OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL COVER SHEET

Complete Only Applicable Items

1. QA: QA

2. ☒ Analysis — Check all that apply

Type of Analysis:
- ☐ Engineering
- ☒ Performance Assessment
- ☐ Scientific

Intended Use of Analysis:
- ☐ Input to Calculation
- ☒ Input to another Analysis or Model
- ☐ Input to Technical Document
- ☐ Input to other Technical Products

Describe use:

Analyze Thermal-Hydrologic-Chemical processes in EBS

3. ☒ Model — Check all that apply

Type of Model:
- ☐ Conceptual Model
- ☐ Abstraction Model
- ☒ Mathematical Model
- ☐ System Model
- ☐ Process Model

Intended Use of Model:
- ☐ Input to Calculation
- ☒ Input to another Model or Analysis
- ☐ Input to Technical Document
- ☐ Input to other Technical Products

Describe use:

Analyze Thermal-Hydrologic-Chemical processes in the EBS

4. Title:

In-Drift Thermal-Hydrological-Chemical Model

5. Document Identifier (including Rev. No. and Change No., if applicable):

ANL-EBS-MD-000026 REV00, ICN 1

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OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL REVISION RECORD

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ANL-EBS-MD-000026 -REV00/ICN 1

4. Revision/Change No.	5. Description of Revision/Change
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00/ICN01	ICN to address compliance of the software NUFT 3.0s, RADPRO Ver 3.22, and XTOOL Ver 10.1 with current requirements of AP-SI.1Q on Software Management

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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 post closure 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 Model* (CRWMS M&O 2000) was prepared which included a completed checklist for the T-H-C Model. The plan documents the AMR Number as E0065 and the corresponding work package as 1231213EM1 for the T-H-C Model. The model shall be a two-dimensional numerical simulation, using the NUFT computer code (**N**on-isothermal **U**nsaturated-saturated **F**low and **T**ransport) (LLNL 1999a and LLNL 1999b). 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 Section 3.0. The model is intended to be used to provide postclosure analysis of temperatures and condensation below the drip shield. It has been determined that condensation below the drip shield is a factor important to the postclosure safety case.

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 1999f). The design analysis, *Classification of the MGR Ex-Container System* (CRWMS M&O 1999c) was performed in accordance with QAP-2-3, *Classification of Permanent Items.* The backfill material and drip shield of the EBS are classified as quality level 1 (CRWMS M&O 1999c). 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. All electronic data used in the preparation of this AMR was obtained from the YMP Technical Data Management System as appropriate.

3. COMPUTER SOFTWARE AND MODEL USAGE

The analysis is performed using the multiphase flow module **usnt** (fully coupled **unsaturated** multiple phases, multiple components model with isothermal and **n**on-iso**thermal** options)of NUFT, developed at Lawrence Livermore National Laboratory (LLNL, 1999a and LLNL, 1999b). The NUFT V2.0s (STN 10095-2.0s-00) is classified as qualified software. NUFT V2.0s is installed on a Sun Ultra 2 Workstation (tag #115488). The NUFT V3.0s (NUFT) software is classified as an unqualified software program (TBV-3828) per AP-SI.1Q, *Software Management*, and is under configuration management (CM) (STN: 10088-3.0s-00). NUFT was run on a Sun Ultra 10 Workstation with SunOS 5.6 operating system. Version 3.0s has been installed on a Sun workstation with CPU Property Tag Number 6524874.

The code is appropriately used for the Engineered Barrier System (EBS) application. 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.

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** 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 (Nitao, 1998b, Appendix C) and Reference Manual (Nitao 1998a).

RADPRO Ver. 3.22 (LLNL, 2000a) 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). RADPRO Ver 3.22 is appropriately used for this subsurface application, and is used within the range of validation.

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. 10.1 (LLNL, 2000b), a postprocessor of NUFT, 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. XTOOL Ver 10.1 is appropriately used for this application within the range of validation.

RADPRO and XTOOL are executed on a Sun Ultra 2 Workstation CPU (tag #6524874). Installation tests for RADPRO and XTOOL have been performed to verify sample output, based on input provided by LLNL. The tests are documented in Attachment III. RADPRO V.3.22 and XTOOL V.10.1 are baselined software under CM and their Computer Software Configuration Item (CSCI) numbers are 10204-3.22-00 and 10208-10.1-00, respectively.

Because NUFT V3.0s is an unqualified software, 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. Although the user's manuals for earlier versions of these software are cited in this document (Daveler, 1998; Nitao 1998b, and LLNL 1998), they can be used for the versions used in the analyses. Software user request forms for RADPRO, and XTOOL are presented in Attachment II.

Model validation is presented in Section 6.6 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 and other inputs 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. Note that the data and input used for input to the THC analysis are appropriate for the intended use.

4.1 DATA AND PARAMETERS

4.1.1 Thicknesses of Individual Stratigraphic Units

The thicknesses of individual stratigraphic units at the repository center point (N233,760m, E170,750m) are presented in DTN SN0003T0571897.013 (TBV-3683). This data is currently unqualified. The locations of the ground surface, the groundwater table, and the repository horizon are discussed Section 5.12.

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 (Section 5.12) (TBV 3490). 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.

4.1.2 Thermal Properties for Individual Stratigraphic Units

The specific heat, and thermal conductivity for the Natural Barrier System (NBS) (See Table 1) are based on data from DTN SN0003T0571897.013 for the coordinates (N233,760m, E170,750m). These data are currently unqualified. The grain density are based upon GS960908312231.004. These data are currently qualified but carry a verification TBV-3618.

4.1.3 Hydrostratigraphic Properties of the Individual Stratigraphic Units

The following hydrostratigraphic properties for the NBS (See Tables 2-3) are derived from the EBS "drift-scale" base case for the 1-D upper-bound infiltration data package DTN LB990861233129.002 (TBV-3502): 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 (Nitao 1988, pp. 11 and 14) (TBV 3586):

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

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

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

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

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

The above abbreviations are explained on page 43.

4.1.4 Radiative Heat Transfer Properties (TBV-3496)

Emissivity of the Simulated Waste Package 0.87 (CRWMS M&O 1999d).
Emissivities of drip shield and invert material are 1.0.

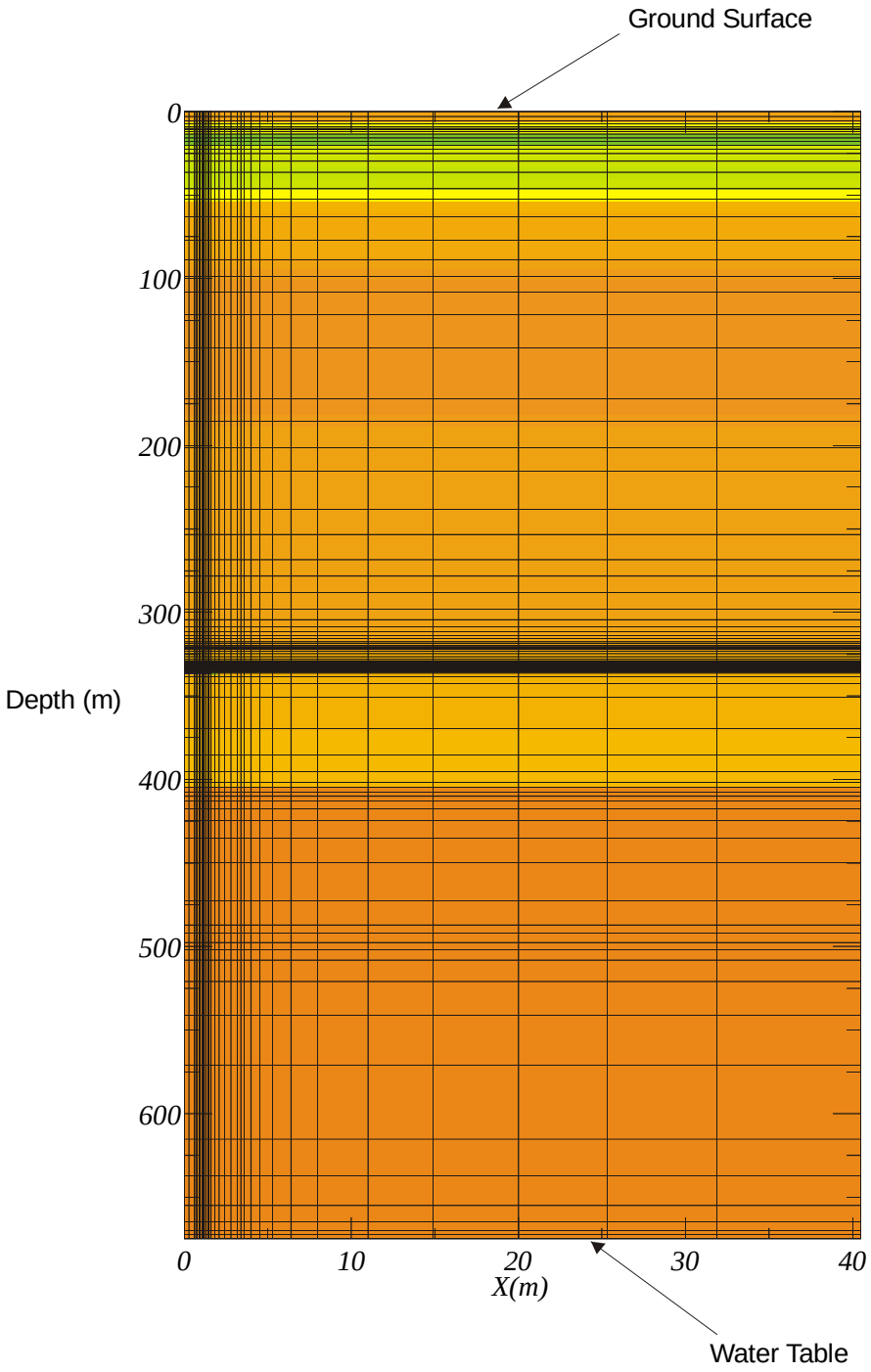

Figure 1. NUFT Simulation Grid

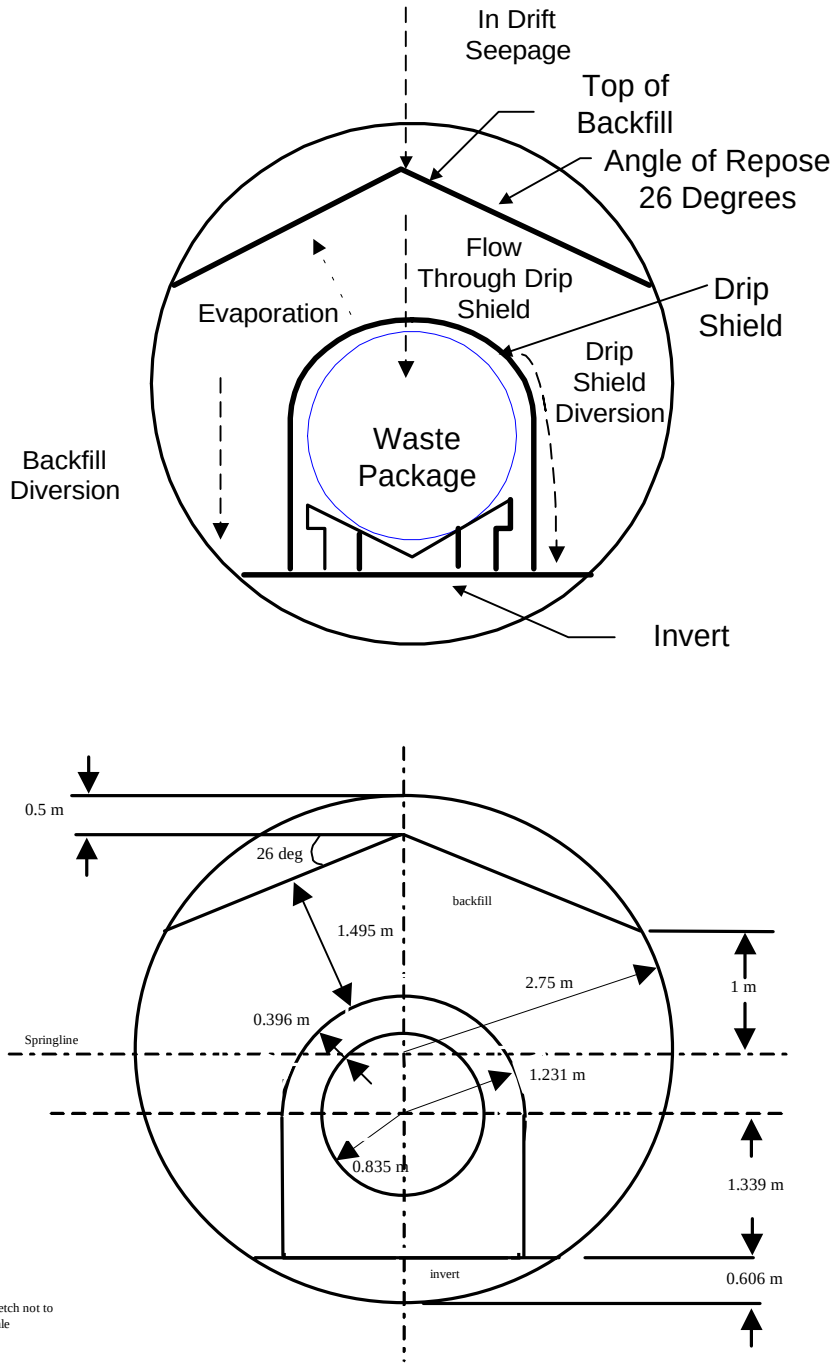

Figure 2. Conceptual Model for Diversion of Water Flow

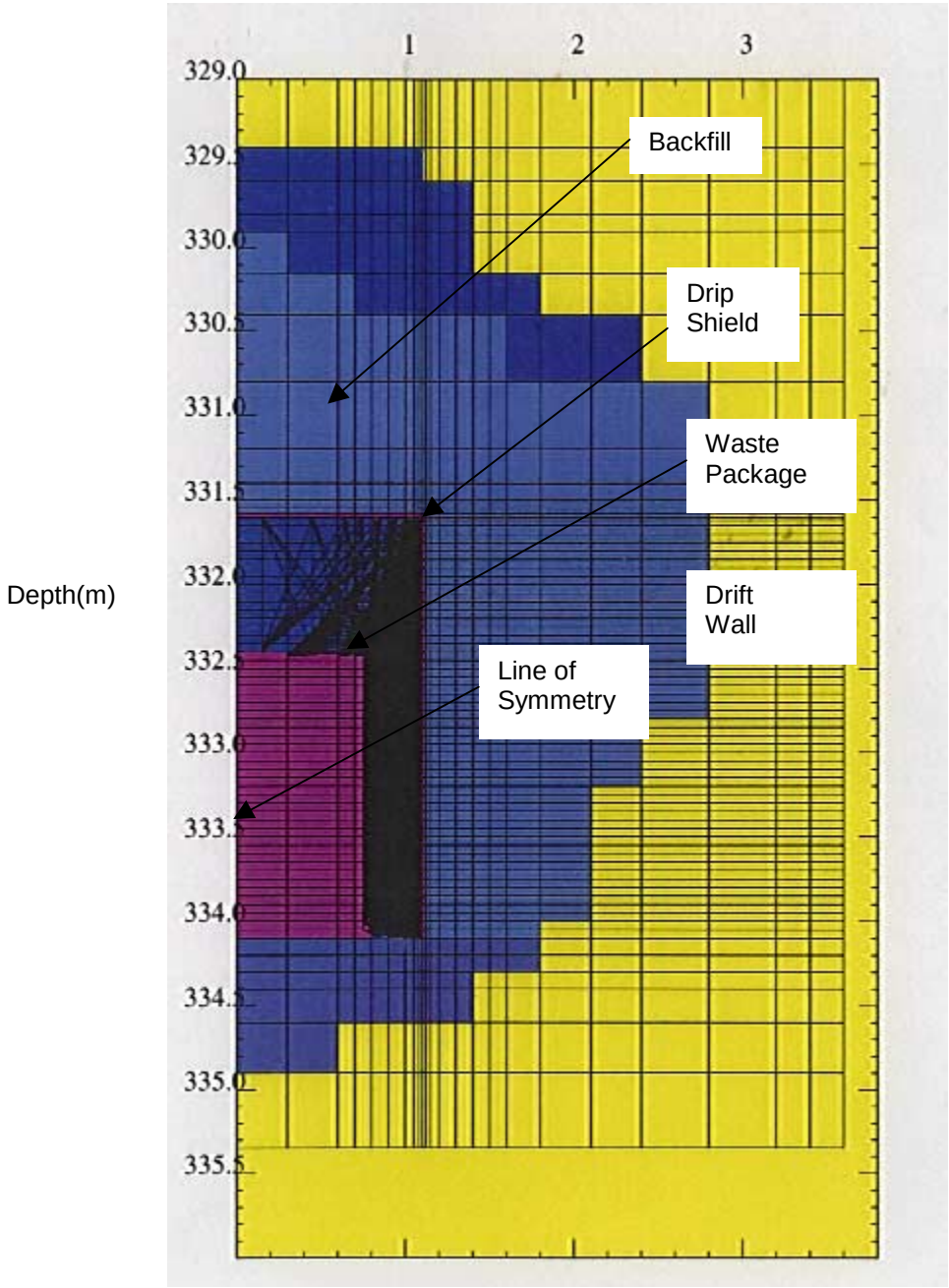

Figure 3. Detailed Grid for Full –Scale Repository Model

Table 1. Thermal Parameters and Tortuosity Factor for NBS (DTN SN0003T0571897.013 and GS960908312231.004)

Unit	Rock Grain Density (Kg/m^3)	Rock Grain Specific Heat (J/Kg K)	Dry Conductivity (W/m K)	Wet Conductivity (W/m K)	Tortuosity
tcw11	2510	847	1.02	1.76	0.7
tcw12	2510	837	1.28	1.88	0.7
tcw13	2470	857	0.54	0.98	0.7
ptn21	2380	1037	0.50	1.07	0.7
ptn22	2340	849	0.44	0.97	0.7
ptn23	2400	1016	0.46	1.02	0.7
ptn24	2370	1330	0.35	0.82	0.7
ptn25	2260	1224	0.23	0.67	0.7
ptn26	2370	1220	0.23	0.67	0.7
tsw31	2510	834	0.37	1.00	0.7
tsw32	2550	866	1.06	1.62	0.7
tsw33	2510	882	0.89	1.58	0.7
tsw34	2530	948	1.56	2.33	0.7
tsw35	2540	900	1.20	2.02	0.7
tsw36	2560	865	1.42	1.84	0.7
tsw37	2560	984	1.69	2.08	0.7
ch1z	2310	1057	0.70	1.31	0.7
ch2z	2350	1201	0.61	1.20	0.7
ch4z	2440	1174	0.61	1.20	0.7

Table 2. Matrix Hydrologic Parameters for NBS (DTN LB990861233129.002)

Model Layer	Permeability	Porosity	Van Genuchten α	Van Genuchten m (L)	Residual Saturation	Satiated Saturation
	k_m (m_2)	f_m (-)	a_m (1/Pa)	m_m (-)	S_{lrm} (-)	S_{lsm} (-)
tcw11	3.98E-15	0.253	4.27E-5	0.484	0.07	1.00
tcw12	3.26E-19	0.082	2.18E-5	0.229	0.19	1.00
tcw13	1.63E-16	0.203	2.17E-6	0.416	0.31	1.00
ptn21	1.26E-13	0.387	1.84E-4	0.199	0.23	1.00
ptn22	5.98E-12	0.439	2.42E-5	0.473	0.16	1.00
ptn23	3.43E-13	0.254	4.06E-6	0.407	0.08	1.00
ptn24	3.93E-13	0.411	5.27E-5	0.271	0.14	1.00
ptn25	1.85E-13	0.499	2.95E-5	0.378	0.06	1.00
ptn26	6.39E-13	0.492	3.54E-4	0.265	0.05	1.00
tsw31	9.25E-17	0.053	7.79E-5	0.299	0.22	1.00
tsw32	5.11E-16	0.157	4.90E-5	0.304	0.07	1.00
tsw33	1.24E-17	0.154	1.97E-5	0.272	0.12	1.00
tsw34	7.94E-19	0.110	3.32E-6	0.324	0.19	1.00
tsw35	1.42E-17	0.131	7.64E-6	0.209	0.12	1.00
tsw36	1.34E-18	0.112	3.37E-6	0.383	0.18	1.00
tsw37	7.04E-19	0.094	2.70E-6	0.447	0.25	1.00
ch1z	8.46E-20	0.288	4.23E-7	0.336	0.33	1.00
ch2z	1.16E-17	0.331	1.13E-6	0.229	0.28	1.00
ch4z	1.16E-17	0.331	1.13E-6	0.229	0.28	1.00

Table 3. Fracture Hydrologic Parameters for NBS (DTN LB990861233129.002)

Model Layer	Permeability	Porosity	Van Genuchten A	Van Genuchten M (L)	Residual Saturation	Satiated Saturation
	K_f (M^2)	F_f (-)	A_f (1/Pa)	M_f (-)	S_{lrf} (-)	S_{lsf} (-)
tcw11	2.75E-12	2.8E-2	4.67E-3	0.636	0.01	1.00
tcw12	1.00E-10	2.0E-2	2.18E-3	0.633	0.01	1.00
tcw13	2.26E-12	1.5E-2	1.71E-3	0.631	0.01	1.00
ptn21	1.00E-11	1.1E-2	2.38E-3	0.611	0.01	1.00
ptn22	1.00E-11	1.2E-2	1.26E-3	0.665	0.01	1.00
ptn23	1.96E-13	2.5E-3	1.25E-3	0.627	0.01	1.00
ptn24	4.38E-13	1.2E-2	2.25E-3	0.631	0.01	1.00
ptn25	6.14E-13	6.2E-3	1.00E-3	0.637	0.01	1.00
ptn26	3.48E-13	3.6E-3	3.98E-4	0.367	0.01	1.00
tsw31	2.55E-11	5.5E-3	1.78E-4	0.577	0.01	1.00
tsw32	7.08E-12	9.5E-3	1.32E-3	0.631	0.01	1.00
tsw33	1.50E-12	6.6E-3	1.50E-3	0.631	0.01	1.00
tsw34	4.63E-13	1.0E-2	4.05E-4	0.579	0.01	1.00
tsw35	5.09E-12	1.1E-2	9.43E-4	0.627	0.01	1.00
tsw36	1.48E-12	1.5E-2	8.21E-4	0.623	0.01	1.00
tsw37	1.48E-12	1.5E-2	8.21E-4	0.623	0.01	1.00
ch1z	5.70E-13	1.7E-4	1.29E-3	0.631	0.01	1.00
ch2z	2.64E-14	4.3E-4	8.45E-4	0.628	0.01	1.00
ch4z	2.64E-14	4.3E-4	8.45E-4	0.628	0.01	1.00

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.

4.1.5 Thermal Properties of Simulated Drift Air at 300° K (Incropera and DeWitt 1996, pg 839) (TBV-3585)

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

4.1.6 Thermal Properties of the Invert Material (DTN: SN9908T0872799.004 – In-driftgeom_rev01.doc, pages 1 and 2) (TBV-3976)

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

4.1.7 Thermal Properties of the Drip Shield (DTN: SN9908T0872799.004) (TBV-3471)

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

4.1.8 Thermal Properties of Waste Package (DTN: SN9908T0872799.004) (TBV-3471)

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

4.1.9 Hydrologic Properties of the Invert Material (SN9908T0872799.004 – MOL.19990901.0312 (TBV-3976)

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.

4.1.10 Thermal and Hydrologic Properties of the Backfill Material (SN9908T0872799.004 – MOL.19990901.0312 TBV-3976)

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.

4.1.11 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).

4.1.12 Universal Constants

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

4.1.13 Measured Temperatures from the Quarter Scale Test

The measured temperatures from the EBS QSDST are used for comparison of the results from the NUFT code. The measured temperatures for the central heater, the outer heater, the drip shield and the invert surface material are taken from SN0003L1011398.003. The data are qualified.

4.2 CRITERIA

The In-Drift T-H-C Model is developed to provide methodology and results for demonstrating compliance with the system criteria specified in the EDA II design (Wilkins and Heath, 1999).

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 – TBV 3507))
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 TBV-3494).

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 (TBV3507)

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 TBV-3493) and is presented in Attachment V. As the 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 this AMR because chemical reactions are not considered in this model.

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. The invert temperature would be overestimated by ignoring the air circulation between the waste package and the invert material. This overestimation of temperature would increase the chance for condensation to form underneath the drip shield and therefore, the assumption is conservative. Furthermore, this assumption would overestimate the temperature of the invert even more because air has a lower thermal condutivity than the invert material and would tend to lower temperature of the invert.

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, TBV3311 and TBV3312) 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 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.

5.9 TORTUOSITY FACTORS (TBV-3508)

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.

5.10 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 4:

Table 4. 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.

5.11 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 5.10. 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.

5.12 GROUND SURFACE AND REPOSITORY CENTER POINT ELEVATIONS

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, TBV-3491). 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, TBV -3491). 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.

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 M&O, 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

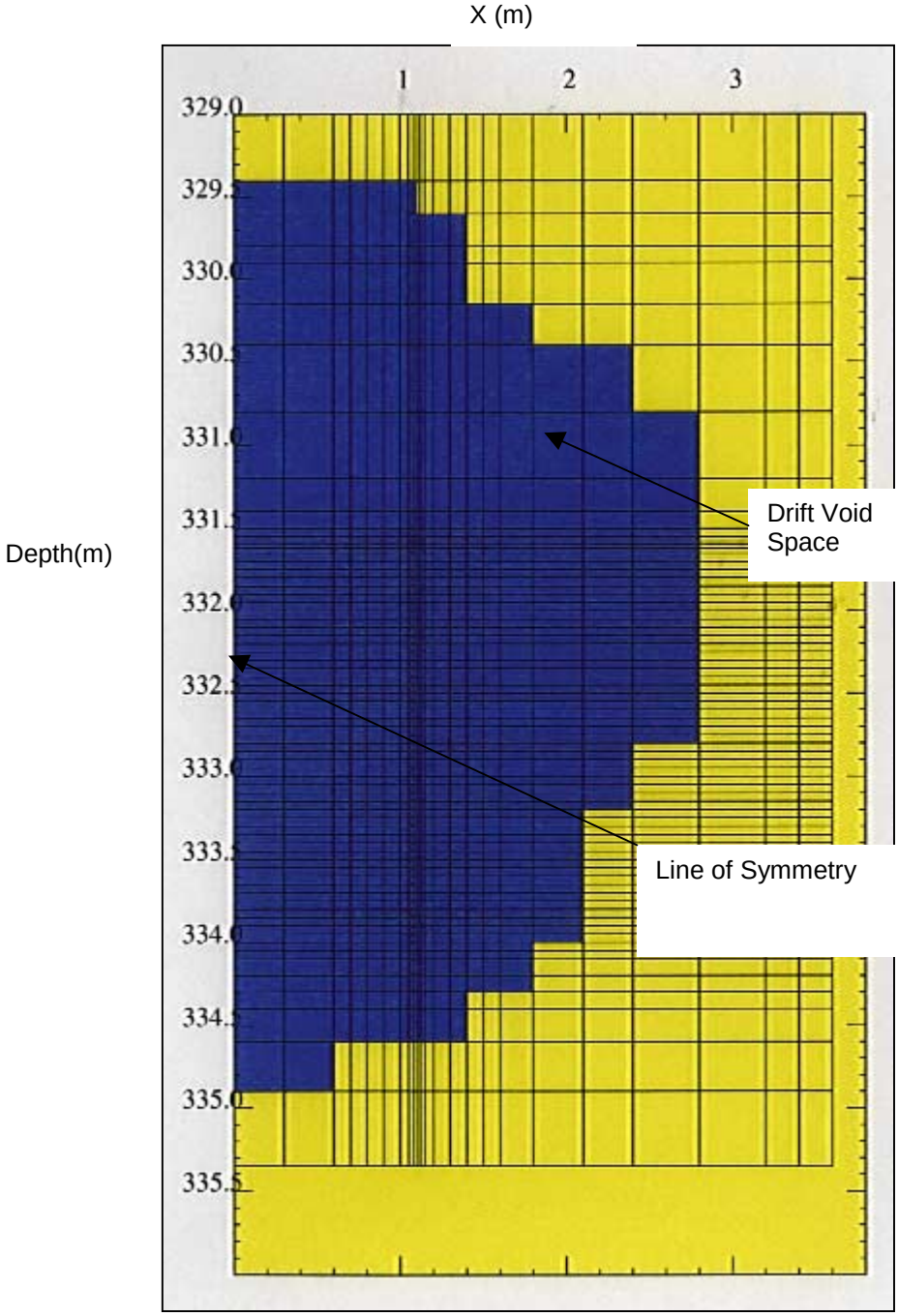

Figure 4. Detailed Grid for Initialization Run

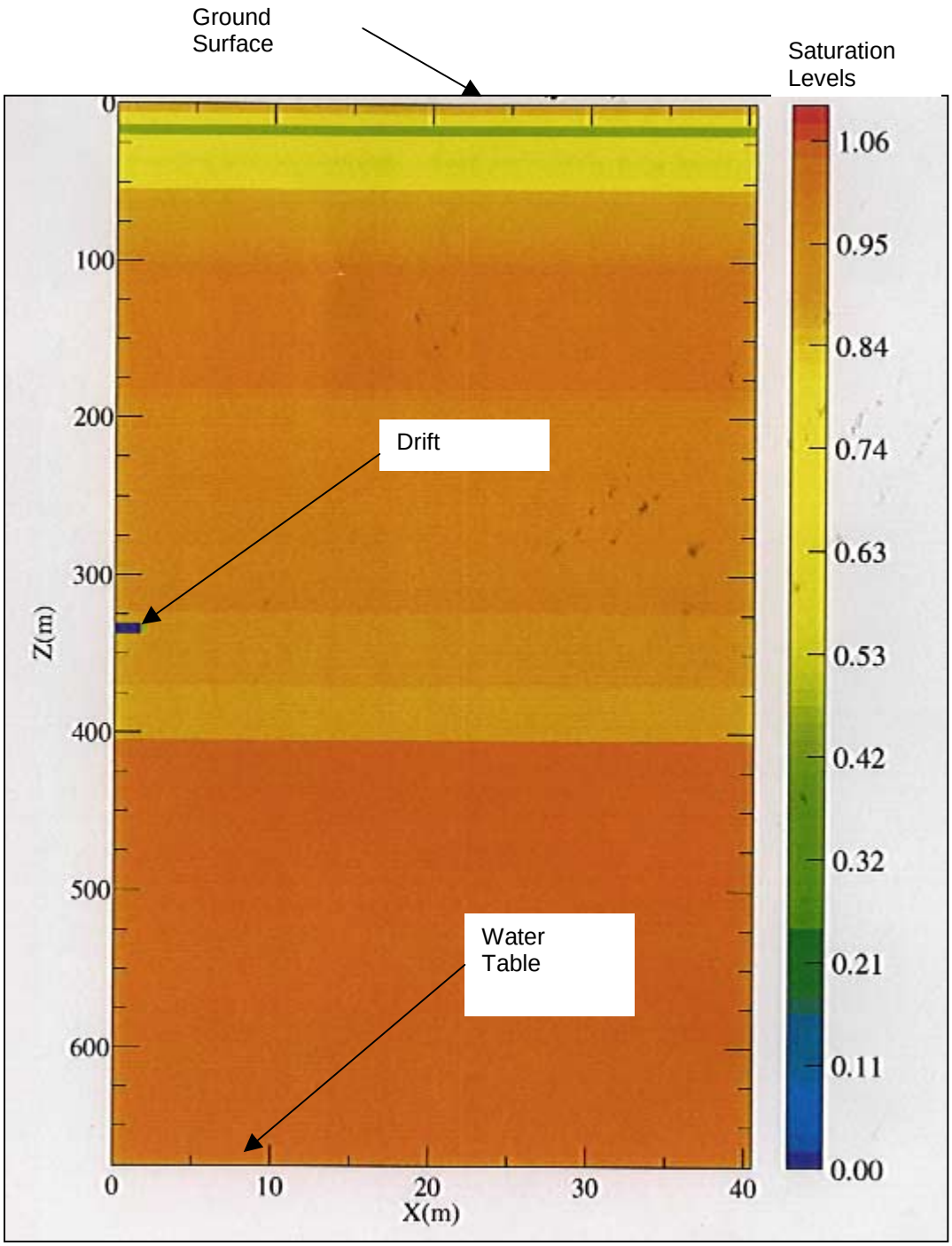

Figure 5. Initial Saturation Contours for the Two-Dimensional T-H Model with a Drip Shield at an Infiltration Rate of 35 mm per year

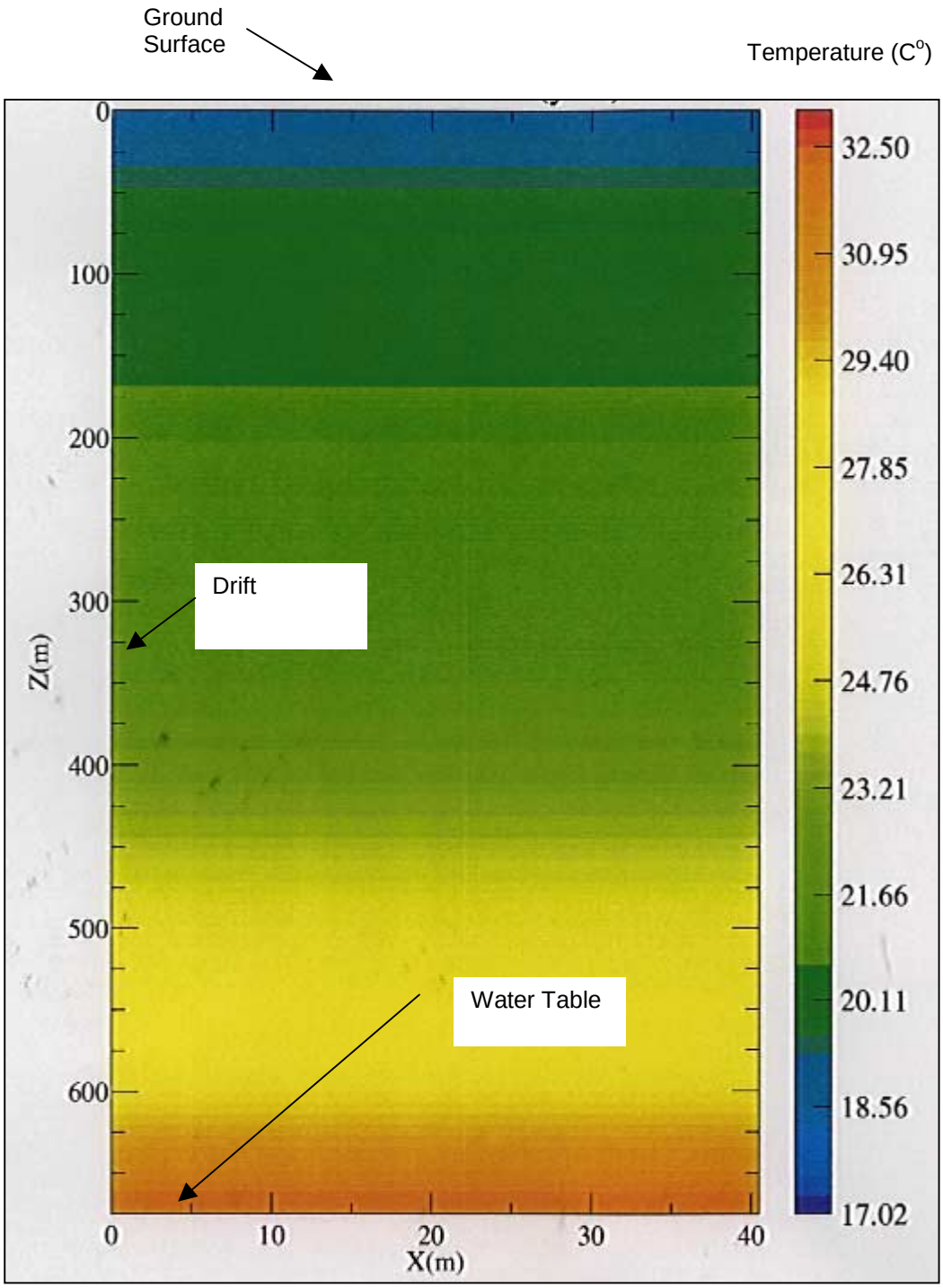

Figure 6. Initial Temperature Contours for the Two-Dimensional T-H Model with a Drip Shield After 100 years at an Infiltration Rate of 35 mm per year

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 M&O, 1998b) which facilitates preferential downward flow rather than horizontal flow. The ECM model was used for the analysis in this AMR (NUFT ver. 2.0s and ver. 3.0s).

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 DTNs: LB990861233129.002 SN0003T0571897.013 and GS960908312231.004, and with the assumptions stated in Section 5. Boundary conditions are stated in Section 5.10 and initial conditions (pressure and saturation) are specified in Section 5.11.

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 (DTN

SN0003L1011398.003) 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 5. Summary of Results for Sensitivity Study
(Temperatures in ^{o}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 5.11
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 5.11

Infiltration flux at ground surface = 68 mm/year
Drip shield in-place
Simulated duration: approximately 1.0×10^6 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.

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.

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 ^{o}C from 50/100 to 1,000 years, and is less than 2 ^{o}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 ^{o}C at any given time (Attachment VII).

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.

5. Water saturation on the flat top surface of the drip shield increases from about 10 percent at 6,000 years to about 60 percent 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.

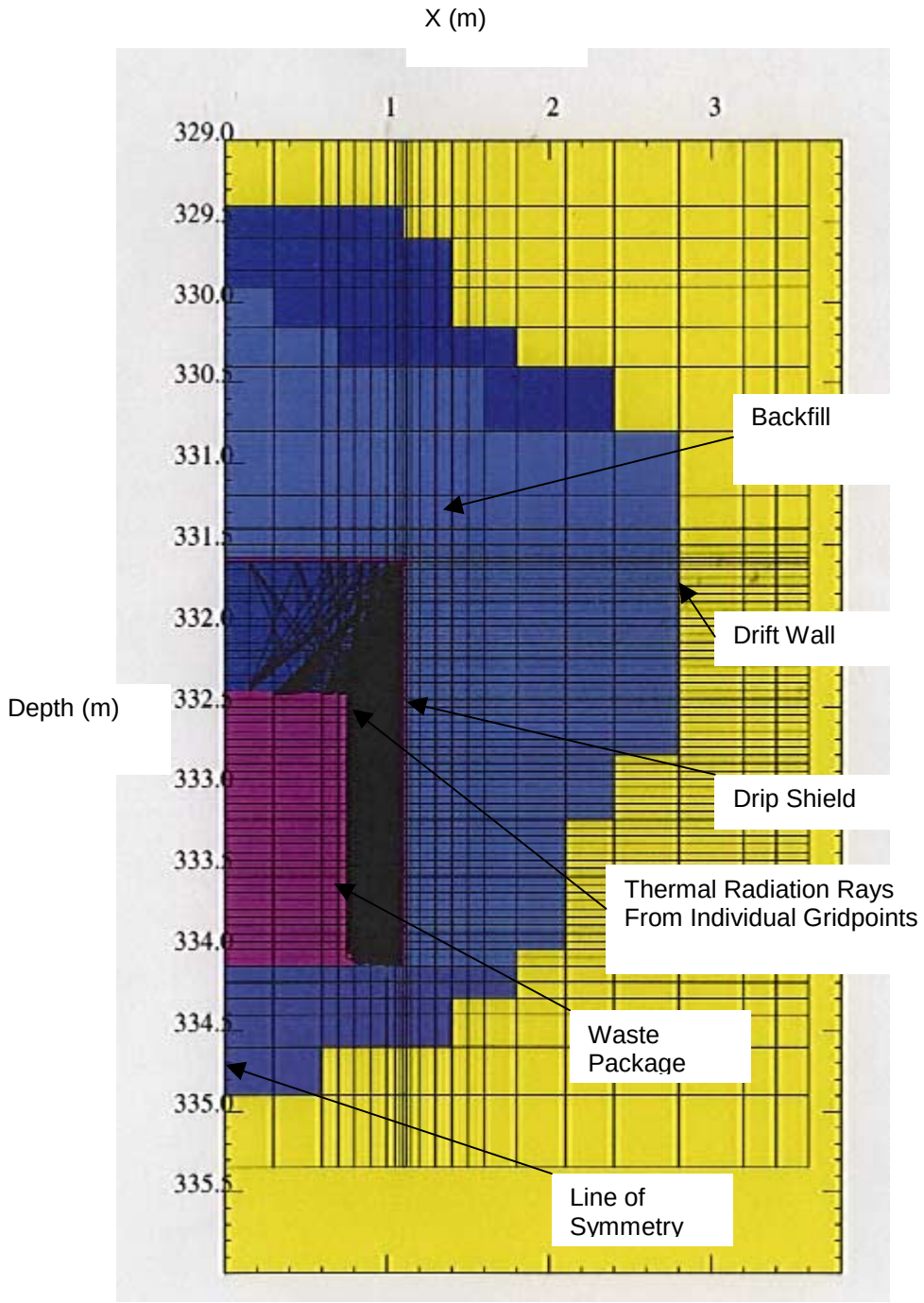

Figure 7. Detailed Grid Showing Thermal Radiation Underneath the Drip Shield

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. Information on relative humidity over time at various locations beneath the drip shield are included 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.

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.

6.6 MODEL VALIDATION

Validation requires review of model calibration parameters for reasonableness and consistency with all relevant data, the T-H-C model input parameters are grouped in the following categories:

- Hydrologic properties for natural and engineered materials
- Thermal properties for natural and engineered materials
- Thermal output of emplaced waste
- Temperature, total pressure, and infiltration flux boundary conditions
- Numerical gridding, convergence criteria, and other model settings

The hydrologic properties used for these models are taken directly from the Unsaturated Zone (UZ) Flow and Transport Model (DTN: LB990861233129.002). Thermal properties are based on laboratory-measured data (DTN: LB990861233129.002). It is noted that values for “wet” thermal conductivity are currently under review. Thermal output of the emplaced waste is based on best-available information for the characteristics of spent fuel and defense high-level waste (Section 5.6).

The temperature and pressure boundary conditions used for these models are based on averages for the ground surface and water table, constrained by measured data. Values for average infiltration flux are also taken directly from the UZ Model, for representative center and edge locations. Alternative infiltration flux boundary conditions are selected from both the "lower" and "upper" infiltration distributions developed for the UZ Model, to represent the range of uncertainty. These alternative values are used comparatively in several cases discussed in this section.

The above descriptions indicate that the model calibration parameters are reasonable since they are consistent with values in the accepted model. It is concluded that the THC models used for analysis is valid for it's intended use. The level of confidence for the model is therefore relatively high. The models are based on appropriate inputs, including properties, boundary conditions, and thermal output. Gridding, convergence, and other model settings used for these models are consistent with past practice.

7. CONCLUSIONS

Descriptions of the models listed above was provided in Sections 6.1 through 6.5. The model validation includes provision of scientific literature, parameter input, assumptions, simplifications, initial and boundary conditions; explanation of how the software are used; expected source of uncertainty (i.e.TBV tracking); comparison with data from measurements or from alternative conceptual models; and computer data files to allow independent repetition of the model simulation. It is determined that these models are validated for their intended use at conceptual level.

These results and conclusions form the basis for analyzing for THC effects in the EBS. (Note that although the model described in this report develops output, it is not used as inputs for other technical products. Only summary of information will be used. Therefore no DTNs are provided for model output at this time.)

The software and most of the inputs used in this AMR are TBV as discussed below. Therefore all conclusions are unqualified. The use of any unqualified technical information or results from this model as input in documents supporting construction, fabrication, or procurement, or as part of a verified design to be released to another organization, is required to be identified and controlled in accordance with appropriate procedures.

The impact of uncertainty of some of the key input variables (e.g., infiltration flux and emissivity of the waste package) were addressed in a previous section of this AMR. Changes to the inputs and/or software will require reproducing this model. This document may be affected by techincal product input information that requires confirmation. Any changes to the document that may occur as a result of completing confirmation activities will be reflected in subsequent revisions. The status of the input information quality may be confirmed by reviw of the Document Input Reference System database. Based upon these caveats, the conclusions are:

Temperature (C^o)

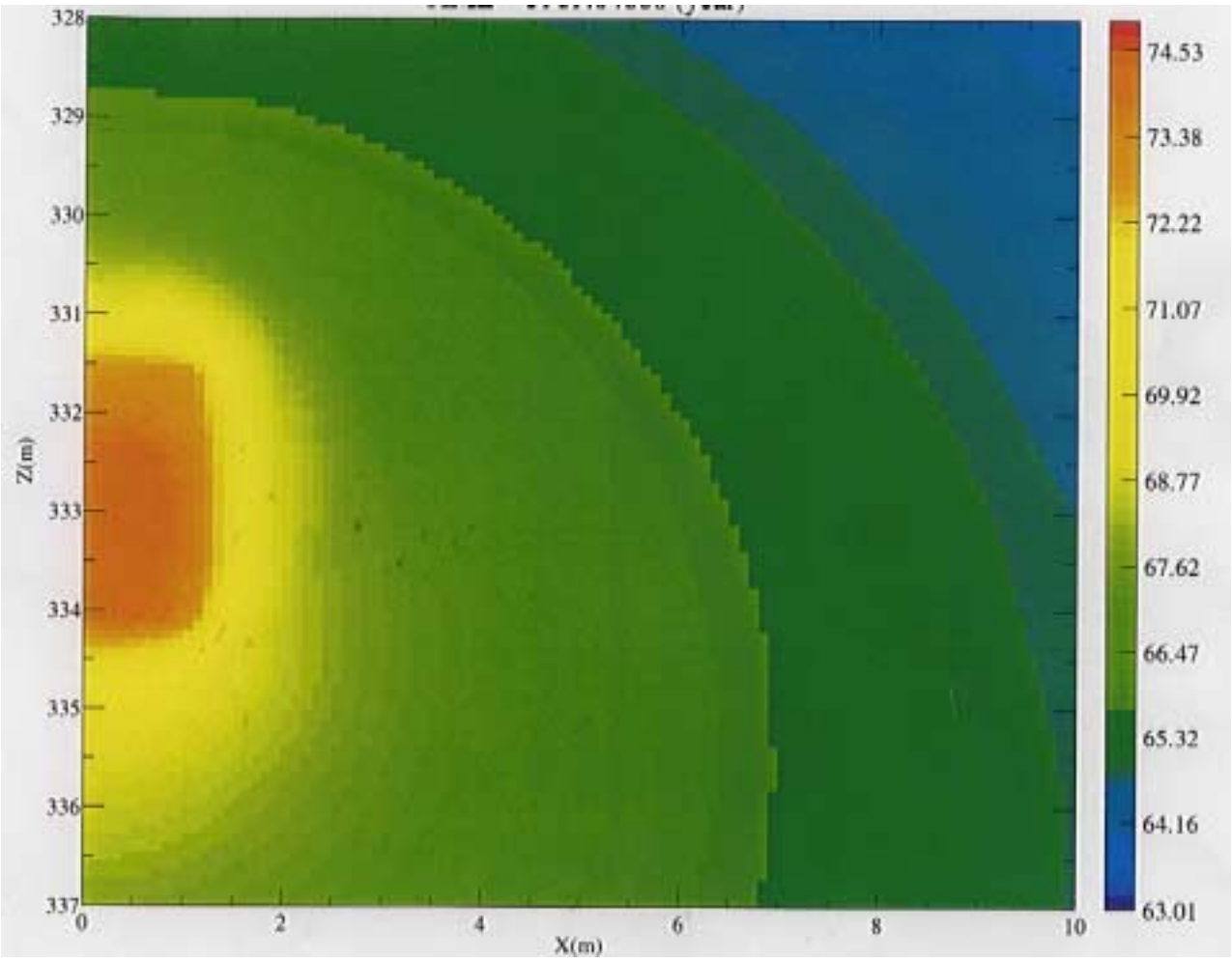

Figure 8. Temperature Contours for the Two-Dimensional T-H Model with a Drip Shield After 6,000 years at an Infiltration Rate of 35 mm per year

Saturation Levels

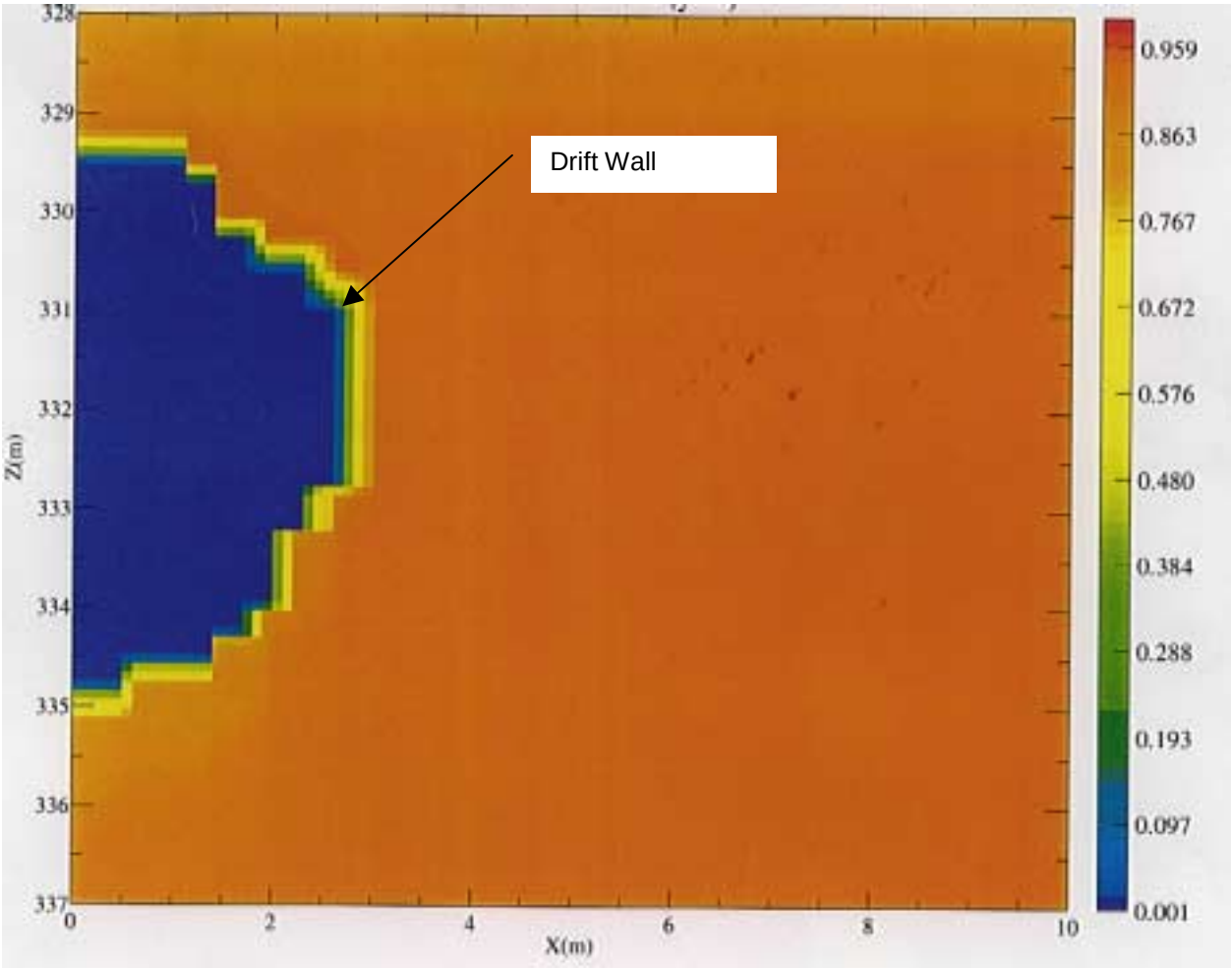

Figure 9. Saturation Contours for the Two-Dimensional T-H Model with a Drip Shield after 6,000 Years at an Infiltration Rate of 35 mm per year

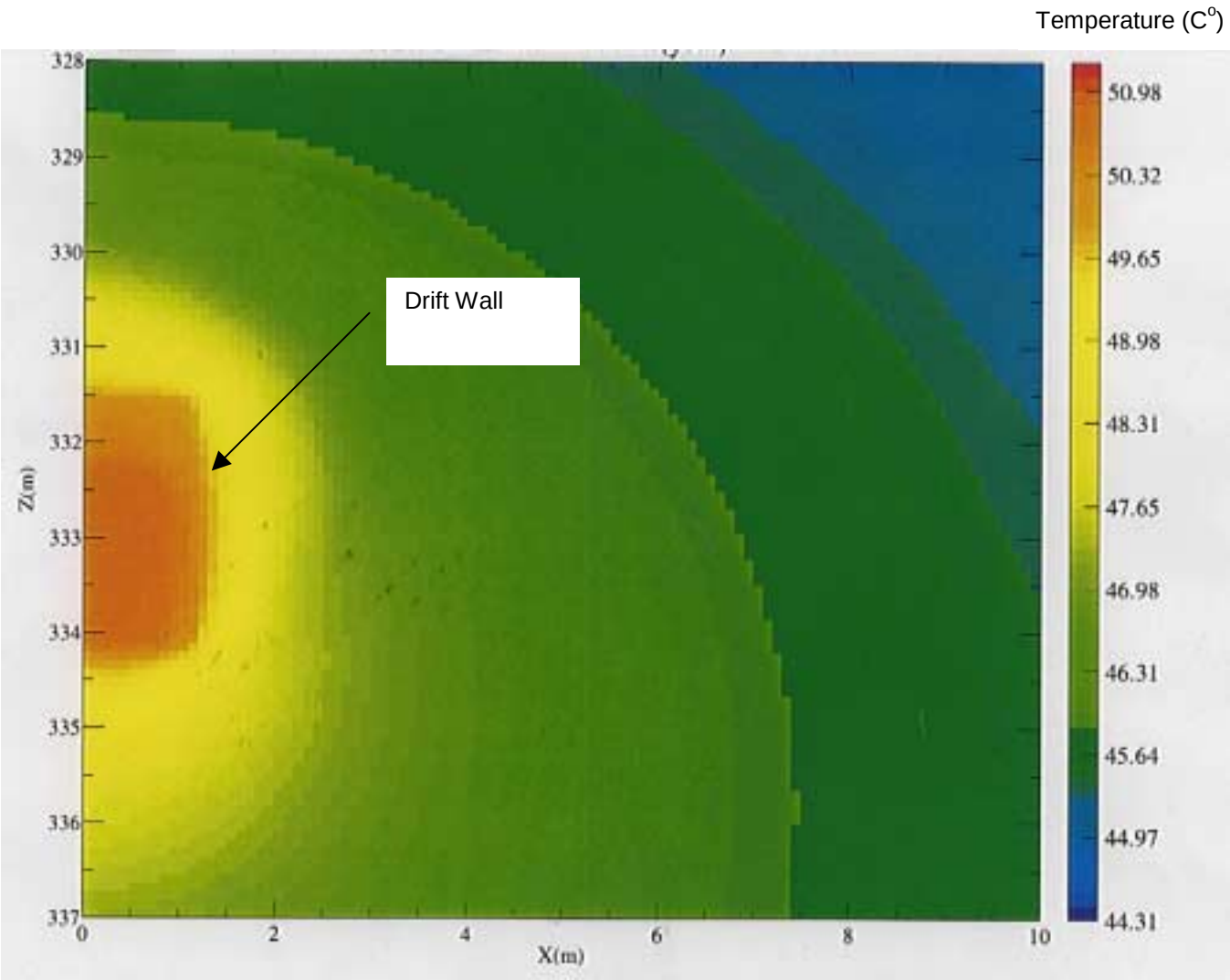

Figure 10. Temperature Contours for the Two-Dimensional T-H Model with a Drip Shield After 15,000 years at an Infiltration Rate of 35 mm per year

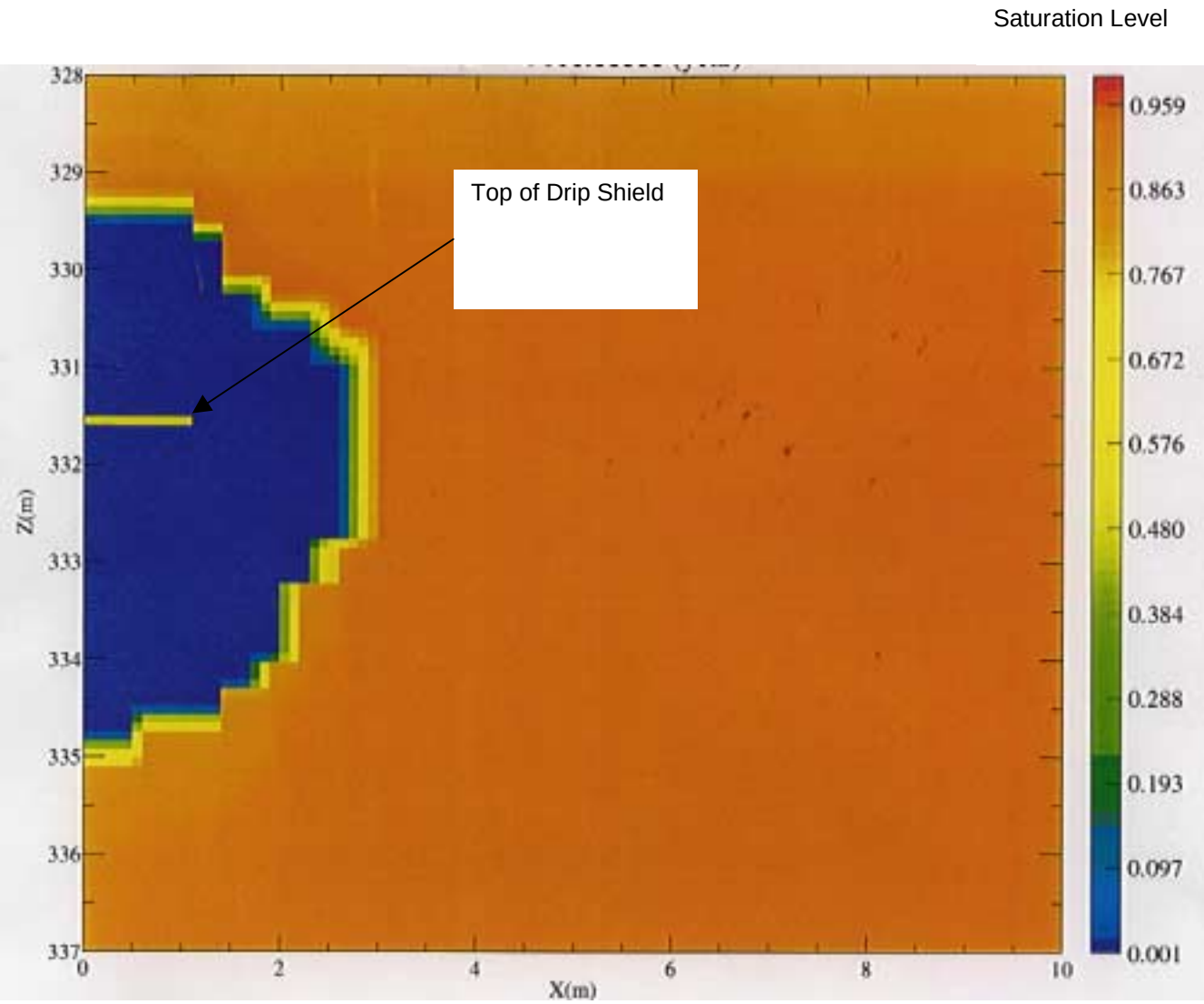

Figure 11. Saturation Contours for the Two-Dimensional T-H Model with a Drip Shield after 15,000 Years at an Infiltration Rate of 35 mm per year

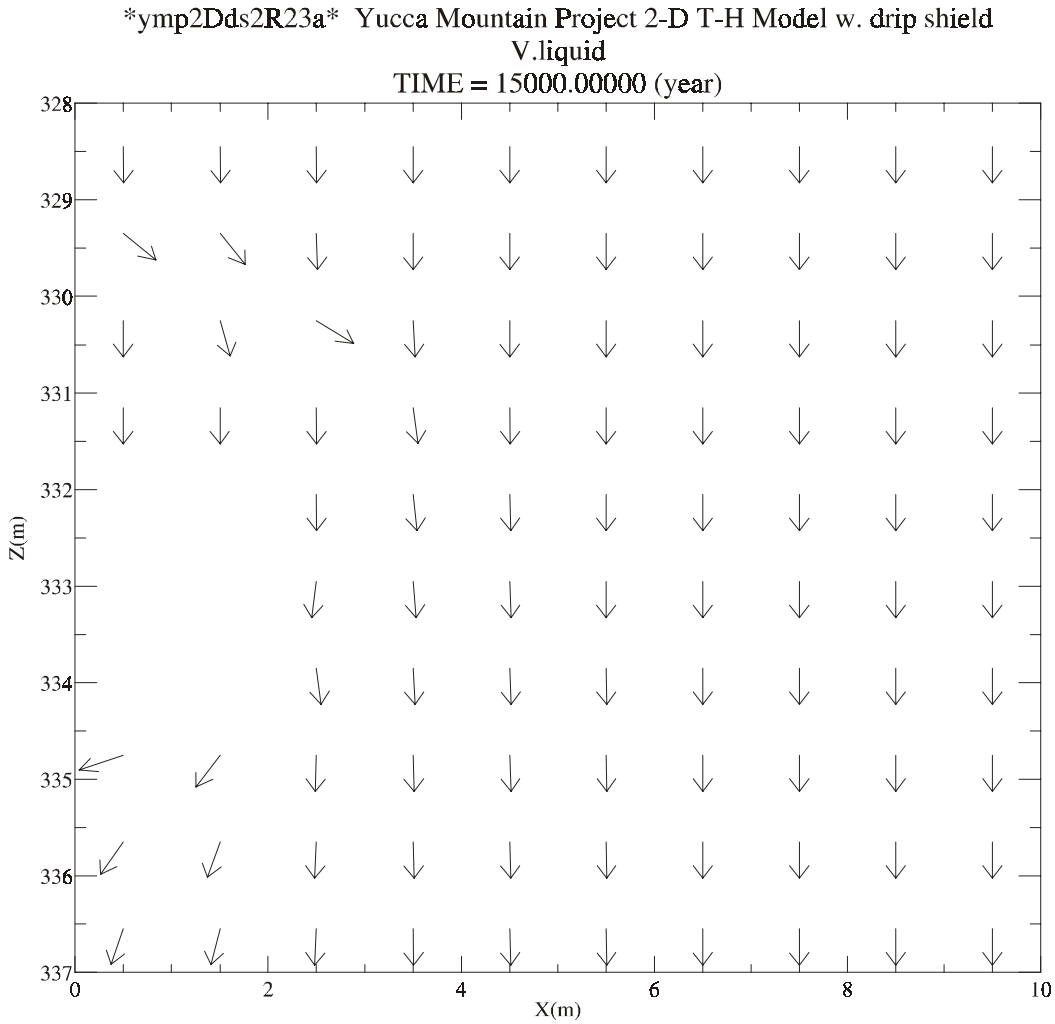

Figure 12. General Direction of Liquid Movement

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. TBV 3471 relates to the thermal properties of the waste package, drip shield, and simulated drift air. It is expected to have a major impact on the results of the analysis.

   B. TBV-3828, which is the result of using the unqualified code, NUFT V3.0s, is the primary TBV item impacting the conclusions of this study. Significant modifications to this code as a result of the qualification process are not anticipated, therefore, the resolution of these TBVs is not expected to significantly impact the results presented in this report.

   C. TBV-3585 and TBV 3471 relate to the thermal properties of the drift air, waste package, and the drip shield respectively. These properties are well established, and would not impact the analysis significantly.

   D. TBV-3490 and 3491 relate the depth of the repository relative to the ground surface and the water table. Since the in-drift THC processes are more affected by the properties of the NBS at the repository horizon, this TBV is expected to have minimal impact.

   E. TBV-3494 relates to the EBS design components configuration and layout.It is expected that this TBV would have a significant impact on the results of the analysis.

   F. TBV-3496 relates to the emissivity of the waste package. It is expected that this TBV would have a minor impact on the results of the analysis.

G. TBV-3502 relates to the hydrostratigraphic properties (calibrated fracture and matrix properties) of the surrounding natural barrier system. These properties have a significant impact on the results of the analysis.

H. TBV-3507 relates to the hydrologic properties of the waste package, and properties of atmospheric air. These properties have a minor impact on the results of the analysis.

I. TBV-3508 relates to the tortuosity factor for rock and soils. The tortuosity is expected to have a minor impact on the analysis.

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

K. The conclusions are not affected by using approximately twice the infiltration rate as specified in TBV-3311 and TBV-3312. This is because the temperature distribution beneath the drip shield is mainly influenced by the thermal properties of the waste and the water vapor below the drip shield.

All other TBV inputs (configuration and properties of all EBS components, rock properties and stratigraphy) are unqualified and along with the unqualified software used. Any change in these unqualified data will require an impact analysis that may modify the conclusions of this report.

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8.3 SOURCE DATA

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8.4 CORRESPONDENCE

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8.5 SOFTWARE SOURCES

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LLNL, 1999b. *Software Code: NUFT V3.0s.* V3.0s. STN: 10088-3.0s-00 (TBV-3828).

LLNL, 2000a, *Software Routine: RADPRO V3.22.* V3.22 STN: 10204-3.22-00.

LLNL, 2000b, *Software Routine: XTOOL V10.1.* V10.1. STN: 10208-10.1-00.

ACRONYMS AND ABBREVIATIONS

ACRONYMS

AMR - Analysis/Model Report

CM - Configuration Management

CPU – Central Processing Unit

CRWMS M&O – Civilian Radioactive 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

NBS – Natural Barrier System

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

NOT USED

ATTACHMENT II

SOFTWARE USER REQUEST

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
SOFTWARE USER REQUEST

QA: QA

Complete Only Applicable Items

1. Software Activity Number:	2. Software Name and Version:	3. Software Tracking Number:
LLNL-2000-037	RADPRO V3.22	10204-3.22-00

4. Organizational and geographical location where software will be used:

M&O, Las Vegas

5. Central Processing Unit (CPU) Number(s) (property tag number(s) or CPU serial number(s):

6524874 115488 - both are SUN WORSTATIONS

6. State the intended use of the software in the new environment:

RADPRO V3.22 is a software routine used to calculate radiation coefficients between grid blocks for a 2 dimensional or 3 dimensional grid and output this information in a format compatible with the program NUFT.

6b.

☒ Distribute Software to a Single Computer

6c.

☐ Server Access
- ☐ Single Access
  - ☐ Read
  - ☐ Write
- ☐ Multiple (Global) Access
  - ☐ Read
  - ☐ Write

7. List of users who are qualified to use the software and will have access to the CPU(s):

Jim Kam

8a. Responsible Manager Name:	8b. Responsible Manager Org.:	8c. Date
Barbara Campbell	LLNL	4/12/00
8d. Responsible Manager Telephone Number:	**8e. Responsible Manager Facsimile Number:**	
925-423-7834	925-423-7346	

9a. Software Configuration Secretariat Name:	9b. Date:
Greg Carlisle	5/5/00

10. ☒ Installation/Reinstallation Successful. Software operating as expected.

Installer Name: Jim Kam Initials: [illegible] Date: 5/15/2000

ATTACHMENT III

SOFTWARE INSTALLATION

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
SOFTWARE USER REQUEST

QA: QA

Complete Only Applicable Items

1. Software Activity Number:	2. Software Name and Version:	3. Software Tracking Number:
LLNL-2000-043	Xtool V10.1	10208.10.100

4. Organizational and geographical location where software will be used:

Subsurface Facilities, Las Vegas

5. Computer Number(s) (property tag number(s) or computer serial number(s)):

6524874 Sun Workstn. 115488 (Sun Workstation)

6a. State the intended use of the software in the new environment:

Postprocessing the NUFT program output files.

6b.

- [x] Distribute Software to a Single Computer

6c.

- [ ] Server Access
  - [ ] Single Access
    - [ ] Read
    - [ ] Read/Write
  - [ ] Multiple (Global) Access
    - [ ] Read
    - [ ] Read/Write

7. List of users who are qualified to use the software and will have access to the CPU(s):

Jim Kam
Ming Lin

8a. Responsible Manager Name:	8b. Responsible Manager Org.:	8c. Date:
Dwayne Chesnut	Subsurface Performance Modeling	03/03/2000
8d. Responsible Manager Telephone Number:	**8e. Responsible Manager Facsimile Number:**	
702-295-3897	702-295-4435	

9a. Software Configuration Secretariat Name:	9b. Date:
Greg Carlisle	5/5/00

10. [x] Installation/Reinstallation Successful. Software operating as expected.

Installer Name: Jim Kam Initials: JK Date: 5/15/2000

1. RADPRO Ver.3.22

The installation test is based on the instructions provided by LLNL in Section 1.3, INSTALLATION AND TESTING, of the following reference:

LLNL, 2000. CRWMS M&O - RADPRO Description and Documentation of Verification and Validation, REV 000, 10204-SRR-3.22-00, Livermore, California: Lawrence Livermore National Laboratory.

The output produced by the installation test using input files "input.3d.1" and "radin01" is presented on page III-4, which is identical to Figure1 on page III-3 provided by LLNL.

2. XTOOL Ver.10.1

The installation test is based on the instructions provided by LLNL in Section 1.3, INSTALLATION AND TESTING, of the following reference:

LLNL, 2000, CRWMS M&O – XTOOL Description and Documentation of Verification and Validation, REV 000, 10208-SRR-10.1-00, Livermore, California: Lawrence Livermore National Laboratory.

The output produced by the installation test using input file "test1.ext" is presented on page III-6, which is identical to Figure1a on page III-5 provided by LLNL.

3. ACCEPTANCE

Based on the results of the installation tests for RADPRO and XTOOL, both software have been installed successfully.

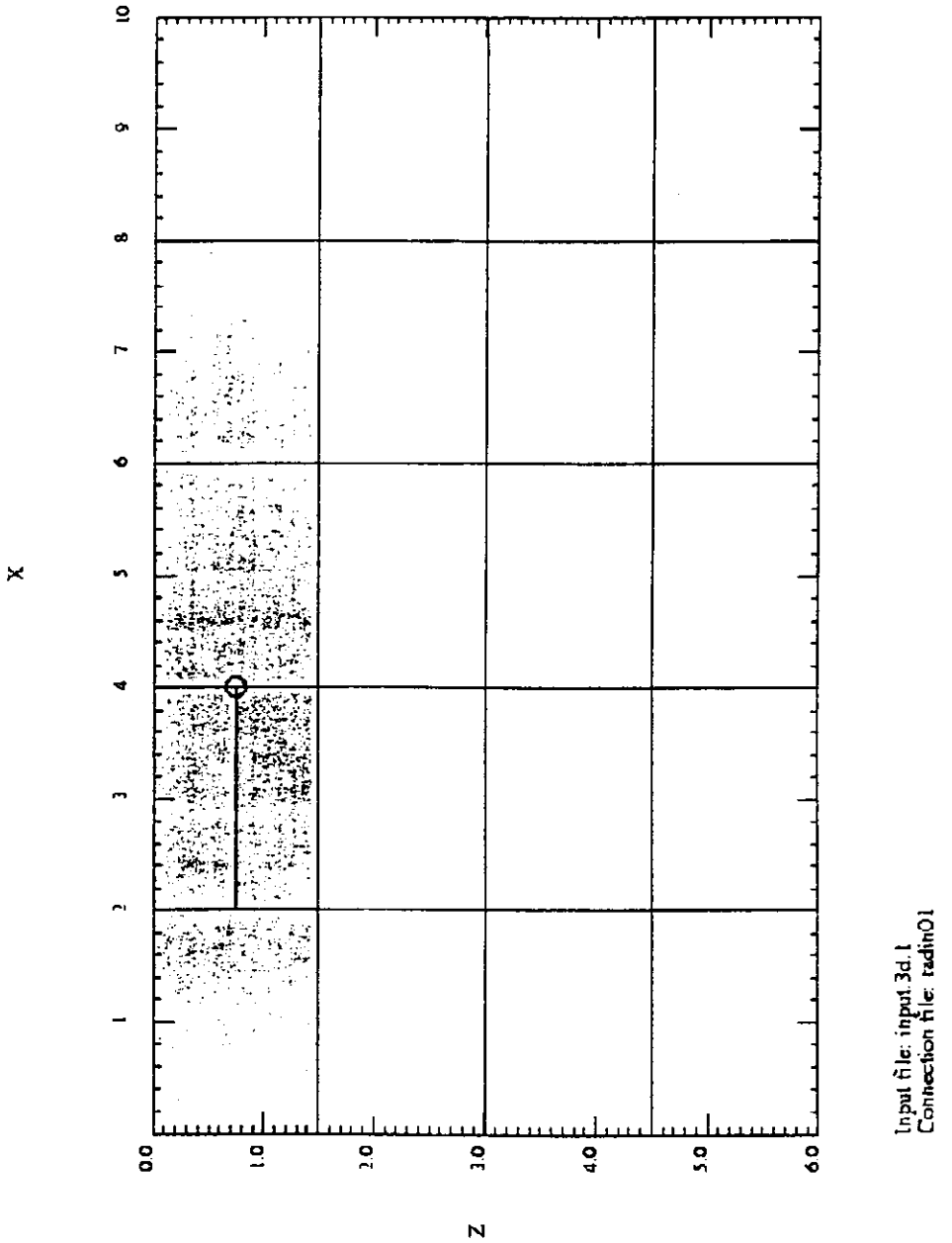
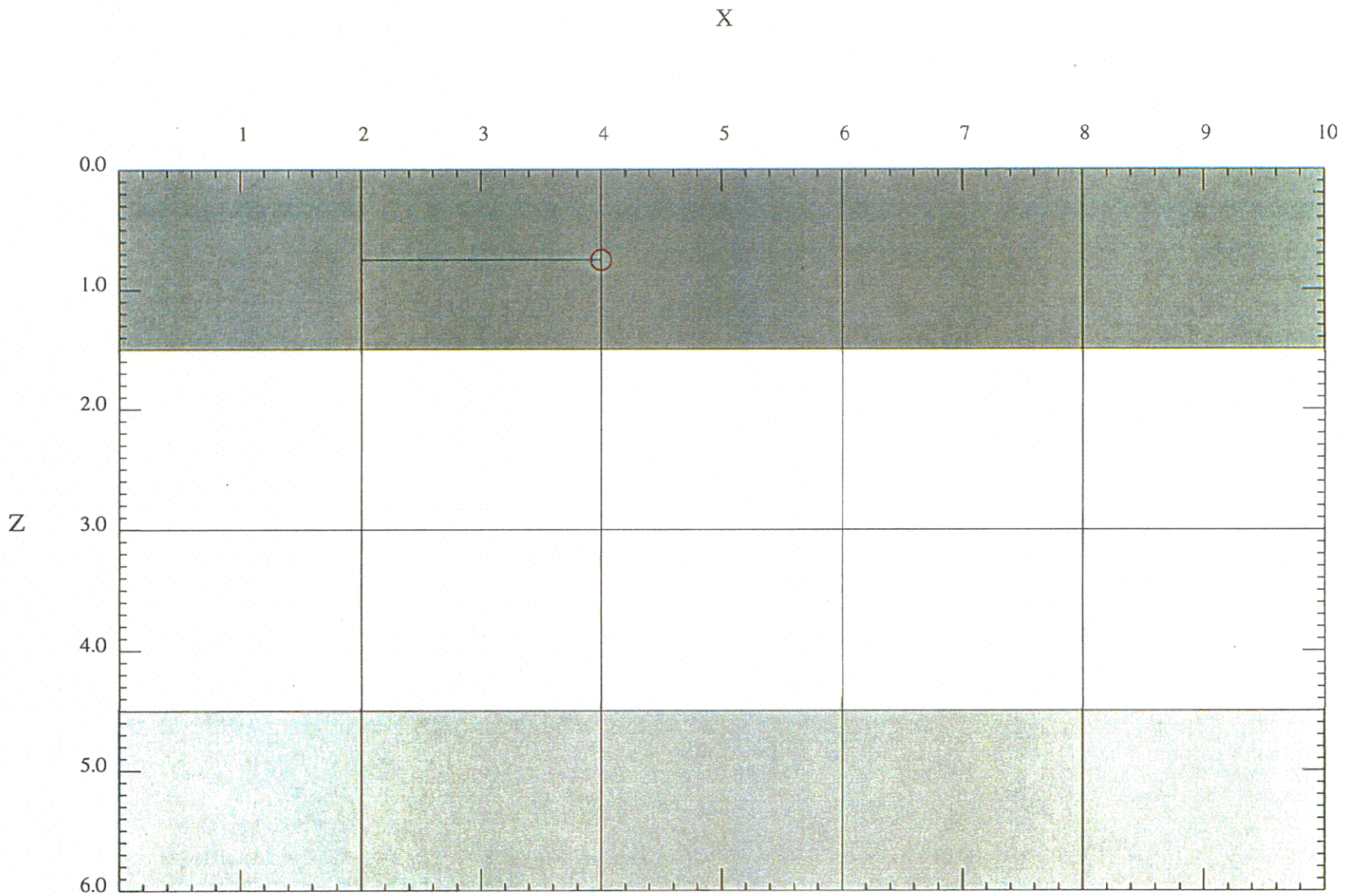


Figure 1. Installation test case picture

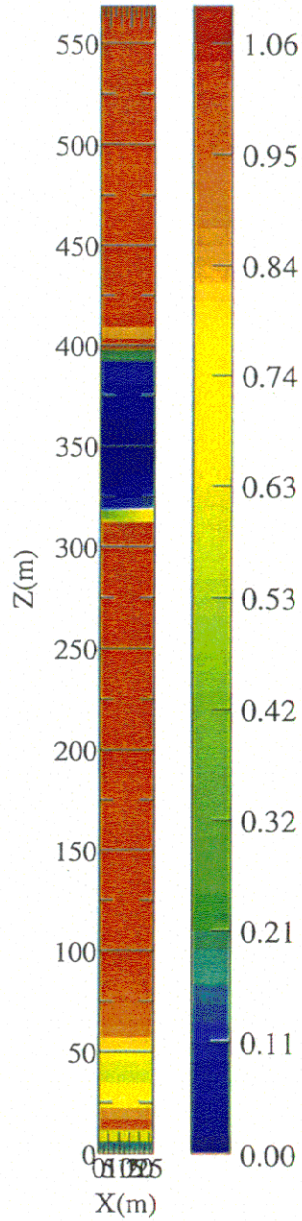


Input file: input.3d.1
Connection file: radin01

bfsmwp1840a 2DRP,flx=0.3,RIBv4,fxdgwt,rmsp53.8m,280md,OFF,base,26y,2024,9.56m

SATURATION OF LIQUID PHASE

TIME = 100.00000 (year)



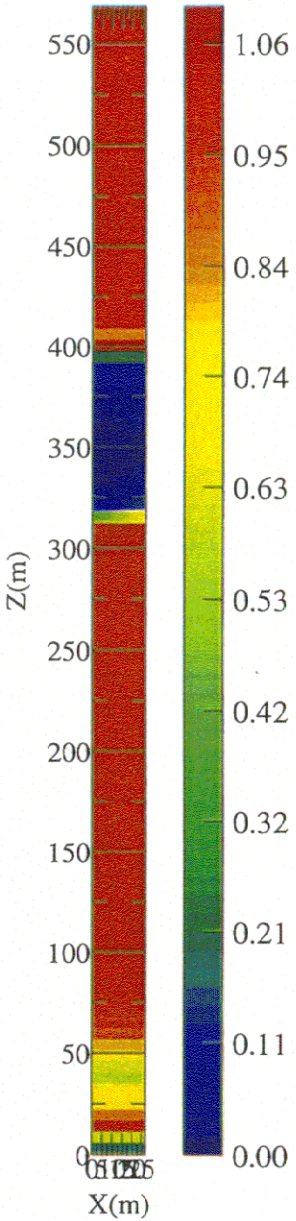
III - 5

levatin /datacvs/xtdir/install Xtool version: 10.1 Fri May 12 13:51:13 2000

bfsmwp1840a 2DRP,flx=0.3,RIBv4,fxdgwt,rmsp53.8m,280md,OFF,base,26y,2024,9.56m

SATURATION OF LIQUID PHASE

TIME = 100.00000 (year)



kam /usr/people/kam Xtool version: 10.1 Mon May 15 12:44:55 2000

Ⅲ-6

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 (DTN: SN9908T0872799.004 - indriftgecm_rev01.doc
~~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)~~

5/16/2000

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)

FOURTH EDITION

Fundamentals of Heat and Mass Transfer

FRANK P. INCROPERA
DAVID P. DEWITT
School of Mechanical Engineering
Purdue University

JOHN WILEY & SONS
New York • Chichester • Brisbane • Toronto • Singapore

IV-3

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10 9 8 7 6 5 4 3

IV-4

TABLE A.1 *Continued*

Composition	Melting Point (K)	Properties at 300 K: ρ (kg/m³)	c_p (J/kg · K)	k (W/m · K)	$\alpha \cdot 10^6$ (m²/s)	Properties at Various Temperatures (K): k (W/m · K)/c_p (J/kg · K) 100	200	400	600	800	1000	1200	1500	2000	2500
Gold	1336	19300	129	317	127	327	323	311	298	284	270	255			
						109	124	131	135	140	145	155			
Iridium	2720	22500	130	147	50.3	172	153	144	138	132	126	120	111		
						90	122	133	138	144	153	161	172		
Iron															
Pure	1810	7870	447	80.2	23.1	134	94.0	69.5	54.7	43.3	32.8	28.3	32.1		
						216	384	490	574	680	975	609	654		
Armco (99.75% pure)		7870	447	72.7	20.7	95.6	80.6	65.7	53.1	42.2	32.3	28.7	31.4		
						215	384	490	574	680	975	609	654		
Carbon steels															
Plain carbon (Mn ≤ 1%, Si ≤ 0.1%)		7854	434	60.5	17.7			56.7	48.0	39.2	30.0				
								487	559	685	1169				
AISI 1010		7832	434	63.9	18.8			58.7	48.8	39.2	31.3				
								487	559	685	1168				
Carbon-silicon (Mn ≤ 1%, 0.1% < Si ≤ 0.6%)		7817	446	51.9	14.9			49.8	44.0	37.4	29.3				
								501	582	699	971				
Carbon-manganese-silicon (1% < Mn ≤ 1.65%, 0.1% < Si ≤ 0.6%)		8131	434	41.0	11.6			42.2	39.7	35.0	27.6				
								487	559	685	1090				
Chromium (low) steels															
½Cr-½Mo-Si (0.18% C, 0.65% Cr, 0.23% Mo, 0.6% Si)		7822	444	37.7	10.9			38.2	36.7	33.3	26.9				
								492	575	688	969				
1 Cr-½Mo (0.16% C, 1% Cr, 0.54% Mo, 0.39% Si)		7858	442	42.3	12.2			42.0	39.1	34.5	27.4				
								492	575	688	969				
1 Cr-V (0.2% C, 1.02% Cr, 0.15% V)		7836	443	48.9	14.1			46.8	42.1	36.3	28.2				
								492	575	688	969				

Stainless steels																	
AISI 302		8055	480	15.1	3.91			17.3 512	20.0 559	22.8 585	25.4 606						
AISI 304	1670	7900	477	14.9	3.95	9.2 272	12.6 402	16.6 515	19.8 557	22.6 582	25.4 611	28.0 640	31.7 682				
AISI 316		8238	468	13.4	3.48			15.2 504	18.3 550	21.3 576	24.2 602						
AISI 347		7978	480	14.2	3.71			15.8 513	18.9 559	21.9 585	24.7 606						
Lead	601	11340	129	35.3	24.1	39.7 118	36.7 125	34.0 132	31.4 142								
Magnesium	923	1740	1024	156	87.6	169 649	159 934	153 1074	149 1170	146 1267							
Molybdenum	2894	10240	251	138	53.7	179 141	143 224	134 261	126 275	118 285	112 295	105 308	98 330	90 380	86 459		
Nickel																	
Pure	1728	8900	444	90.7	23.0	164 232	107 383	80.2 485	65.6 592	67.6 530	71.8 562	76.2 594	82.6 616				
Nichrome (80% Ni, 20% Cr)	1672	8400	420	12	3.4			14 480	16 525	21 545							
Inconel X-750 (73% Ni, 15% Cr, 6.7% Fe)	1665	8510	439	11.7	3.1	8.7 —	10.3 372	13.5 473	17.0 510	20.5 546	24.0 626	27.6 —	33.0 —				
Niobium	2741	8570	265	53.7	23.6	55.2 188	52.6 249	55.2 274	58.2 283	61.3 292	64.4 301	67.5 310	72.1 324	79.1 347			
Palladium	1827	12020	244	71.8	24.5	76.5 168	71.6 227	73.6 251	79.7 261	86.9 271	94.2 281	102 291	110 307				
Platinum																	
Pure	2045	21450	133	71.6	25.1	77.5 100	72.6 125	71.8 136	73.2 141	75.6 146	78.7 152	82.6 157	89.5 165	99.4 179			
Alloy 60Pt–40Rh (60% Pt, 40% Rh)	1800	16630	162	47	17.4			52 —	59 —	65 —	69 —	73 —	76 —				
Rhenium	3453	21100	136	47.9	16.7	58.9 97	51.0 127	46.1 139	44.2 145	44.1 151	44.6 156	45.7 162	47.8 171	51.9 186			
Rhodium	2236	12450	243	150	49.6	186 147	154 220	146 253	136 274	127 293	121 311	116 327	110 349	112 376			
Silicon	1685	2330	712	148	89.2	884 259	264 556	98.9 790	61.9 867	42.2 913	31.2 946	25.7 967	22.7 992				
Silver	1235	10500	235	429	174	444 187	430 225	425 239	412 250	396 262	379 277	361 292					
Tantalum	3269	16600	140	57.5	24.7	59.2 110	57.5 133	57.8 144	58.6 146	59.4 149	60.2 152	61.0 155	62.2 160	64.1 172	65.6 189		
Thorium	2023	11700	118	54.0	39.1	59.8 99	54.6 112	54.5 124	55.8 134	56.9 145	56.9 156	58.7 167					
Tin	505	7310	227	66.6	40.1	85.2 188	73.3 215	62.2 243									

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TABLE A.4 Thermophysical Properties of Gases at Atmospheric Pressure[a]

T (K)	ρ (kg/m³)	c_p (kJ/kg · K)	$\mu \cdot 10^7$ (N · s/m²)	$\nu \cdot 10^6$ (m²/s)	$k \cdot 10^3$ (W/m · K)	$\alpha \cdot 10^6$ (m²/s)	Pr
Air							
100	3.5562	1.032	71.1	2.00	9.34	2.54	0.786
150	2.3364	1.012	103.4	4.426	13.8	5.84	0.758
200	1.7458	1.007	132.5	7.590	18.1	10.3	0.737
250	1.3947	1.006	159.6	11.44	22.3	15.9	0.720
300	1.1614	1.007	184.6	15.89	26.3	22.5	0.707
350	0.9950	1.009	208.2	20.92	30.0	29.9	0.700
400	0.8711	1.014	230.1	26.41	33.8	38.3	0.690
450	0.7740	1.021	250.7	32.39	37.3	47.2	0.686
500	0.6964	1.030	270.1	38.79	40.7	56.7	0.684
550	0.6329	1.040	288.4	45.57	43.9	66.7	0.683
600	0.5804	1.051	305.8	52.69	46.9	76.9	0.685
650	0.5356	1.063	322.5	60.21	49.7	87.3	0.690
700	0.4975	1.075	338.8	68.10	52.4	98.0	0.695
750	0.4643	1.087	354.6	76.37	54.9	109	0.702
800	0.4354	1.099	369.8	84.93	57.3	120	0.709
850	0.4097	1.110	384.3	93.80	59.6	131	0.716
900	0.3868	1.121	398.1	102.9	62.0	143	0.720
950	0.3666	1.131	411.3	112.2	64.3	155	0.723
1000	0.3482	1.141	424.4	121.9	66.7	168	0.726
1100	0.3166	1.159	449.0	141.8	71.5	195	0.728
1200	0.2902	1.175	473.0	162.9	76.3	224	0.728
1300	0.2679	1.189	496.0	185.1	82	238	0.719
1400	0.2488	1.207	530	213	91	303	0.703
1500	0.2322	1.230	557	240	100	350	0.685
1600	0.2177	1.248	584	268	106	390	0.688
1700	0.2049	1.267	611	298	113	435	0.685
1800	0.1935	1.286	637	329	120	482	0.683
1900	0.1833	1.307	663	362	128	534	0.677
2000	0.1741	1.337	689	396	137	589	0.672
2100	0.1658	1.372	715	431	147	646	0.667
2200	0.1582	1.417	740	468	160	714	0.655
2300	0.1513	1.478	766	506	175	783	0.647
2400	0.1448	1.558	792	547	196	869	0.630
2500	0.1389	1.665	818	589	222	960	0.613
3000	0.1135	2.726	955	841	486	1570	0.536
Ammonia (NH_3)							
300	0.6894	2.158	101.5	14.7	24.7	16.6	0.887
320	0.6448	2.170	109	16.9	27.2	19.4	0.870
340	0.6059	2.192	116.5	19.2	29.3	22.1	0.872
360	0.5716	2.221	124	21.7	31.6	24.9	0.872
380	0.5410	2.254	131	24.2	34.0	27.9	0.869

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

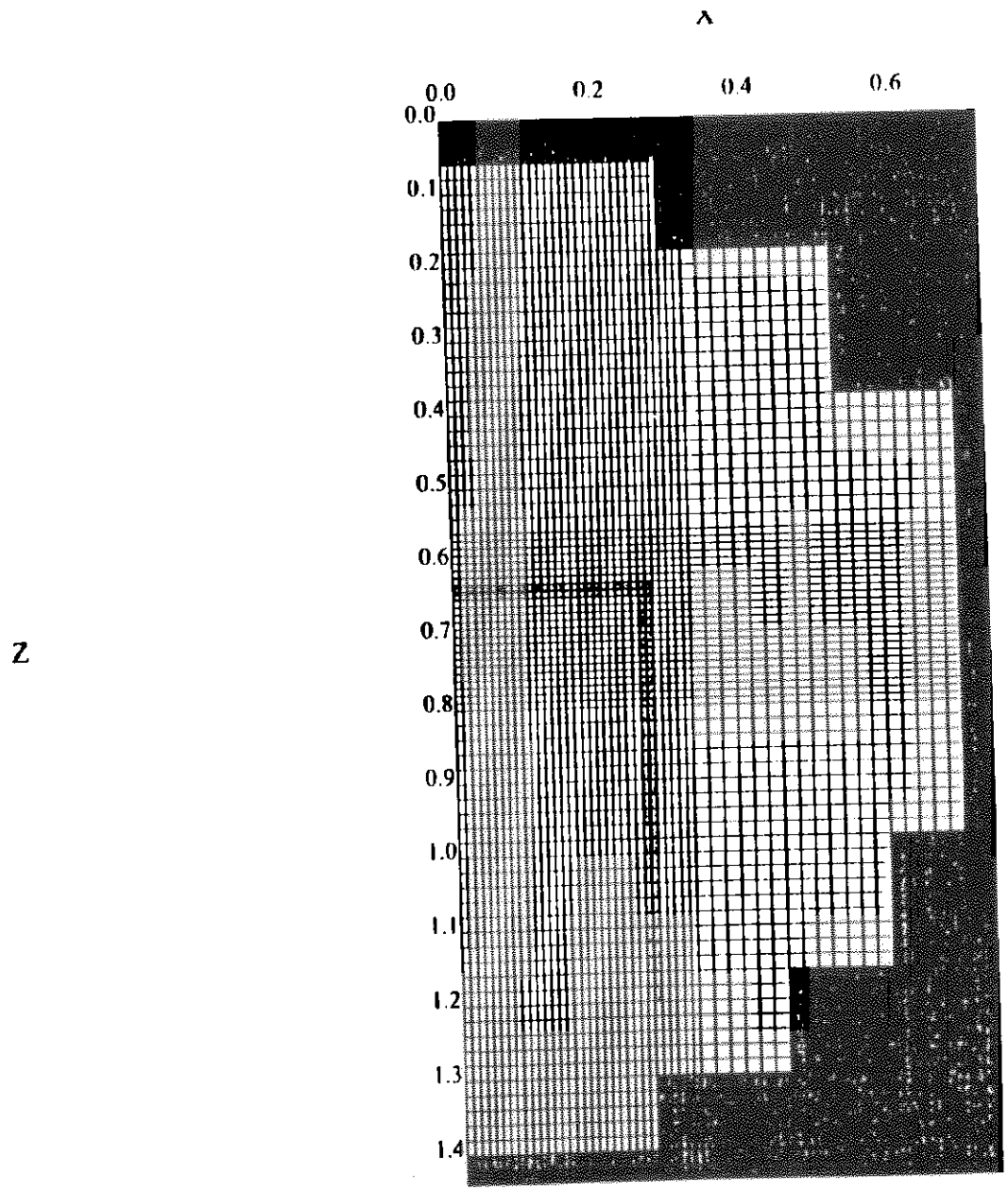
$k = 0.030$ W/m.K
$\beta = 0.0029$ K^{-1}
$\nu = 2.092E\text{-}5$ m^2/s
$\alpha = 2.990E\text{-}5$ m^2/s

$Pr = 0.70$

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

$k_{eff} = 0.1666$

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



Input file: radymp2Ddst9
Connection file:

```
  (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 ".ral")
    ;;     )



   ;;     (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 ".ral")
     ;;     )



    ;;     (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)
                         ("drl**" 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) ("drl**"
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 ".ral")
    ;;)


      (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
c
radiating_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
connections     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
c
radiating_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 ".ral")
     )

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



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

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

    (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.ga
                (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 ".ral")
     ;;)



      (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)
         )
```

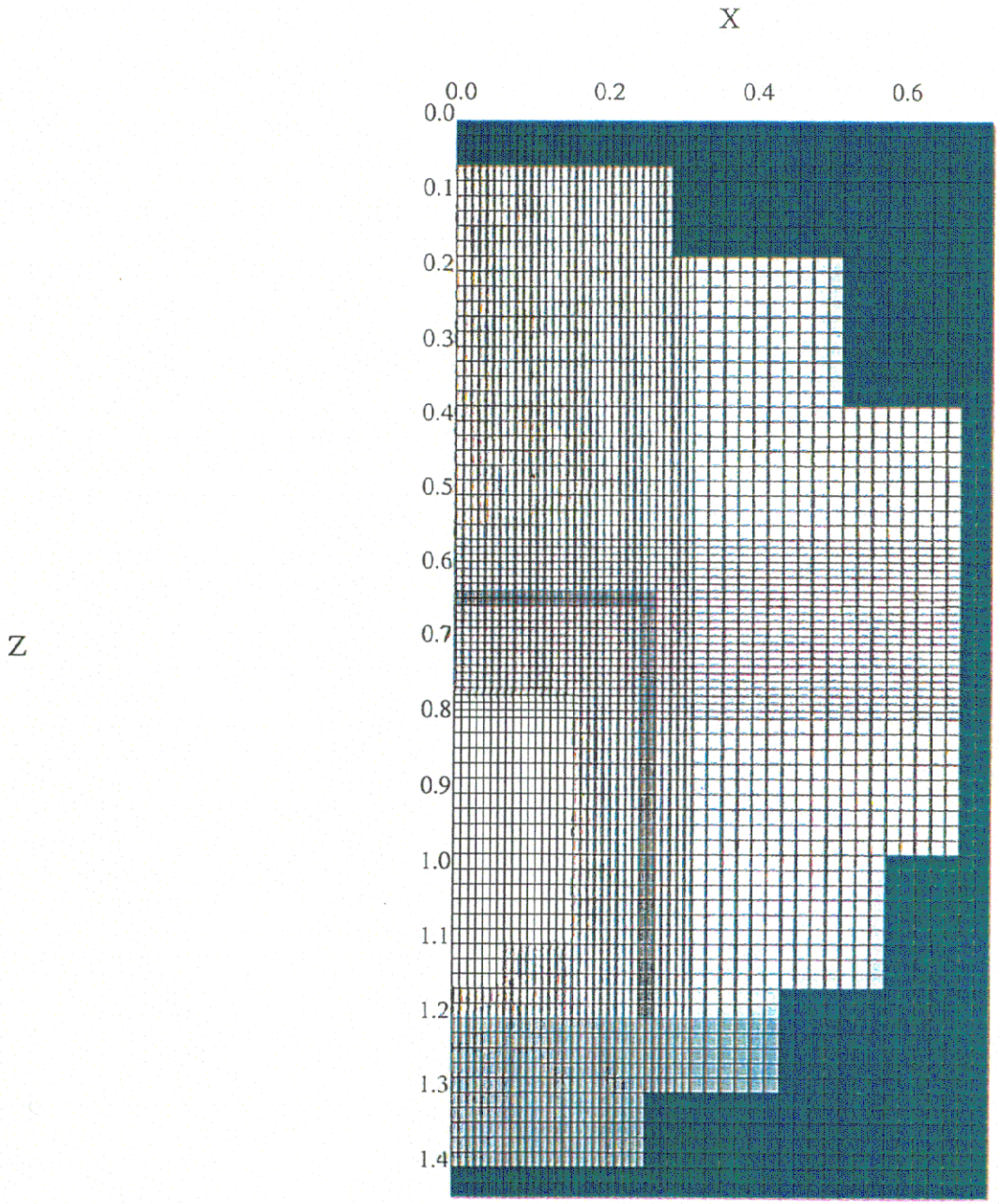
```
        (X.air by-key ("** -1.0)  ("at** 0.999) ("dr** 0.999) ("dr1**
0.999)
                      ("ht** 1.0) ("dr2** 0.999) ("sh** 1.0))

       ) ;; 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
c
radiating_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
connections     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
c
radiating_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
c
radiating_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
```

```
  (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
```

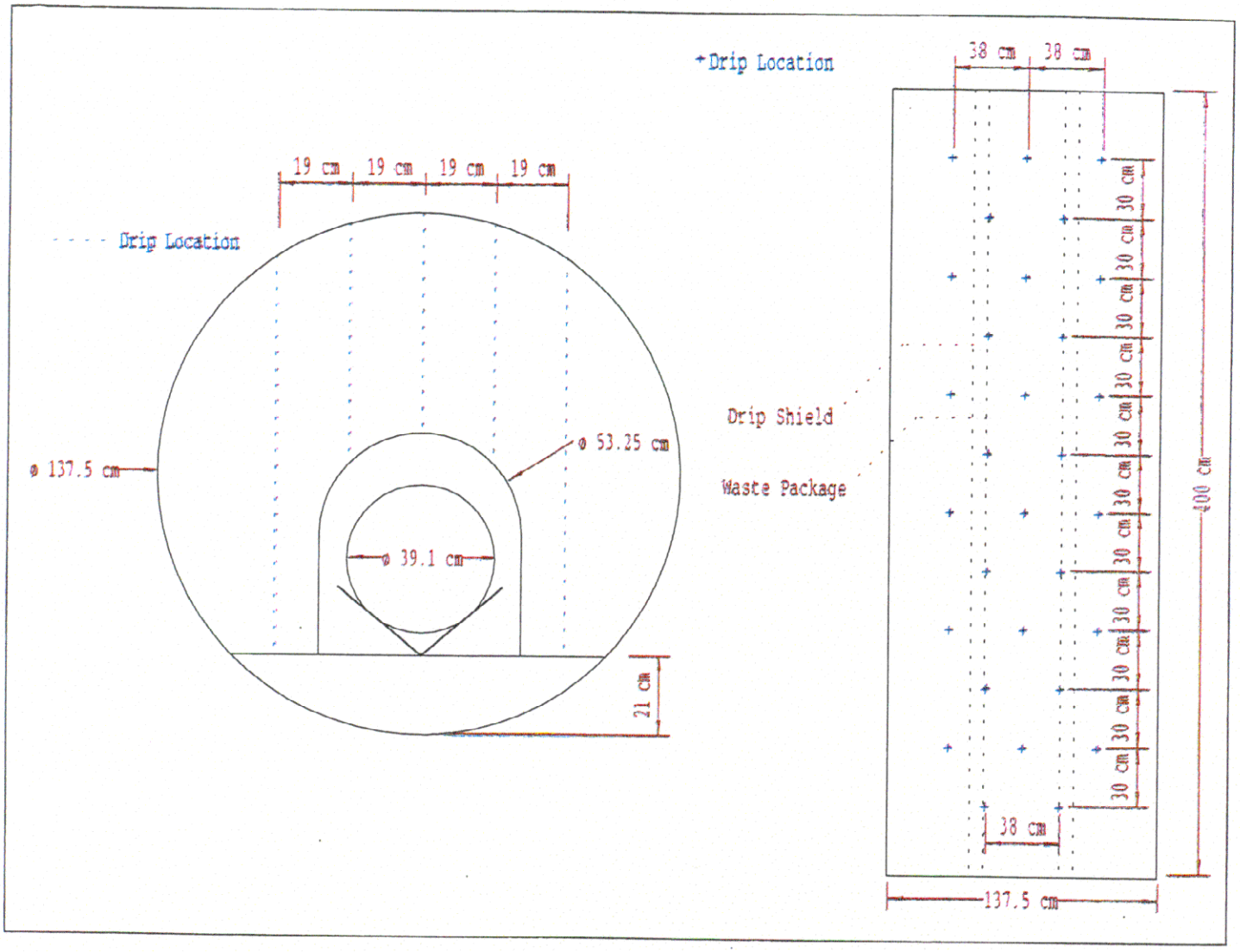


Figure 1. Quarter Scale Test Configuration

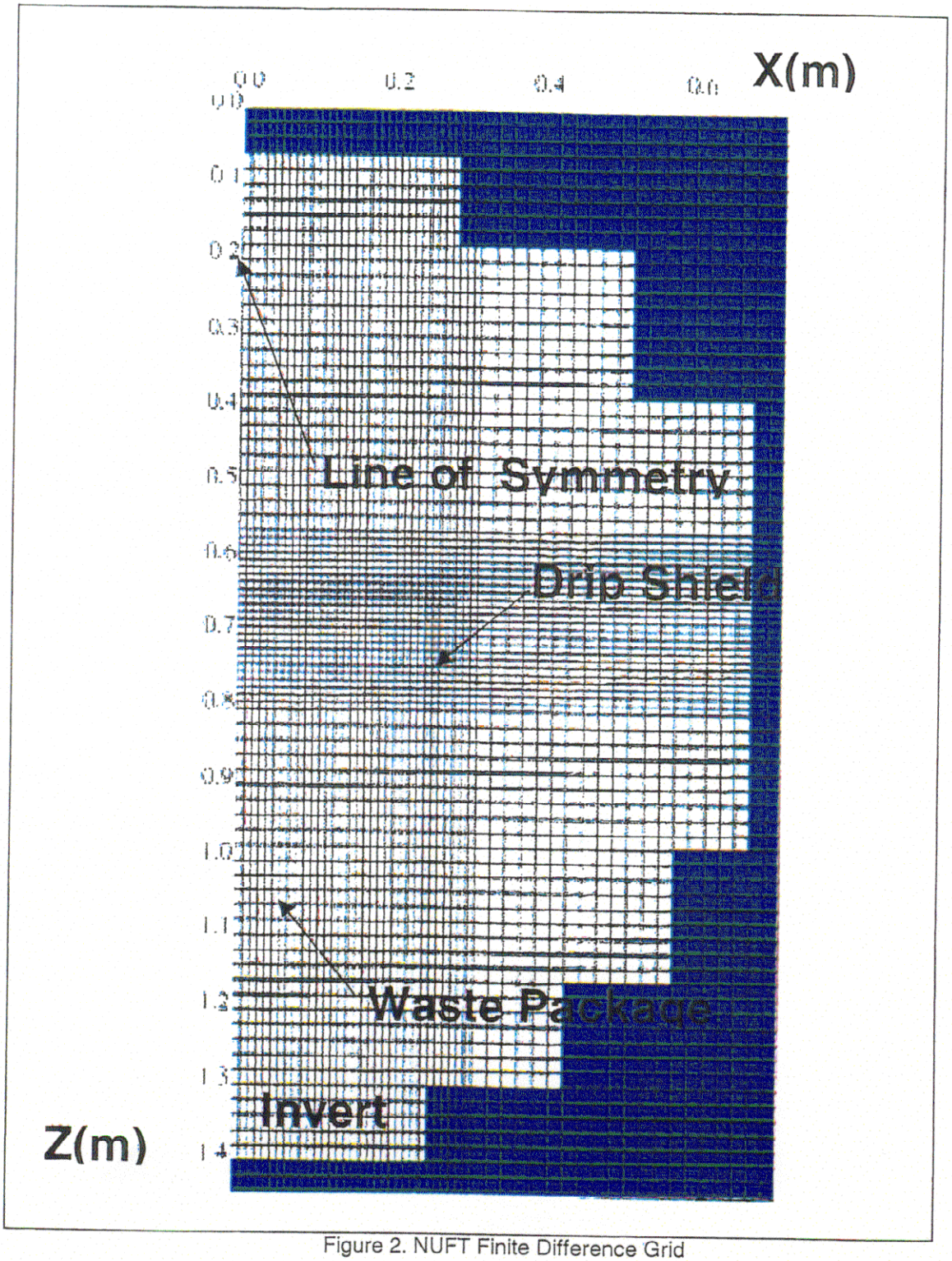


Figure 2. NUFT Finite Difference Grid

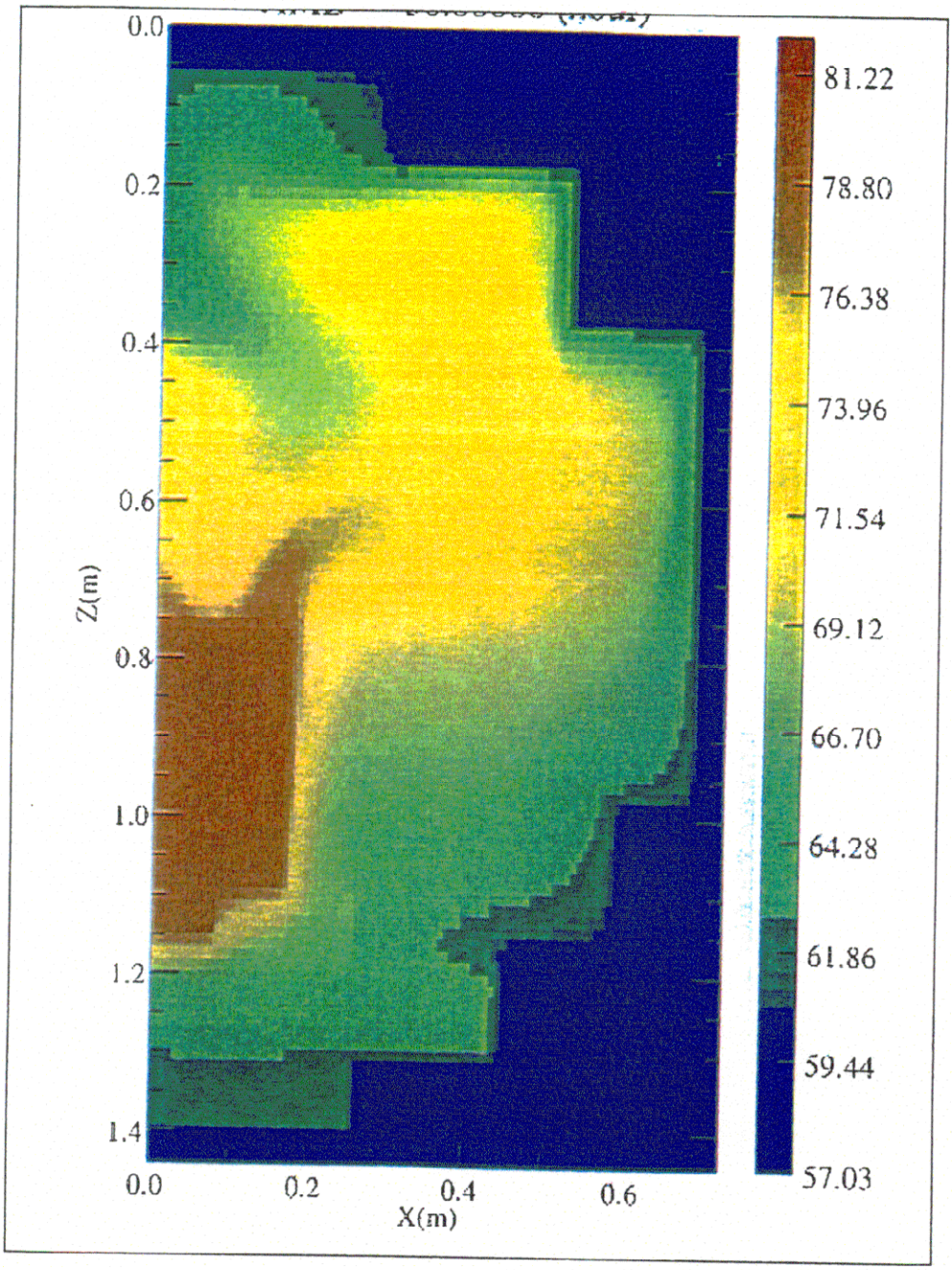


Figure 3 T-H NUFT Analysis for the Case of No Drip Shield After 36 Hours

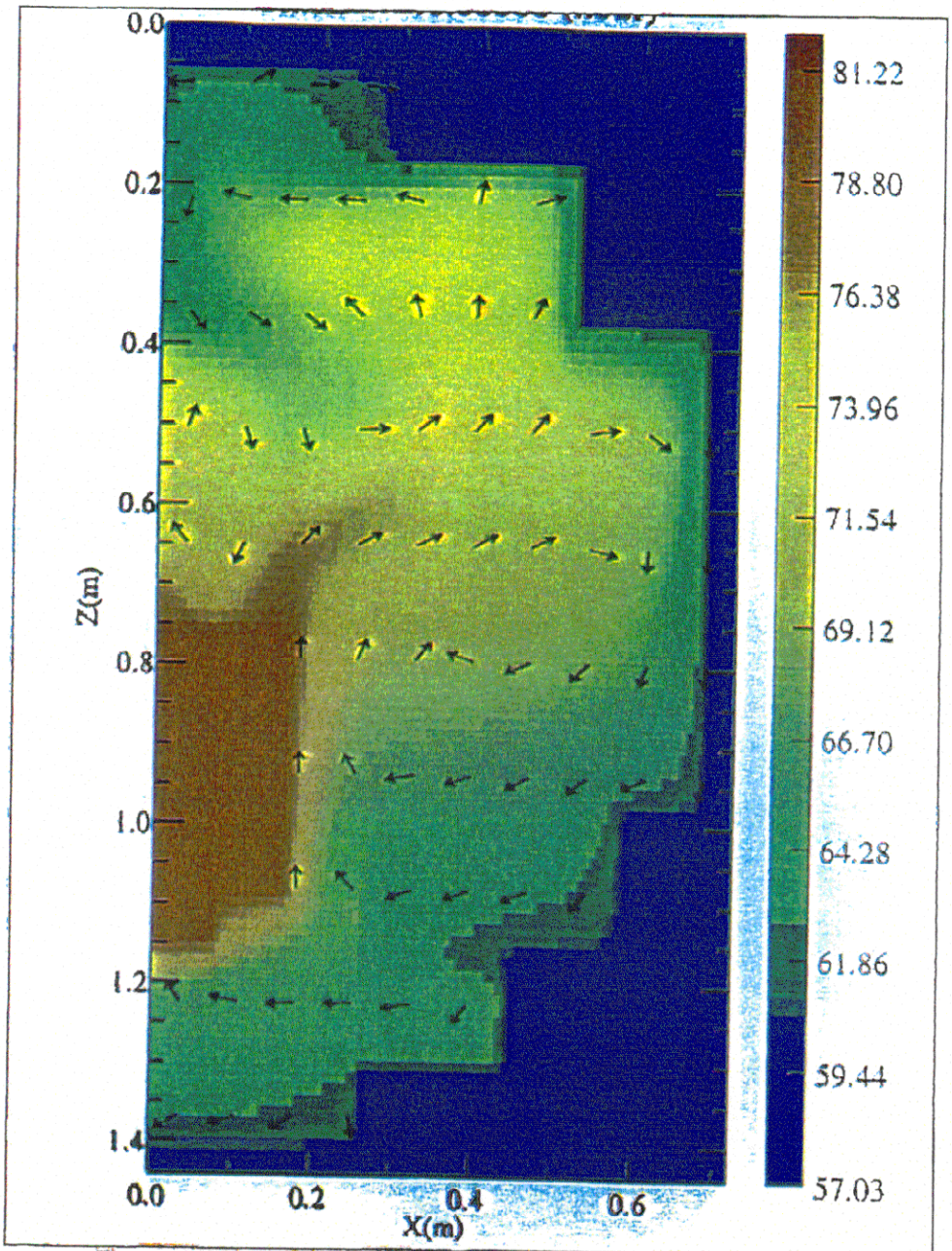


Figure 4 T-H NUFT Analysis for the Case of No Drip Shield After 48 Hours

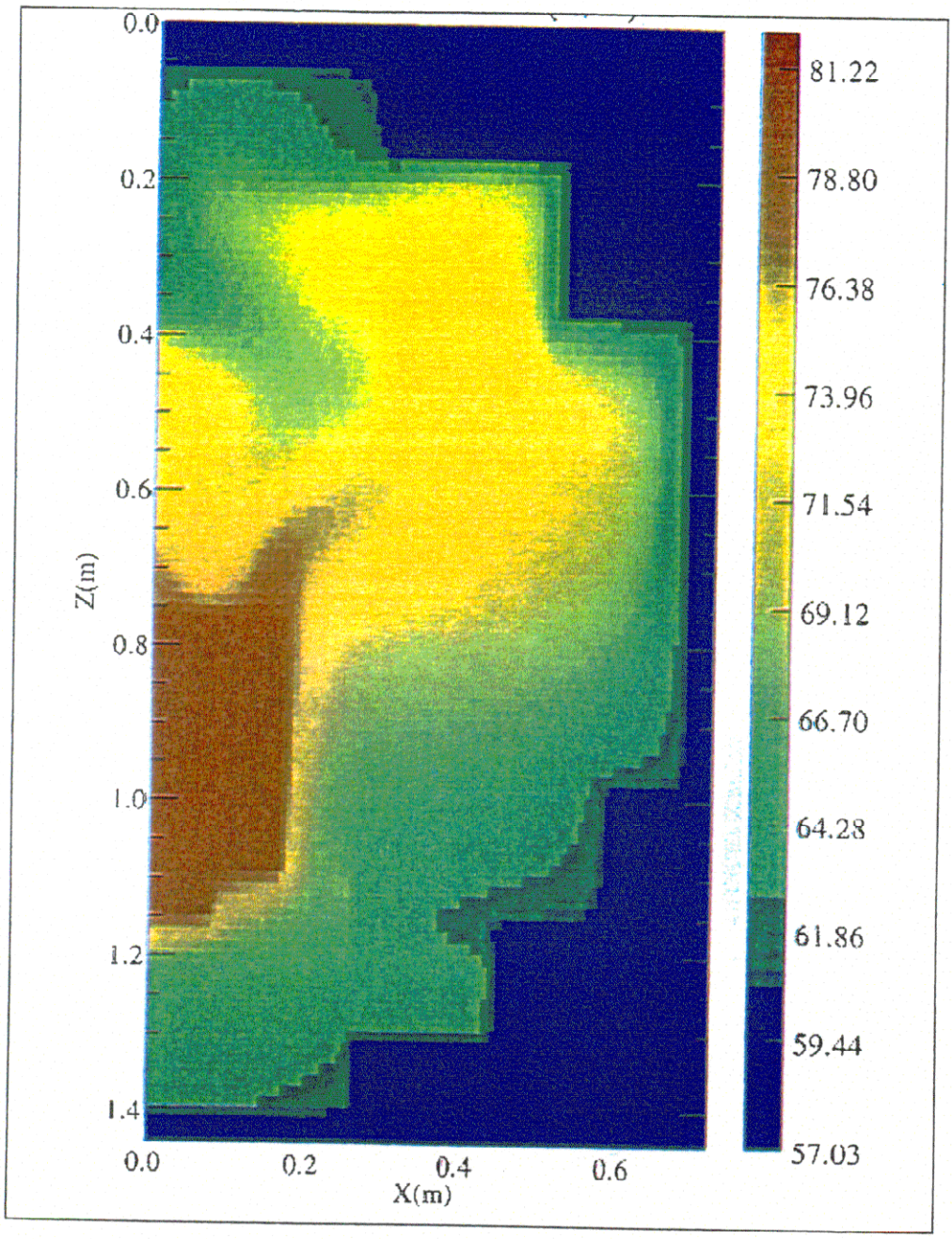


Figure 5 T-H NUFT Analysis for the Case of No Drip Shield After 72 Hours

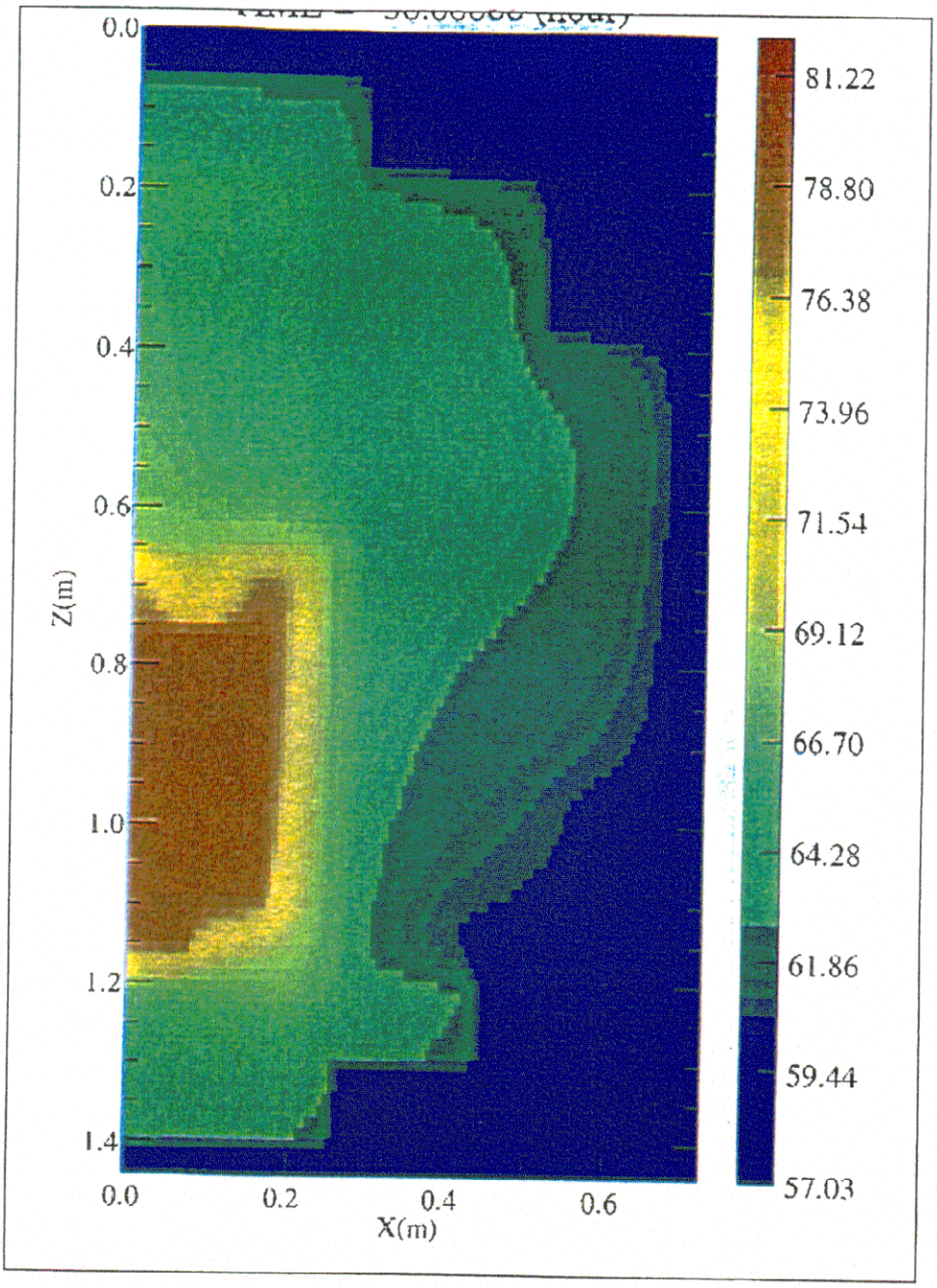


Figure 6 T-H NUFT Analysis for the Case of a Drip Shield After 36 Hours

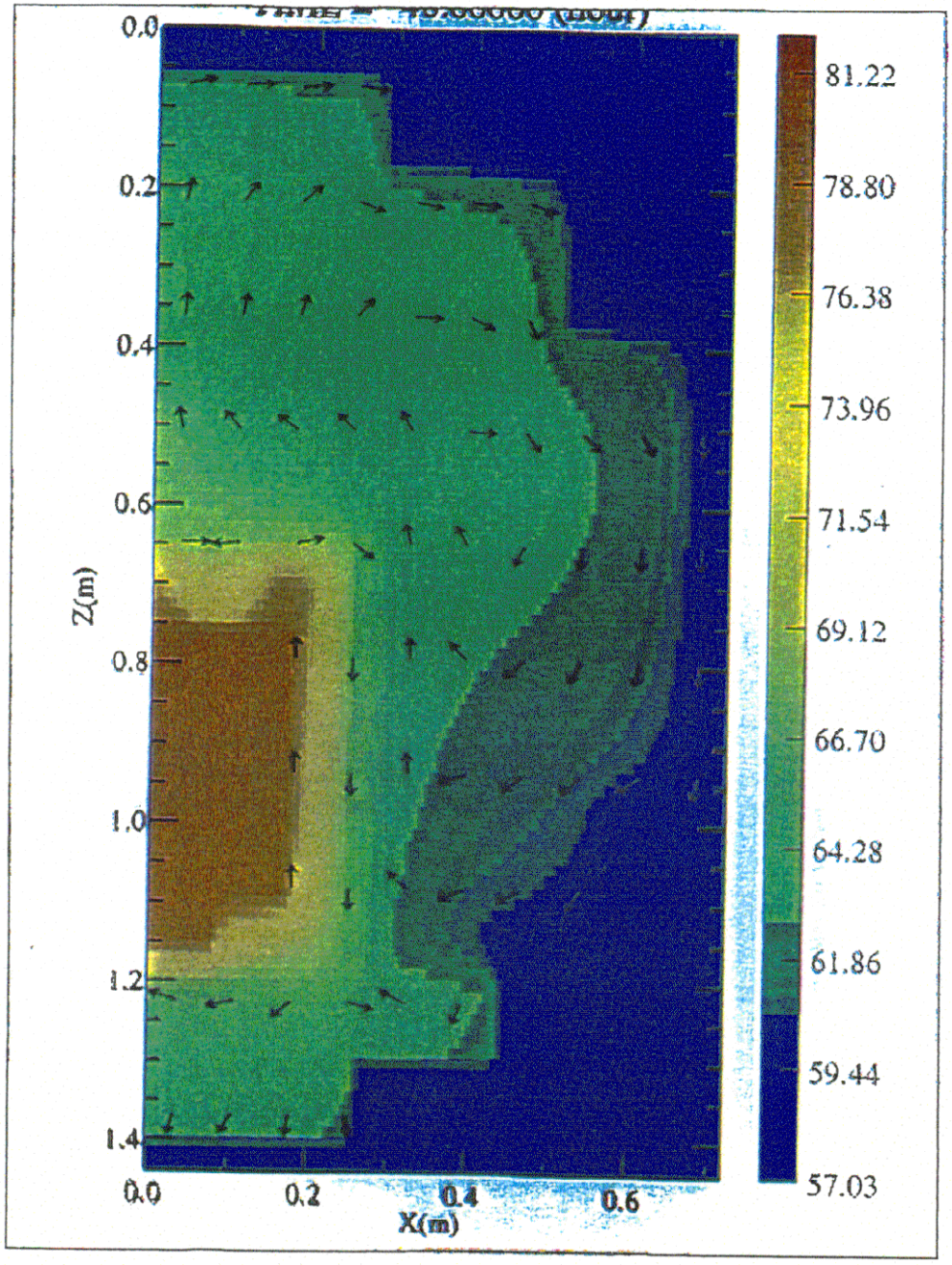


Figure 7 T-H NUFT Analysis for the Case of a Drip Shield After 48 Hours

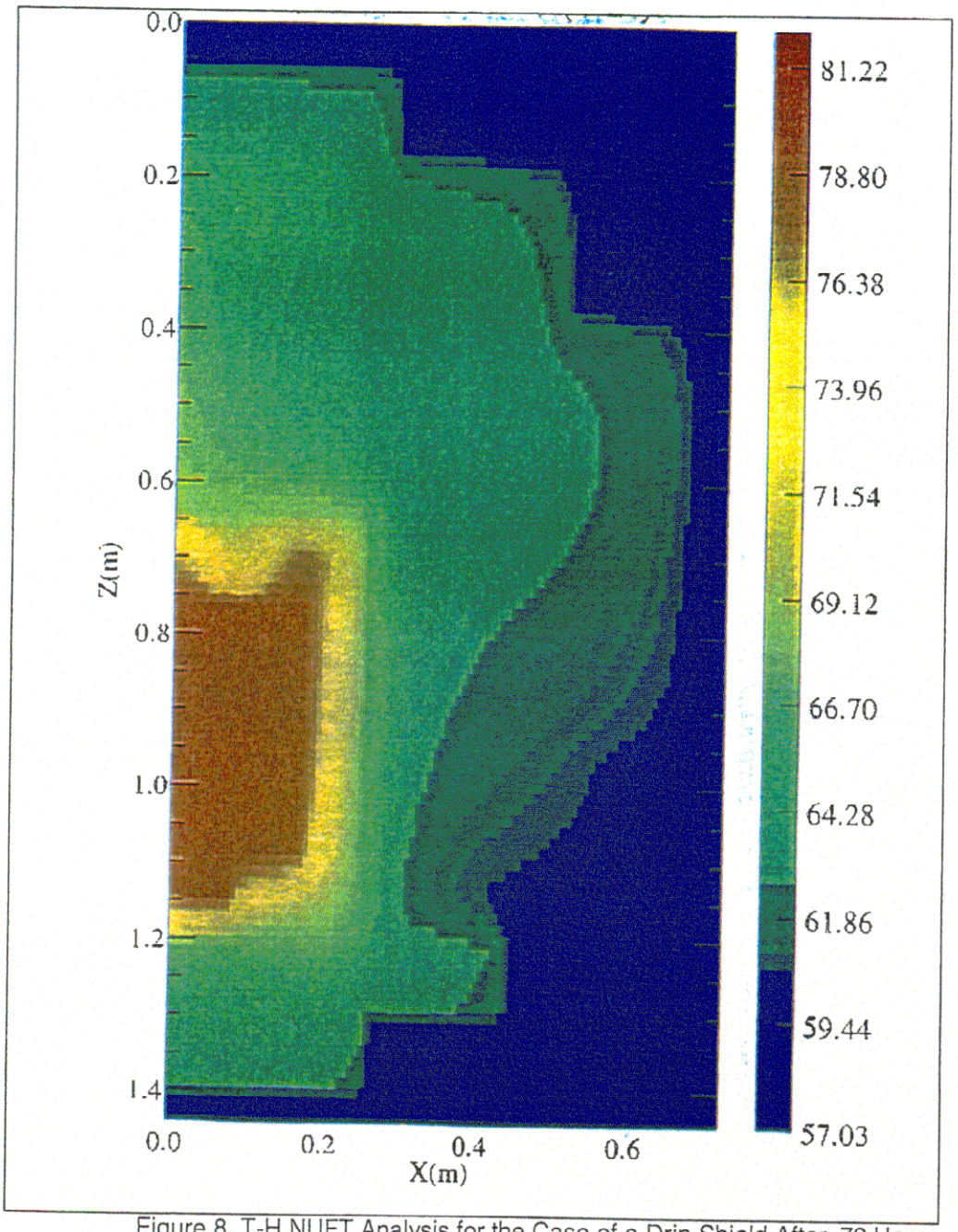


Figure 8 T-H NUFT Analysis for the Case of a Drip Shield After 72 Hours

Cliff Howard
09/13/99 01:54 PM

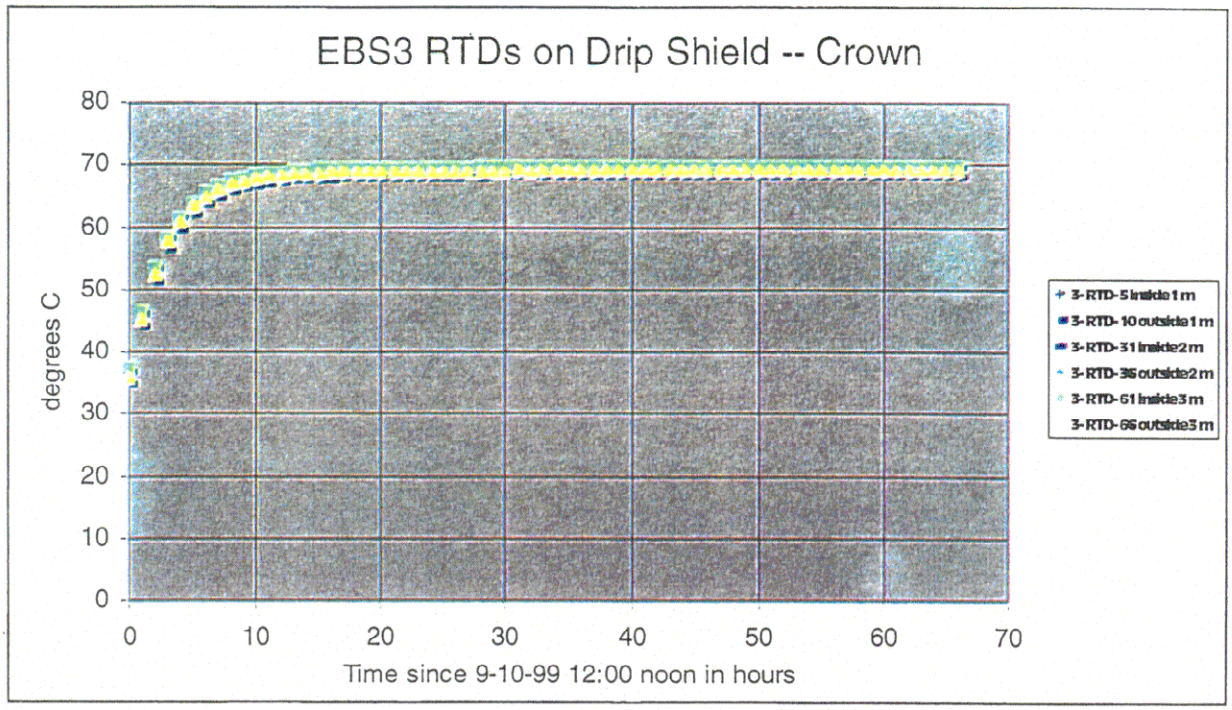
To: Jim Kam/YM/RWDOE@CRWMS, John Case/YM/RWDOE@CRWMS, swwebb@sandia.gov, Randolph Schreiner/YM/RWDOE@CRWMS, Dwayne Chestnut/YM/RWDOE@CRWMS

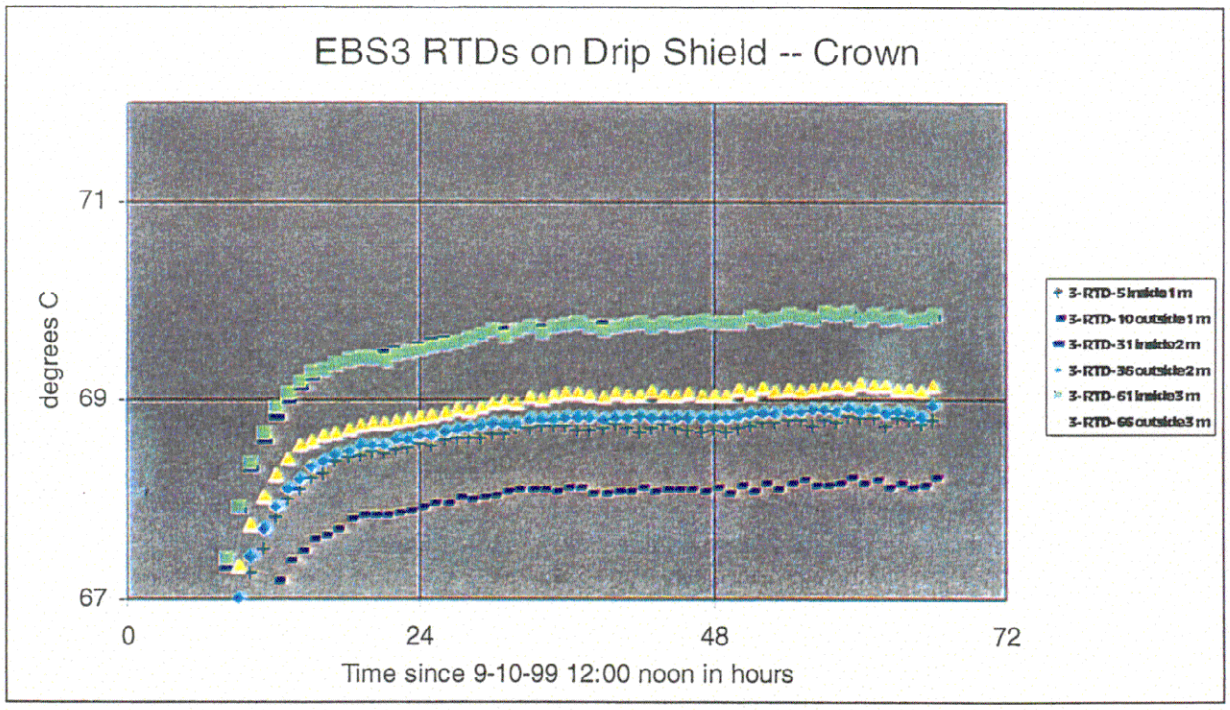
cc: John Pye/YM/RWDOE@CRWMS, Hemendra Kalia/YM/RWDOE@CRWMS, REFINLE@SANDIA.GOV, Fred Homuth/YM/RWDOE@CRWMS, Douglas Weaver/YM/RWDOE@CRWMS, David Kessel/YM/RWDOE@CRWMS, Ron Taylor/YM/RWDOE@CRWMS, William Lowry/YM/RWDOE@CRWMS, jtgeorg@sandia.gov, Roy Johnston/YM/RWDOE@CRWMS, Troy Williams/YM/RWDOE@CRWMS,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

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

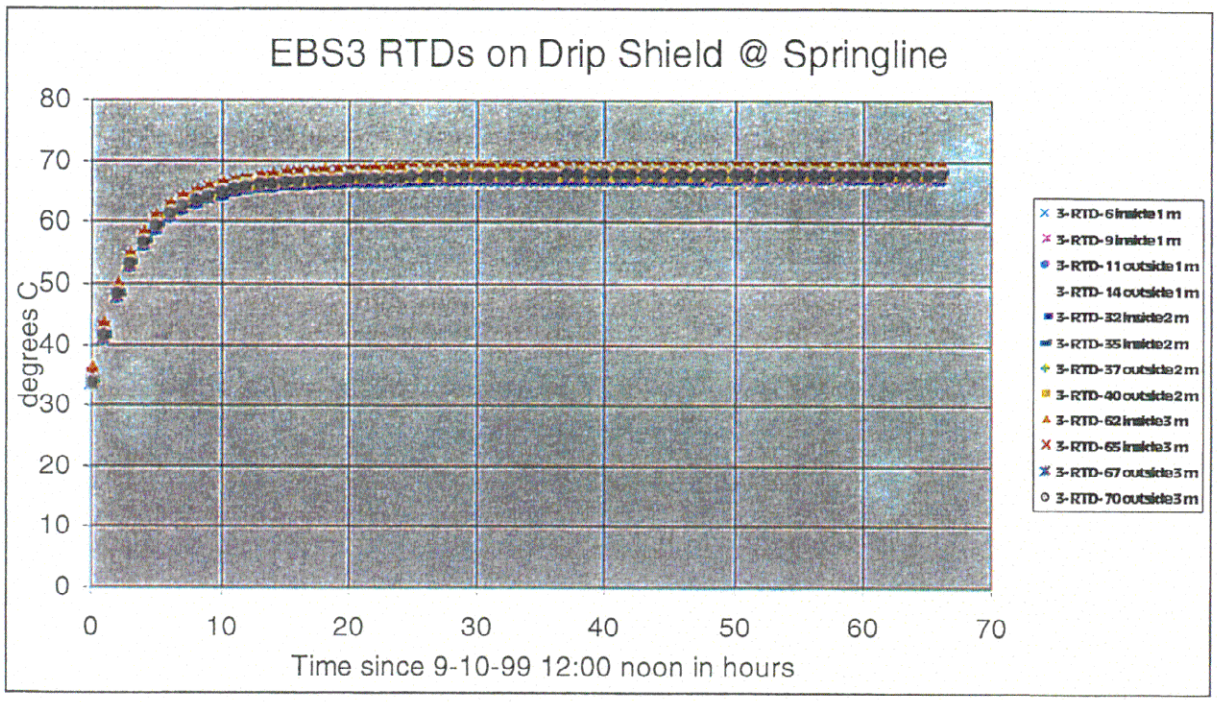
Gentlemen,
In my previous E-mail, I did not include data from the test that showed the 60 degree and 80 degree set points. This is because this data is driven by the power control circuit and I thought the other data would provide the more definitive evidence of steady state heat flow and distribution. 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

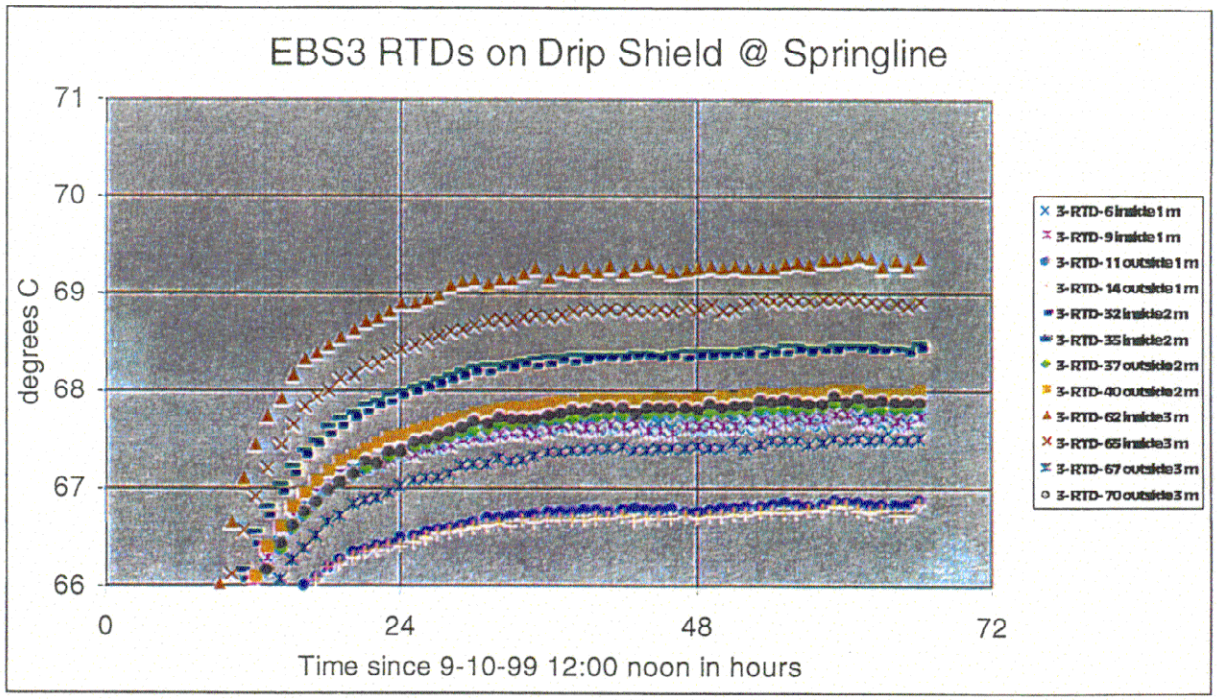
DripShieldTurnOn.do



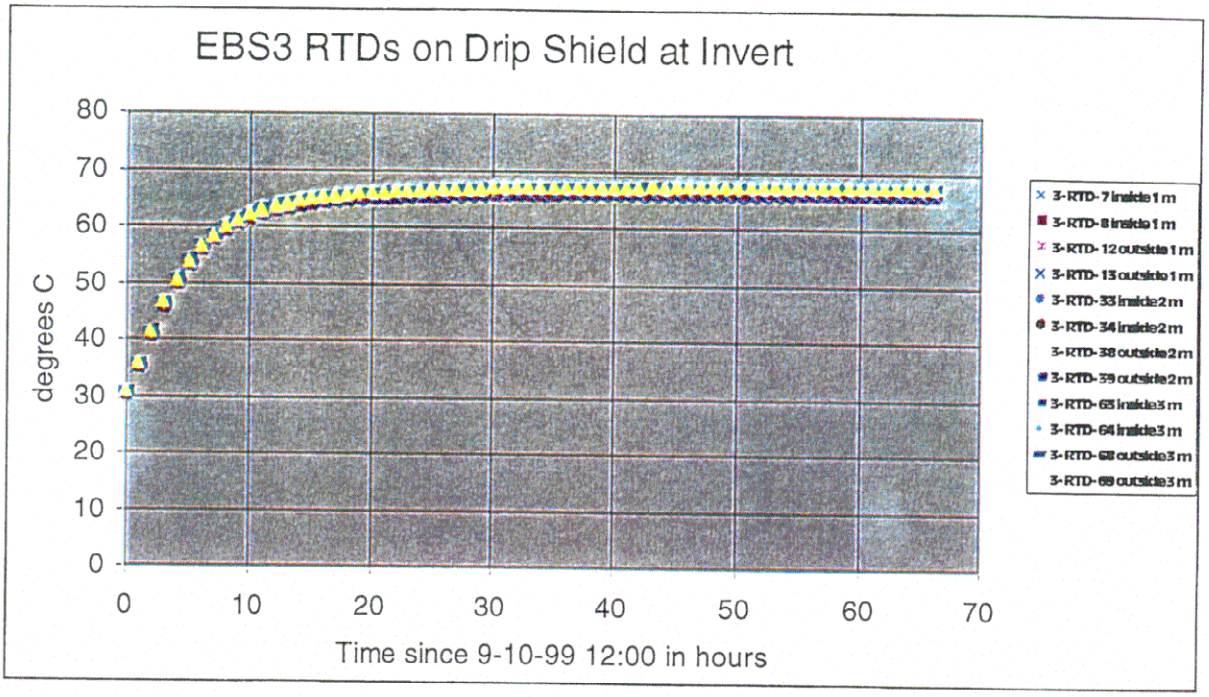


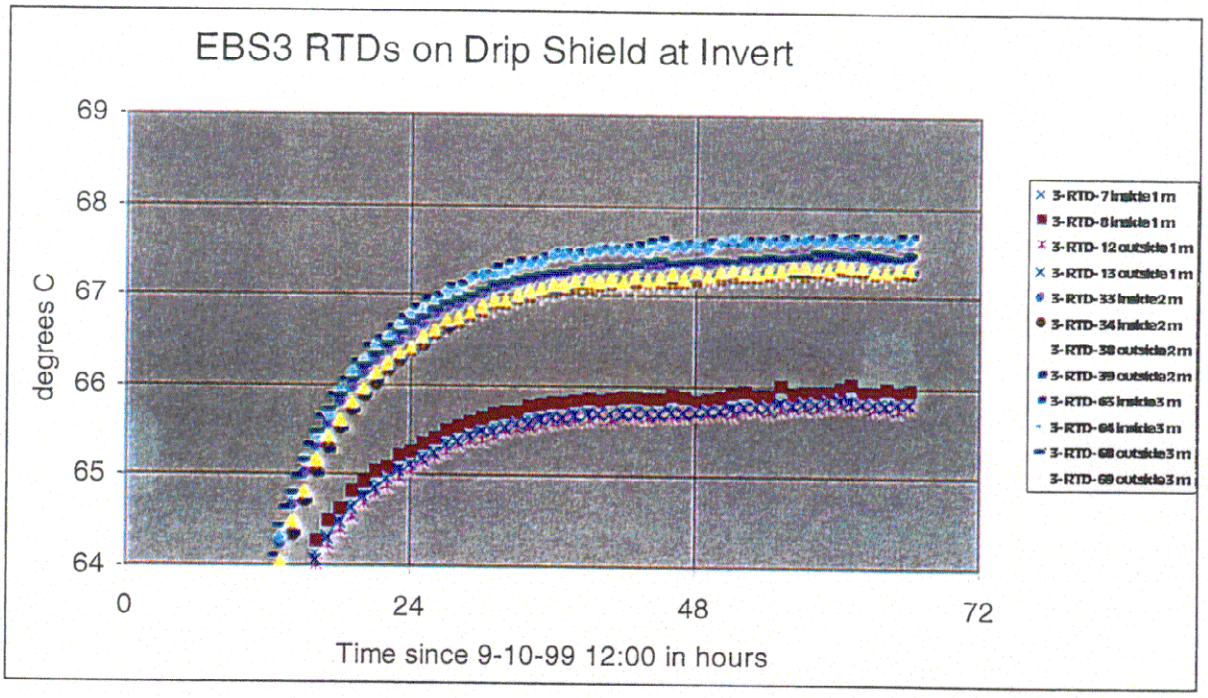
Preliminary Data – Not yet qualified to project standards – approximate conversions used from raw data
Power turned on about 11:30 am on 9-10-99



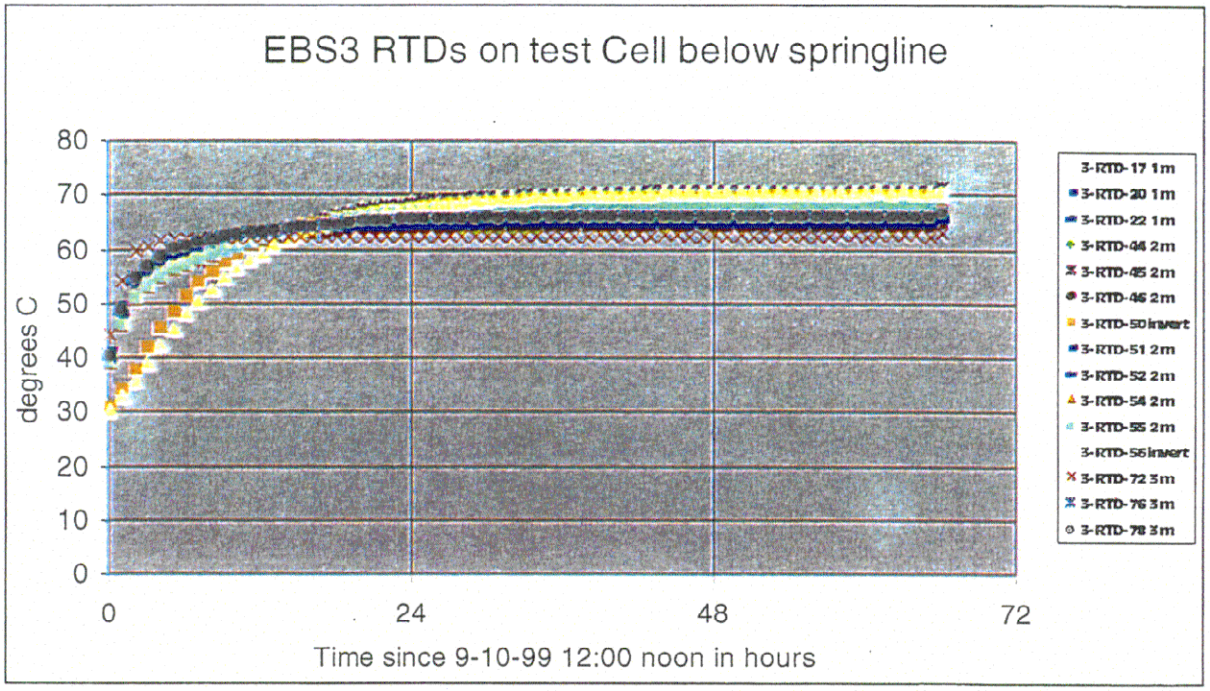


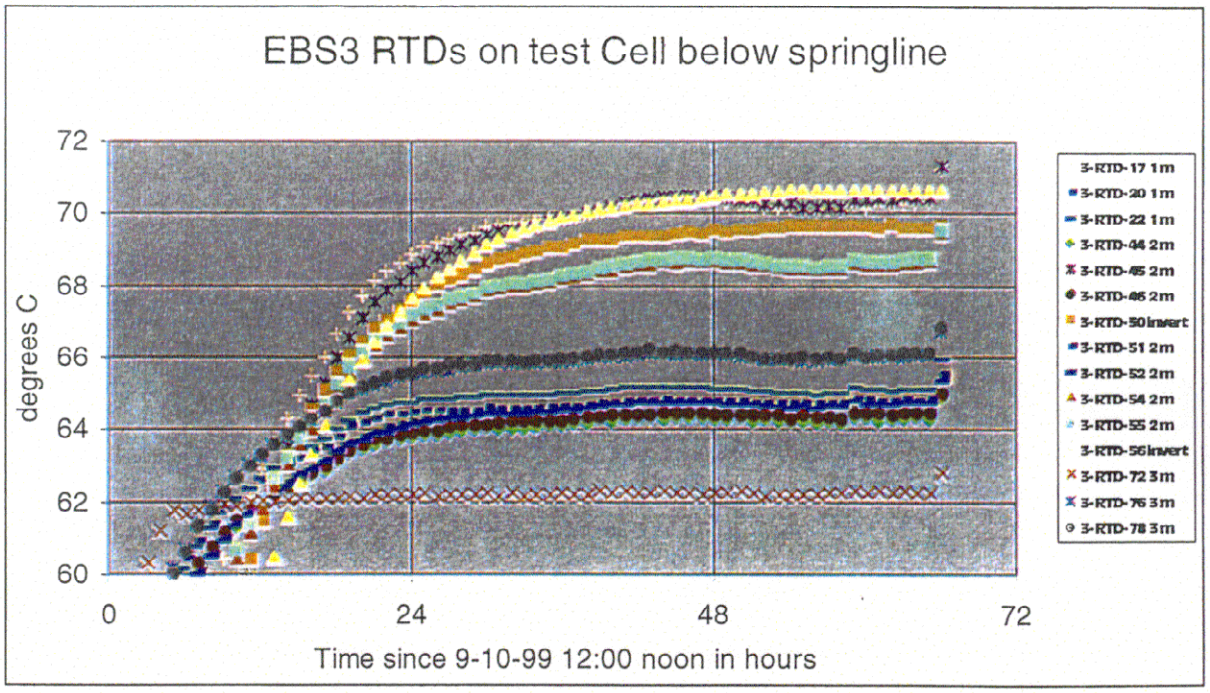
Preliminary Data – Not yet qualified to project standards – approximate conversions used from raw data
Power turned on about 11:30 am on 9-10-99



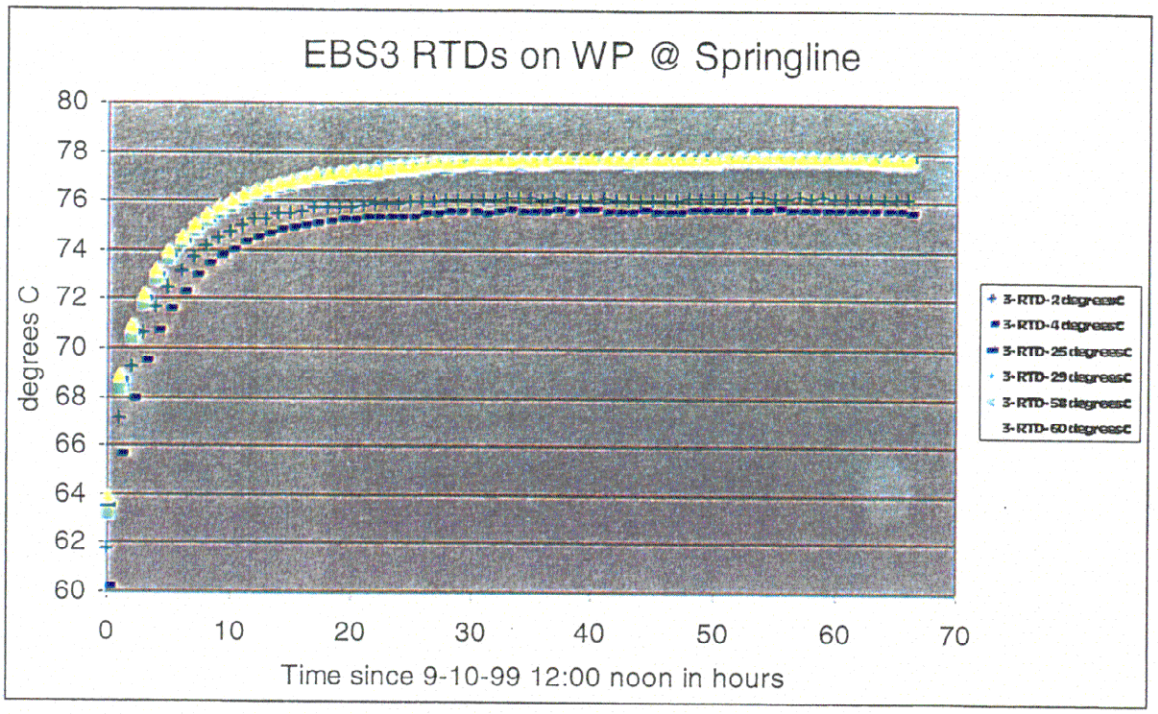


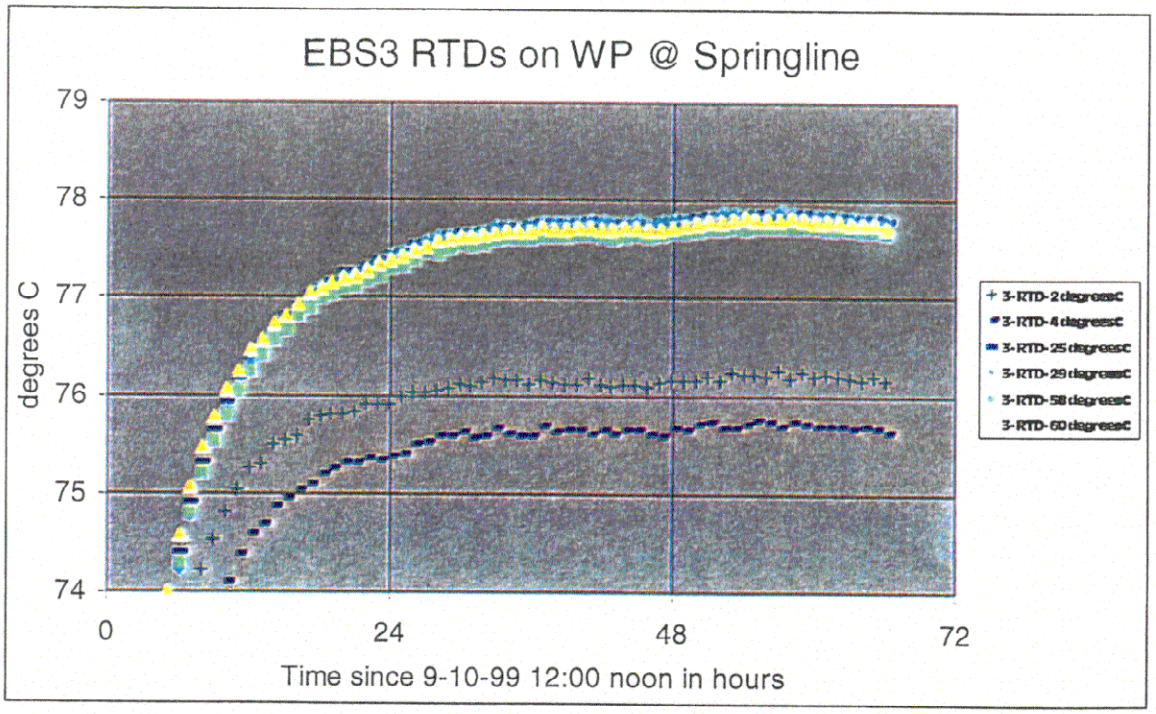
Preliminary Data – Not yet qualified to project standards – approximate conversions used from raw data
Power turned on about 11:30 am on 9-10-99



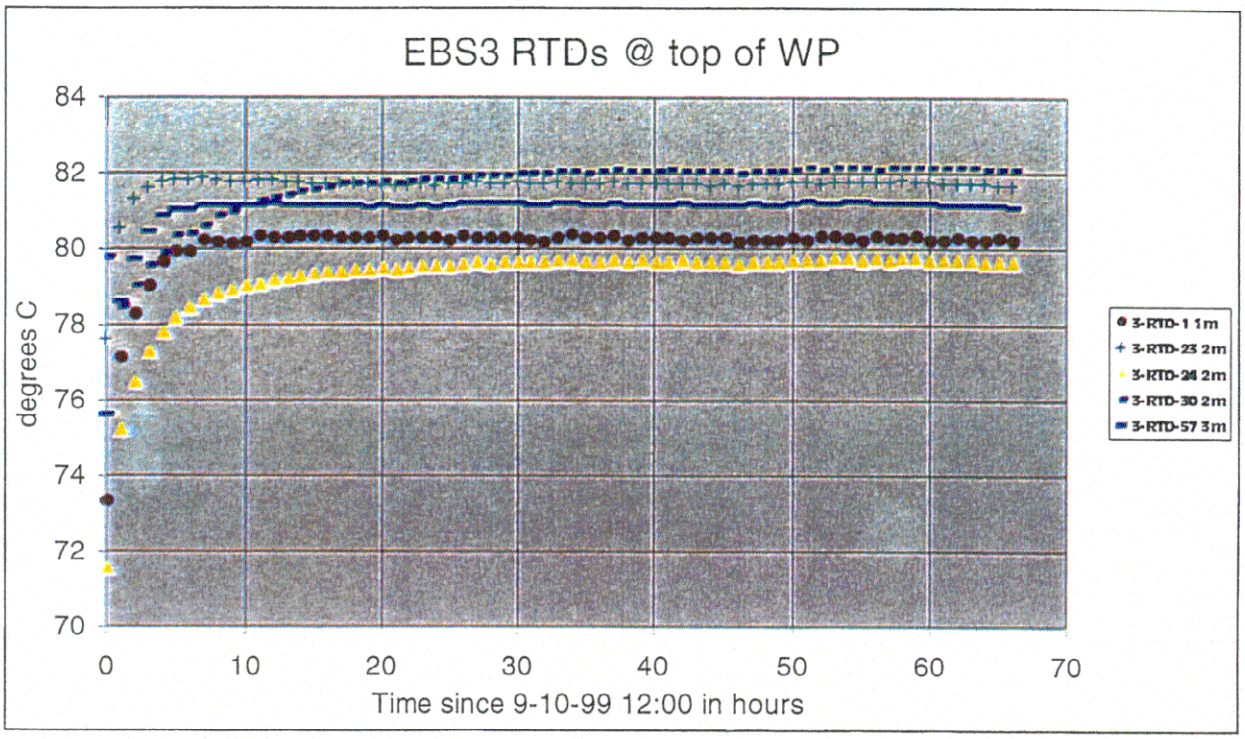


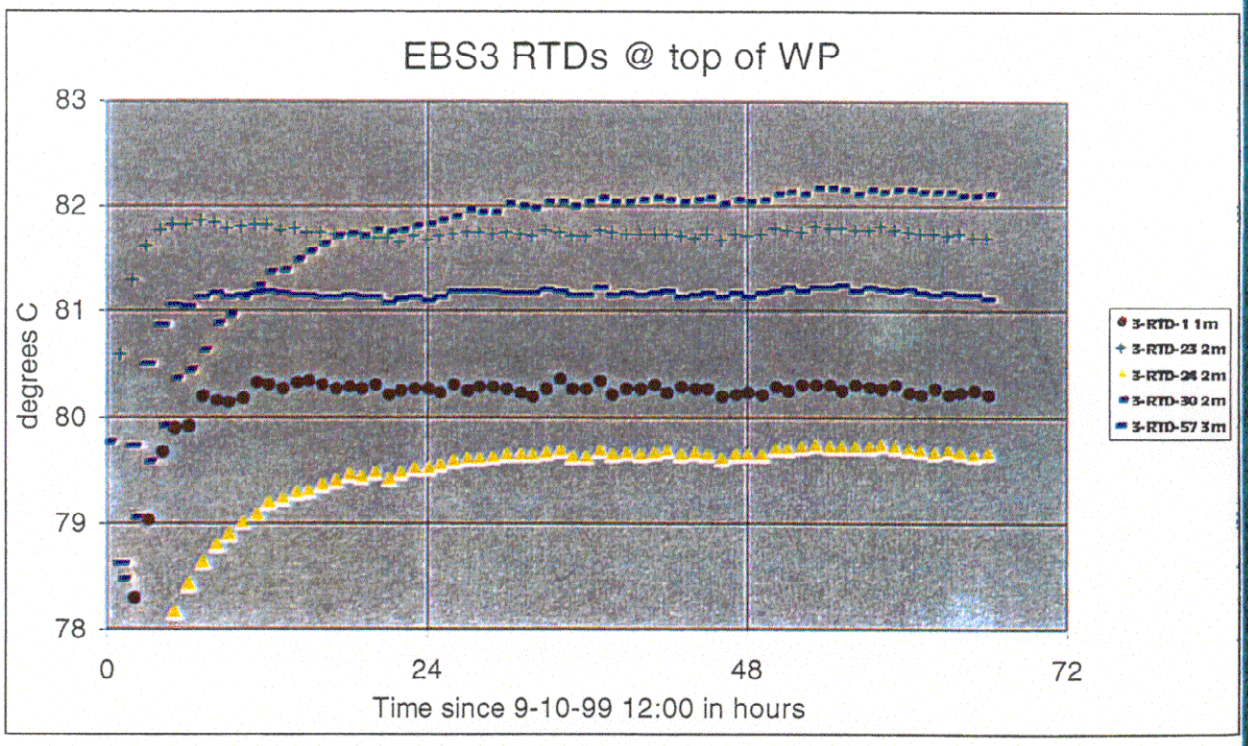
Preliminary Data – Not yet qualified to project standards – approximate conversions used from raw data
Power turned on about 11:30 am on 9-10-99



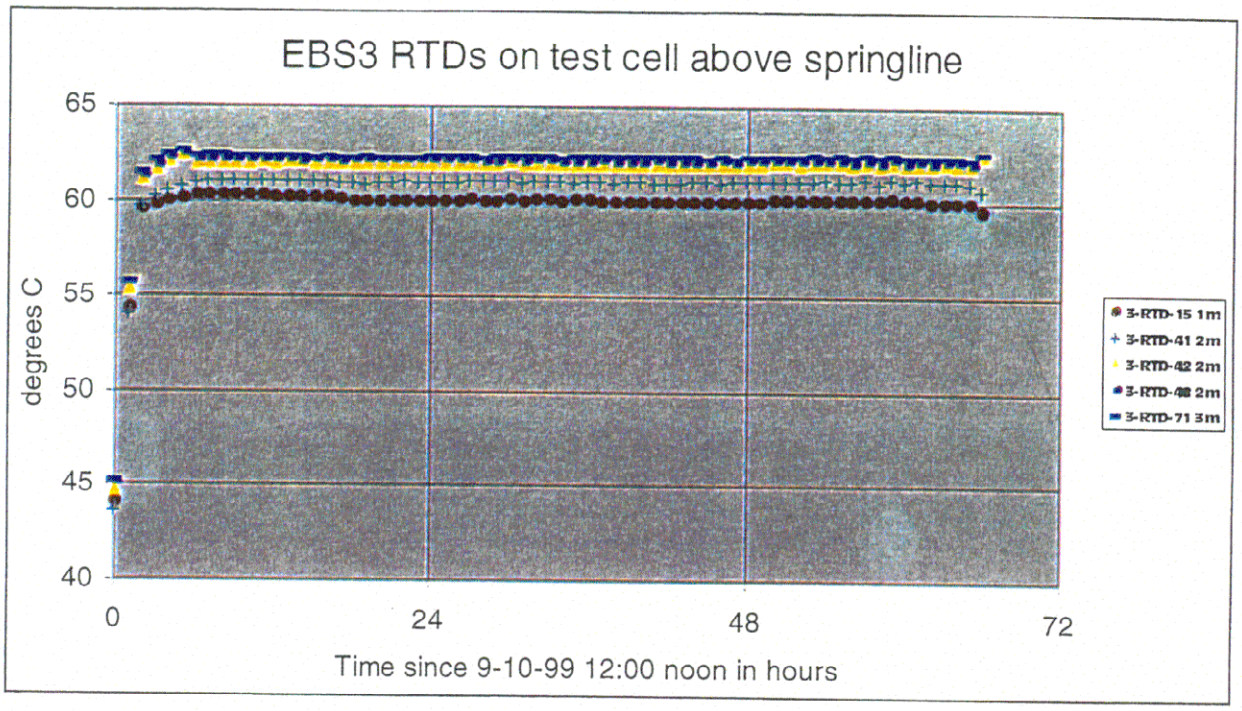


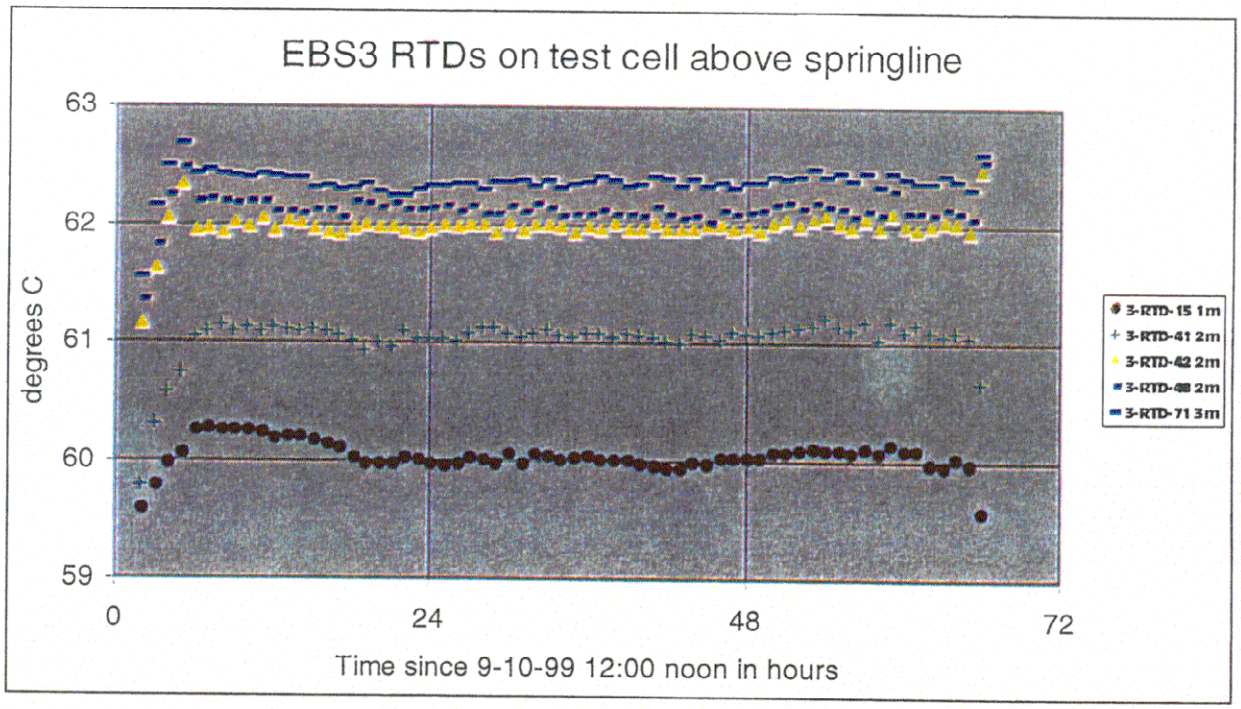
Preliminary Data – Not yet qualified to project standards – approximate conversions used from raw data
Power turned on about 11:30 am on 9-10-99



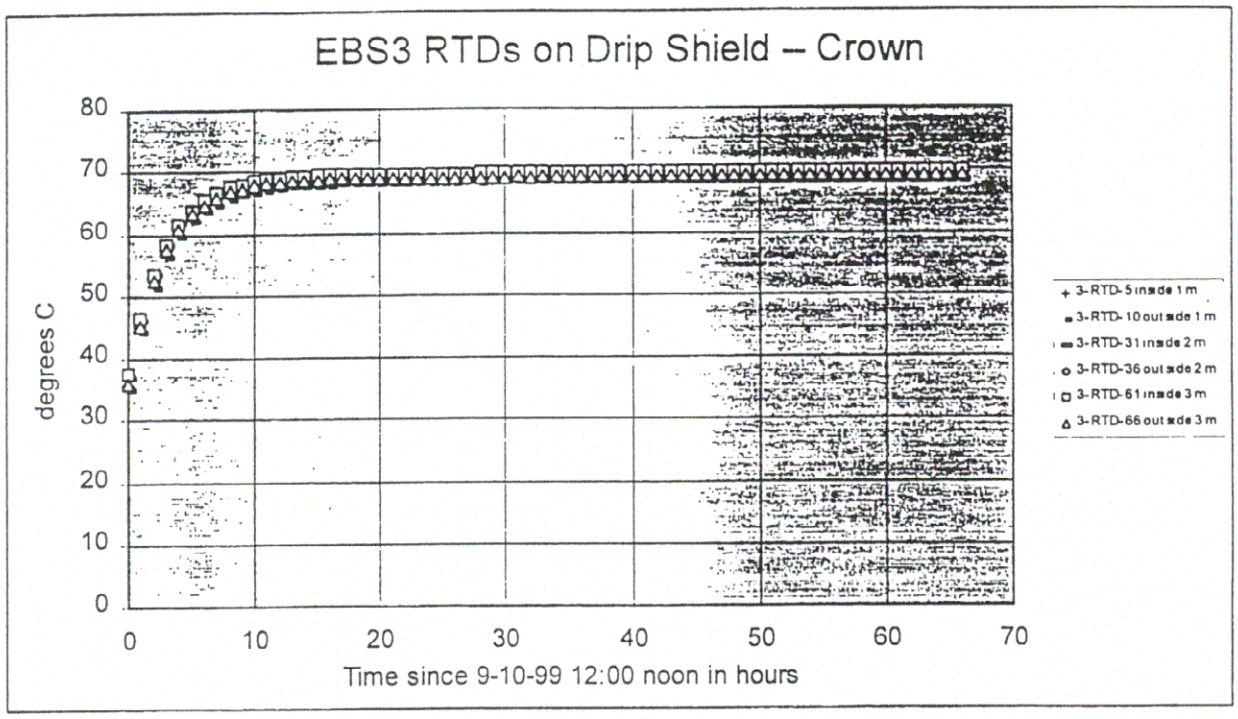


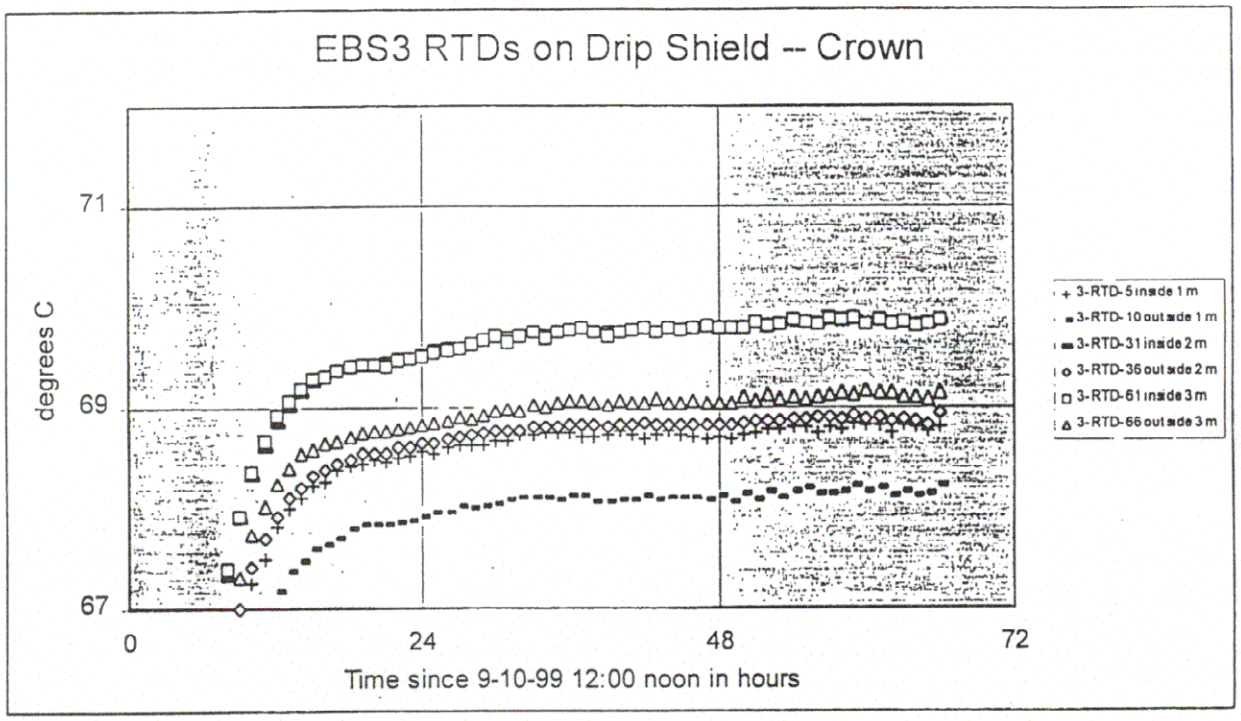
Preliminary Data – Not yet qualified to project standards – approximate conversions used from raw data
Power turned on about 11:30 am on 9-10-99



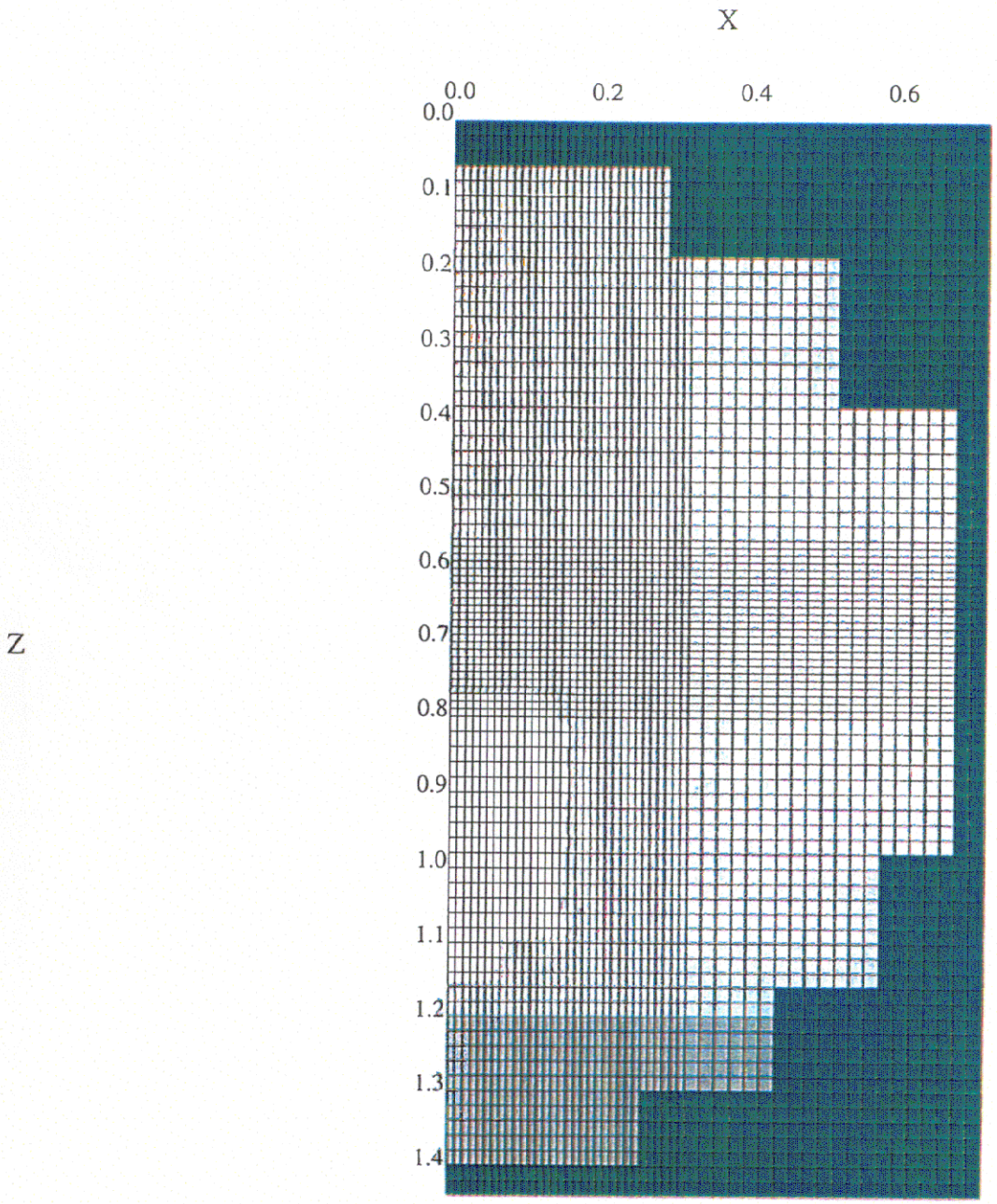


Preliminary Data – Not yet qualified to project standards – approximate conversions used from raw data
Power turned on about 11:30 am on 9-10-99





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

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, ΔT = 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

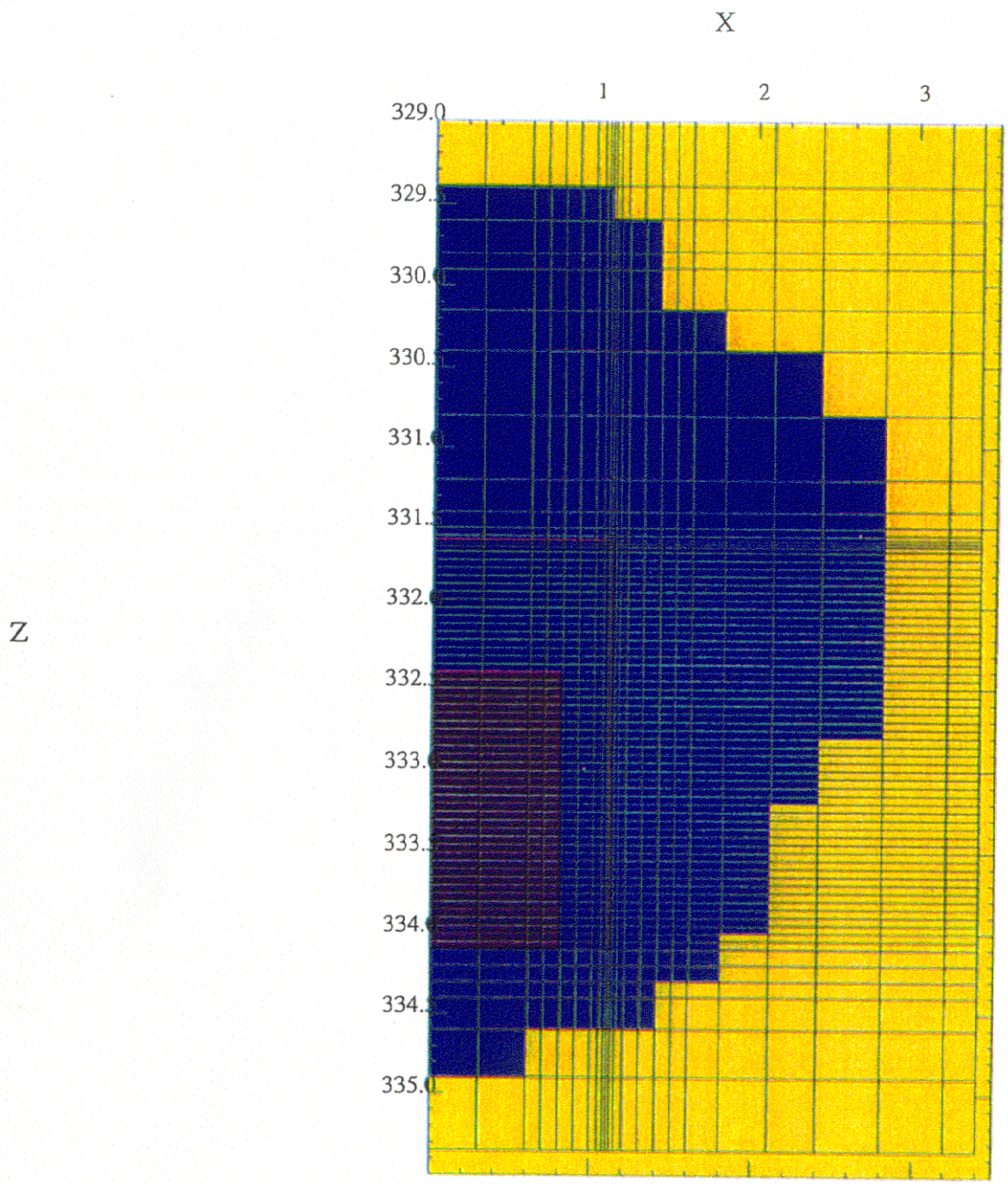
At 334.85 K, air properties are:

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

$Pr = 0.70$

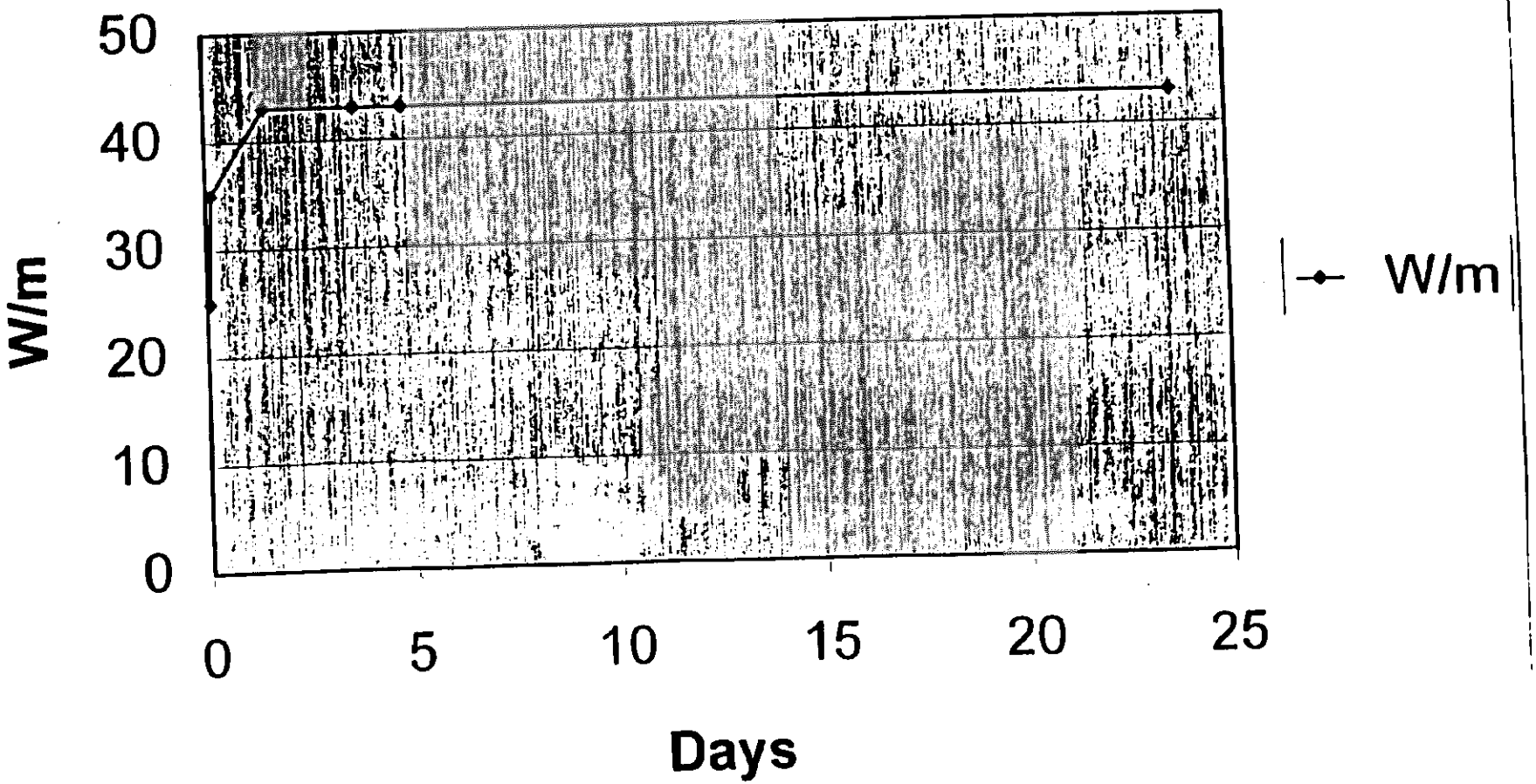
$Ra_L = 3.222E+7$
$Ra_c^* = 3.514E+6$
$k_{eff} = 0.395$

$q' = 17.8$ W/m

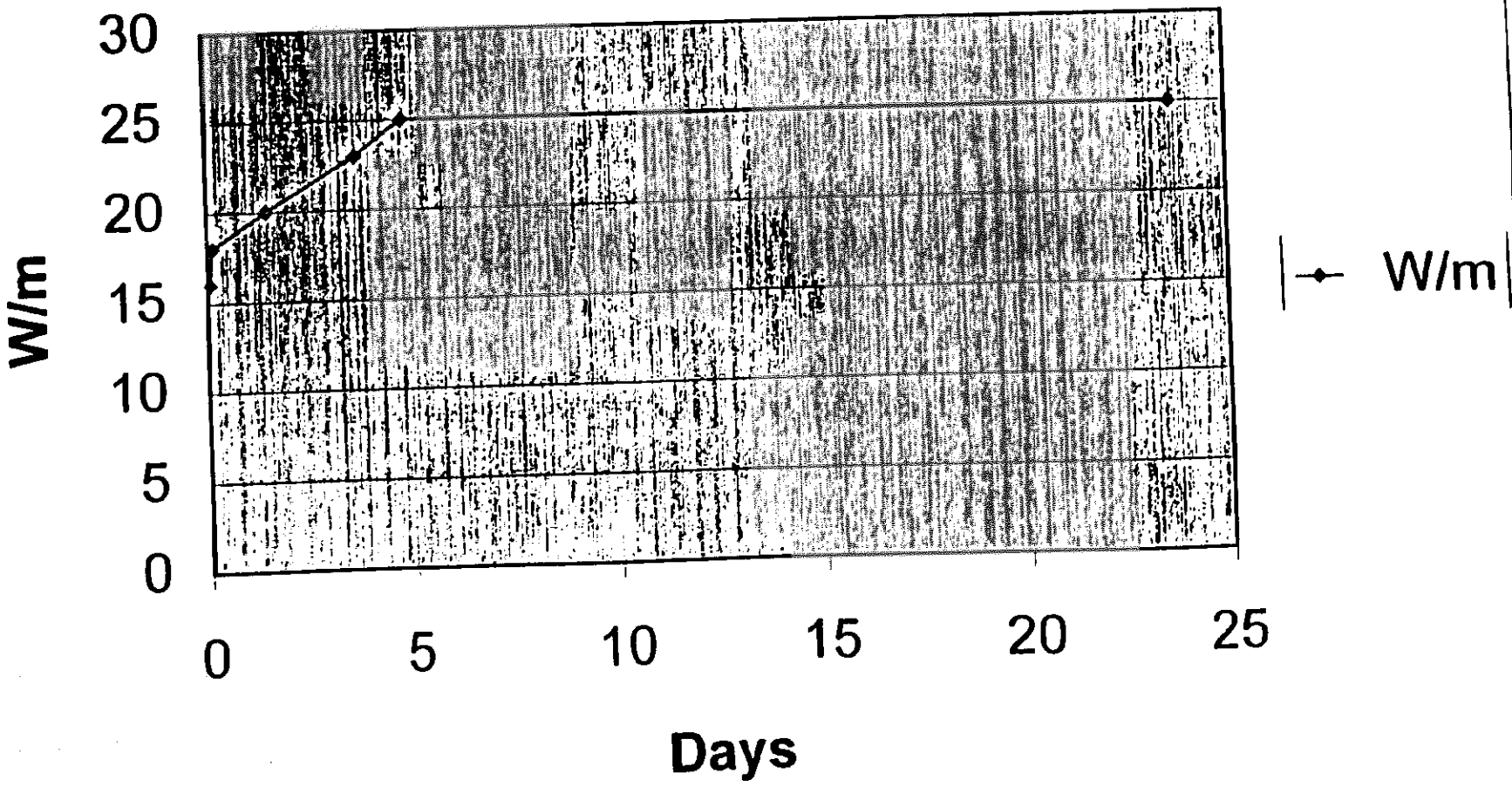


Input file: radymp
Connection file: 2Ddst0.rad

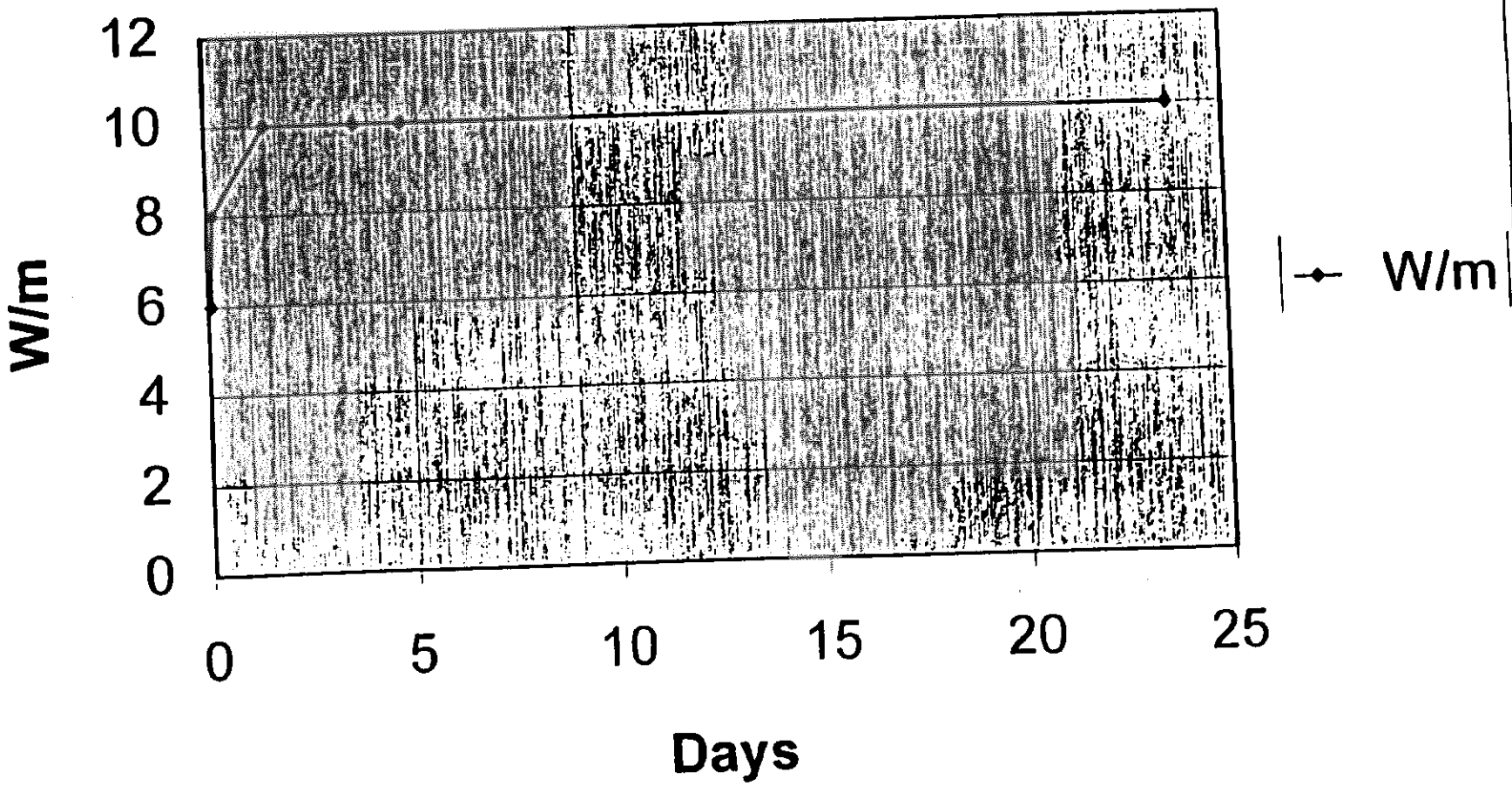
Case 1. Thermal Loading vs. Time



Case 2. Thermal Loading vs. Time



Case 3. Thermal Loading vs. Time



FOURTH EDITION

Fundamentals of Heat and Mass Transfer

FRANK P. INCROPERA
DAVID P. DEWITT
School of Mechanical Engineering
Purdue University

JOHN WILEY & SONS
New York • Chichester • Brisbane • Toronto • Singapore

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aspect ratios Catton [26] suggests that reasonable results may be obtained from a correlation of the form

$$\overline{Nu}_L = \overline{Nu}_L(\tau = 0)\left[\frac{\overline{Nu}_L(\tau = 90)}{\overline{Nu}_L(\tau = 0)}\right]^{\tau/\tau^*}(\sin\tau^*)^{(\tau/4\tau^*)} \qquad \begin{bmatrix} \dfrac{H}{L} \geq 12 \\ 0 < \tau \leq \tau^* \end{bmatrix} \tag{9.55}$$

Beyond the critical tilt angle, the following correlations due to Ayyaswamy and Catton [31] and Arnold et al. [34], respectively, have been recommended [26] for all aspect ratios (H/L):

$$\overline{Nu}_L = \overline{Nu}_L(\tau = 90°)(\sin\tau)^{1/4} \qquad \tau^* < \tau < 90° \tag{9.56}$$

$$\overline{Nu}_L = 1 + [\overline{Nu}_L(\tau = 90°) - 1]\sin\tau \qquad 90° < \tau < 180° \tag{9.57}$$

9.8.2 Concentric Cylinders

Free convection heat transfer in the annular space between *long*, horizontal concentric cylinders (Figure 9.14) has been considered by Raithby and Hollands [37]. Flow in the annular region is characterized by two cells that are symmetric about the vertical midplane. If the inner cylinder is heated and the outer cylinder is cooled ($T_i > T_o$), fluid ascends and descends along the inner and outer cylinders, respectively. If $T_i < T_o$, the cellular flows are reversed. The heat transfer rate per unit length of cylinder (W/m) may be expressed as

$$q' = \frac{2\pi k_{\text{eff}}}{\ln(D_o/D_i)}(T_i - T_o) \tag{9.58}$$

where the *effective thermal conductivity* k_{eff} is the thermal conductivity that a stationary fluid should have to transfer the same amount of heat as the moving fluid. The suggested correlation for k_{eff} is

$$\frac{k_{\text{eff}}}{k} = 0.386\left(\frac{Pr}{0.861 + Pr}\right)^{1/4}(Ra_c^*)^{1/4} \tag{9.59}$$

where

$$Ra_c^* = \frac{[\ln(D_o/D_i)]^4}{L^3(D_i^{-3/5} + D_o^{-3/5})^5}Ra_L \tag{9.60}$$

Equation 9.59 may be used for the range $10^2 \leq Ra_c^* \leq 10^7$. For $Ra_c^* < 100$, $k_{\text{eff}} = k$. A more detailed correlation, which accounts for cylinder eccentricity effects, has been developed by Kuehn and Goldstein [38].

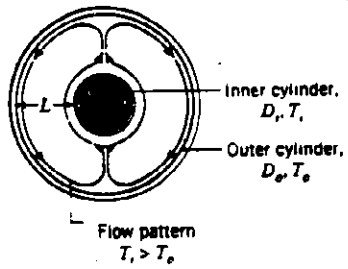

FIGURE 9.14
Free convection flow in the annular space between long, horizontal, concentric cylinders or concentric spheres.

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9.8.3 Concentric Spheres

Raithby and Hollands [37] have also considered free convection heat transfer between concentric spheres (Figure 9.14) and express the total heat transfer rate as

$$q = k_{\text{eff}}\pi\left(\frac{D_i D_o}{L}\right)(T_i - T_o) \tag{9.61}$$

The effective thermal conductivity is

$$\frac{k_{\text{eff}}}{k} = 0.74\left(\frac{Pr}{0.861 + Pr}\right)^{1/4}(Ra_s^*)^{1/4} \tag{9.62}$$

where

$$Ra_s^* = \left[\frac{L}{(D_o D_i)^4}\frac{Ra_L}{(D_i^{-7/5} + D_o^{-7/5})^5}\right] \tag{9.63}$$

The result may be used to a reasonable approximation for $10^2 \le Ra_s^* \le 10^4$.

EXAMPLE 9.5

A long tube of 0.1-m diameter is maintained at 120°C by passing steam through its interior. A radiation shield is installed concentric to the tube with an air gap of 10 mm. If the shield is at 35°C, estimate the heat transfer by free convection from the tube per unit length. What is the heat loss if the space between the tube and the shield is filled with glass-fiber blanket insulation?

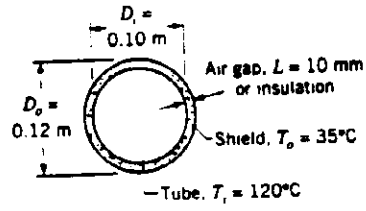
SOLUTION

Known: Temperatures and diameters of a steam tube and a concentric radiation shield.

Find:

1. Heat loss per unit length of tube.
2. Heat loss if air space is filled with glass-fiber blanket insulation.

Schematic:



Assumptions:

1. Radiation heat transfer may be neglected.
2. Contact resistance with insulation is negligible.

IV-91

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Known: Temperatures and diameters of a steam tube and a concentric radiation shield.

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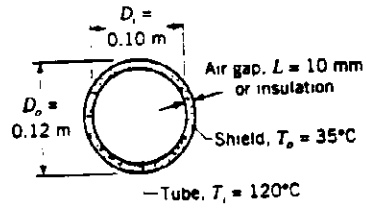

Assumptions:

1. Radiation heat transfer may be neglected.
2. Contact resistance with insulation is negligible.

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Properties: Table A.4, air [$T = (T_i - T_o)/2 = 350$ K]: $k = 0.030$ W/m · K, $\nu = 20.92 \times 10^{-6}$ m²/s, $\alpha = 29.9 \times 10^{-6}$ m²/s, $Pr = 0.70$, $\beta = 0.00285$ K⁻¹. Table A.3, insulation, glass-fiber ($T \approx 300$ K): $k = 0.038$ W/m · K.

Analysis:

1. From Equation 9.58 the heat loss by free convection is

$$q' = \frac{2\pi k_{\text{eff}}}{\ln (D_o/D_i)} (T_i - T_o)$$

where k_{eff} may be obtained from Equations 9.59 and 9.60. With

$$Ra_L = \frac{g\beta(T_i - T_o)L^3}{\nu\alpha}$$

$$Ra_L = \frac{9.8 \text{ m/s}^2 \times 0.00285 \text{ K}^{-1} \times (120 - 35)^\circ\text{C} \, (0.01 \text{ m})^3}{20.92 \times 10^{-6} \text{ m}^2/\text{s} \times 29.9 \times 10^{-6} \text{ m}^2/\text{s}} = 3795$$

it follows that

$$Ra_c^* = \frac{[\ln (D_o/D_i)]^4 Ra_L}{L^3(D_i^{-3/5} + D_o^{-3/5})^5}$$

$$Ra_c^* = \frac{[\ln (0.12 \text{ m}/0.10 \text{ m})]^4 (3795)}{(0.01 \text{ m})^3[(0.10 \text{ m})^{-3/5} + (0.12 \text{ m})^{-3/5}]^5} = 171$$

Hence

$$\frac{k_{\text{eff}}}{k} = 0.386 \left(\frac{Pr}{0.861 + Pr}\right)^{1/4} (Ra_c^*)^{1/4}$$

$$\frac{k_{\text{eff}}}{k} = 0.386 \left(\frac{0.70}{0.861 + 0.70}\right)^{1/4} (171)^{1/4} = 1.14$$

The effective thermal conductivity is then

$$k_{\text{eff}} = 1.14(0.030 \text{ W/m} \cdot \text{K}) = 0.0343 \text{ W/m} \cdot \text{K}$$

and the heat loss is

$$q' = \frac{2\pi(0.0343 \text{ W/m} \cdot \text{K})}{\ln (0.12 \text{ m}/0.10 \text{ m})} (120 - 35)^\circ\text{C} = 100 \text{ W/m}$$

2. With insulation in the space between the tube and the shield, heat loss is conduction and from Equation 3.27

$$q' = \frac{2\pi k(T_i - T_o)}{\ln (D_o/D_i)}$$

$$q' = \frac{2\pi(0.038 \text{ W/m} \cdot \text{K})}{\ln (0.12 \text{ m}/0.10 \text{ m})} (120 - 35)^\circ\text{C} = 111 \text{ W/m}$$

Comments: Although there is slightly more heat loss by conduction thro the insulation than by free convection across the air space, the total heat

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across the air space may exceed that through the insulation because of the effects of radiation. The heat loss due to radiation may be minimized by using a radiation shield of low emissivity, and the means for calculating the loss will be developed in Chapter 13.

9.9 Combined Free and Forced Convection

In dealing with forced convection (Chapters 6 to 8), we ignored the effects of free convection. This was, of course, an assumption; for, as we now know, free convection is likely when there is an unstable temperature gradient. Similarly, in the preceding sections of this chapter, we assumed that forced convection was negligible. It is now time to acknowledge that situations may arise for which free and forced convection effects are comparable, in which case it is inappropriate to neglect either process. In Section 9.3 we indicated that free convection is negligible if $(Gr_L/Re_L^2) \ll 1$ and that forced convection is negligible if $(Gr_L/Re_L^2) \gg 1$. Hence the *combined free* and *forced* (or *mixed*) *convection* regime is generally one for which $(Gr_L/Re_L^2) \approx 1$.

The effect of buoyancy on heat transfer in a forced flow is strongly influenced by the direction of the buoyancy force relative to that of the flow. Three special cases that have been studied extensively correspond to buoyancy-induced and forced motions having the same direction (*assisting* flow), opposite directions (*opposing* flow), and perpendicular directions (*transverse* flow). Upward and downward forced motions over a heated vertical plate are examples of assisting and opposing flows, respectively. Examples of transverse flow include horizontal motion over a heated cylinder, sphere, or horizontal plate. In assisting and transverse flows, buoyancy acts to enhance the rate of heat transfer associated with pure forced convection; in opposing flows, it acts to decrease this rate.

It has become common practice to correlate mixed convection heat transfer results for external and internal flows by an expression of the form

$$Nu^n = Nu_F^n \pm Nu_N^n \tag{9.64}$$

For the specific geometry of interest, the Nusselt numbers Nu_F and Nu_N are determined from existing correlations for pure forced and natural (free) convection, respectively. The plus sign on the right-hand side of Equation 9.64 applies for assisting and transverse flows, while the minus sign applies for opposing flow. The best correlation of data is often obtained for $n = 3$, although values of $\frac{7}{2}$ and 4 may be better suited for transverse flows involving horizontal plates and cylinders (or spheres), respectively.

Equation 9.64 should be viewed as a first approximation, and any serious treatment of a mixed convection problem should be accompanied by an examination of the open literature. Mixed convection flows received considerable attention in the late 1970s to middle 1980s, and comprehensive literature reviews are available [39–42]. The flows are endowed with a variety of rich and un-

TABLE A.4 Thermophysical Properties of Gases at Atmospheric Pressure[a]

T (K)	ρ (kg/m³)	c_p (kJ/kg · K)	$\mu \cdot 10^7$ (N · s/m²)	$\nu \cdot 10^6$ (m²/s)	$k \cdot 10^3$ (W/m · K)	$\alpha \cdot 10^6$ (m²/s)	Pr
Air							
100	3.5562	1.032	71.1	2.00	9.34	2.54	0.786
150	2.3364	1.012	103.4	4.426	13.8	5.84	0.758
200	1.7458	1.007	132.5	7.590	18.1	10.3	0.737
250	1.3947	1.006	159.6	11.44	22.3	15.9	0.720
300	1.1614	1.007	184.6	15.89	26.3	22.5	0.707
350	0.9950	1.009	208.2	20.92	30.0	29.9	0.700
400	0.8711	1.014	230.1	26.41	33.8	38.3	0.690
450	0.7740	1.021	250.7	32.39	37.3	47.2	0.686
500	0.6964	1.030	270.1	38.79	40.7	56.7	0.684
550	0.6329	1.040	288.4	45.57	43.9	66.7	0.683
600	0.5804	1.051	305.8	52.69	46.9	76.9	0.685
650	0.5356	1.063	322.5	60.21	49.7	87.3	0.690
700	0.4975	1.075	338.8	68.10	52.4	98.0	0.695
750	0.4643	1.087	354.6	76.37	54.9	109	0.702
800	0.4354	1.099	369.8	84.93	57.3	120	0.709
850	0.4097	1.110	384.3	93.80	59.6	131	0.716
900	0.3868	1.121	398.1	102.9	62.0	143	0.720
950	0.3666	1.131	411.3	112.2	64.3	155	0.723
1000	0.3482	1.141	424.4	121.9	66.7	168	0.726
1100	0.3166	1.159	449.0	141.8	71.5	195	0.728
1200	0.2902	1.175	473.0	162.9	76.3	224	0.728
1300	0.2679	1.189	496.0	185.1	82	238	0.719
1400	0.2488	1.207	530	213	91	303	0.703
1500	0.2322	1.230	557	240	100	350	0.685
1600	0.2177	1.248	584	268	106	390	0.688
1700	0.2049	1.267	611	298	113	435	0.685
1800	0.1935	1.286	637	329	120	482	0.683
1900	0.1833	1.307	663	362	128	534	0.677
2000	0.1741	1.337	689	396	137	589	0.672
2100	0.1658	1.372	715	431	147	646	0.667
2200	0.1582	1.417	740	468	160	714	0.655
2300	0.1513	1.478	766	506	175	783	0.647
2400	0.1448	1.558	792	547	196	869	0.630
2500	0.1389	1.665	818	589	222	960	0.613
3000	0.1135	2.726	955	841	486	1570	0.536
Ammonia (NH_3)							
300	0.6894	2.158	101.5	14.7	24.7	16.6	0.887
320	0.6448	2.170	109	16.9	27.2	19.4	0.870
340	0.6059	2.192	116.5	19.2	29.3	22.1	0.872
360	0.5716	2.221	124	21.7	31.6	24.9	0.872
380	0.5410	2.254	131	24.2	34.0	27.9	0.869

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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 (same as results99) – output radiation file from radymp and radymp.con used as input to NUFT. (Note: File "results99" exists in the Sun workstation and during transfer to a PC, the filename is changed to results9.9 – only maximum of 8 characters allowed in filename before the extension)

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
ddsr2 (ddymp2DdsR2)	Initialization Run with Infiltration Rate = 35 mm/yr
ddsr2b (ddymp2DdsR2b)	Initialization Run with Infiltration Rate = 68 mm/yr
ds2r22 (ymp2Dds2R22)	Production Run with Infiltration Rate = 35 mm/yr and 100% heat removal in the first 50 yr ; emissivity = 0.87
ds2r23 (ymp2Dds2R23)	Production Run with Infiltration Rate = 35 mm/yr and 100% heat removal in the first 100 yr ; emissivity = 0.87
ds2r23a (ymp2Dds2R23a)	Same as ymp2Dds2R23 or ds2r23 except in addition, outputs Vapor and Liquid Fluxes ; emissivity = 0.87
ds2r23b (ymp2Dds2R23b)	Production Run with Infiltration Rate = 68 mm/yr and 100% heat removal in the first 100 yr ; emissivity = 0.87
ds2r23c (ymp2Dds2R23c)	Same as ymp2Dds2R23a or ds2r23a except emissivity = 0.70

Note: Filenames in parenthesis are used in Sun workstation. These names are changed when transferred to a PC.

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
ddsr2.ext (ddymp2DdsR2.ext)	Output from ddymp2DdsR2
ddsr2b.ext (ddymp2DdsR2b.ext)	Output from ddymp2DdsR2b
ds2r22.ext (ymp2Dds2R22.ext)	Output from ymp2Dds2R22
ds2r23.ext (ymp2Dds2R23.ext)	Output from ymp2Dds2R23
ds2r23a.ext (ymp2Dds2R23a.ext)	Output from ymp2Dds2R23a
ds2r23b.ext (ymp2Dds2R23b.ext)	Output from ymp2Dds2R23b
ds2r23c.ext (ymp2Dds2R23c.ext)	Output from ymp2Dds2R23c
ds2r23a.gid (ymp2Dds2R23a.gid)	Gas Flux from Invert Mat. to Air Gap underneath the Drip Shield (from ymp2Dds2R23a).
ds2r23a.lid (ymp2Dds2R23a.lid)	Liquid Flux from Invert Mat. to Air Gap underneath the Drip Shield (from ymp2Dds2R23a).
ds2r23a.lti (ymp2Dds2R23a.lti)	Liquid Flux from Host Rock to Invert Mat. (from ymp2Dds2R23a).
ds2r23a.gti (ymp2Dds2R23a.gti)	Gas Flux from Host Rock to Invert Mat. (from ymp2Dds2R23a).
ds2r23a.lbi (ymp2Dds2R23a.lbi)	Liquid Flux from Backfill to Invert Mat. (from ymp2Dds2R23a).
ds2r23a.gbi (ymp2Dds2R23a.gbi)	Gas Flux from Backfill to Invert Mat. (from ymp2Dds2R23a).
ds2r23a.ltb (ymp2Dds2R23a.ltb)	Liquid Flux from Host Rock to Backfill (from ymp2Dds2R23a).
ds2r23a.gtb (ymp2Dds2R23a.gtb)	Gas Flux from Host Rock to Backfill (from ymp2Dds2R23a).

Note: Filenames in parenthesis are used in Sun workstation. These names are changed when transferred to a PC.