALYSIS

(See files in directory Attachment 7 of CD-ROM)

RESULTS OF ANALYSIS
(Explanation of files in directory Attachment 7 of CD-ROM)

The following output files are the results of analysis using the input from Attachment VI. They all have the extension **.ext** and are to be used by the computer code XTOOL for graphical display.

File Name	File Description
ddymp2DdsR2.ext or ddsr2.ext	Output from ddymp2DdsR2
ddymp2DdsR2b.ext or ddsr2b.ext	Output from ddymp2DdsR2b
ymp2Dds2R22.ext or ds2r22.ext	Output from ymp2Dds2R22
ymp2Dds2R23.ext or ds2r23.ext	Output from ymp2Dds2R23
ymp2Dds2R23a.ext or ds2r23a.ext	Output from ymp2Dds2R23a
ymp2dds2R23b.ext or ds2r23b.ext	Output from ymp2Dds2R23b
ymp2Dds2R23c.ext or ds2r23c.ext	Output from ymp2Dds2R23c
ymp2Dds2R23a.gid or ds2r23a.gid	Gas Flux from Invert Mat. to Air Gap underneath the Drip Shield (from ymp2Dds2R23a).
ymp2Dds2R23a.lid or ds2r23a.lid	Liquid Flux from Invert Mat. to Air Gap underneath the Drip Shield (from ymp2Dds2R23a).
ymp2Dds2R23a.lti or ds2r23a.lti	Liquid Flux from Host Rock to Invert Mat. (from ymp2Dds2R23a).
ymp2Dds2R23a.gti or ds2r23a.gti	Gas Flux from Host Rock to Invert Mat. (from ymp2Dds2R23a).
ymp2Dds2R23a.lbi or ds2r23a.lbi	Liquid Flux from Backfill to Invert Mat. (from ymp2Dds2R23a).
ymp2Dds2R23a.gbi or ds2r23a.gbi	Gas Flux from Backfill to Invert Mat. (from ymp2Dds2R23a).
ymp2Dds2R23a.ltb or ds2r23a.ltb	Liquid Flux from Host Rock to Backfill (from ymp2Dds2R23a).
ymp2Dds2R23a.gtb or ds2r23a.gtb	Gas Flux from Host Rock to Backfill (from ymp2Dds2R23a).



Detailed Grid Showing Thermal Radiation Underneath the Drip Shield

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