EVALUATION OF A THERMAL ANALYSIS MODEL FOR THE ENGINEERED BARRIER SYSTEM PERFORMANCE ASSESSMENT CODE

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INTRODUCTION

The Center for Nuclear Waste Regulatory Analyses (Center) contracted Systems Support, Inc. (SSI) in 1989 to survey available thermal analysis codes that could be used to support the Engineered Barrier System Performance Assessment Code (EBSPAC) development. Also, SSI was to recommend at least one candidate thermal analysis code for the Center to obtain and consider for integration into the EBSPAC.

While conducting the thermal model survey, SSI reviewed more than twenty-nine thermal model computer codes. Most of the surveyed thermal codes were formulated using the finite element or the finite difference numerical methodology; however, three of the codes use analytical solutions to calculate the temperature distributions. The final code selection was based on the overall capability, availability, and utility of the code [Ref. 1]. For completeness, a copy of the SSI report is included at the end of this document as Appendix A.

SSI recommended TOPAZ3D [Ref. 1] as the preferred candidate thermal analysis code. TOPAZ3D has three ancillary codes--INGRID, FACET, and TAURUS. INGRID can be used as a mesh generator and a data input generator for TOPAZ3D. FACET can be used as a view factor calculator for TOPAZ3D when radiative heat transfer is considered. TAURUS can be used for graphical display of TOPAZ3D analysis results and various geometry plots. Subsequent to the SSI recommendation, TOPAZ3D and its ancillary codes were obtained by SSI and transferred to the Center. SSI was also contracted to run sample problems for each code and to debug the sample problems/codes as needed for proper execution of the given data. However, to date SSI has had problems in getting TOPAZ3D to execute on the IBM system at NIH. A change of scope in SSI work is planned. This effort will be directed toward providing support in developing a data/analysis package for TOPAZ3D. The Center has initiated the task of identifying the conditions under which TOPAZ3D can be incorporated into EBSPAC.

The purpose of this report is to present the Center-generated results from its TOPAZ3D thermal code checkout analysis. The objective of the thermal code checkout analysis was to exercise certain portions of the TOPAZ3D code and to ascertain the ease of use and the suitability of the TOPAZ3D thermal modelling/analysis capabilities for inclusion into EBSPAC. The following report contains results from the TOPAZ3D thermal code checkout, a discussion of some thermal modelling considerations for TOPAZ3D-based analyses of the canister and near-rock region, and a discussion of how TOPAZ3D may be integrated into EBSPAC.

Review of TOPAZ3D

Computer Code Capabilities

TOPAZ3D [Ref. 2] is a three-dimensional implicit finite element computer code for heat transfer analysis. It can be used to analyze steady state and

transient problems with or without phase change. The computer code allows one to specify the material properties as constants or as temperature dependent values with isotropic or orthotropic material behavior. Problems with temperature, flux, convection and radiation boundary conditions may be analyzed. The applied boundary conditions may be specified as time dependent or temperature dependent functions incorporated in the analysis through the input data stream or through a user supplied subroutine. A specified condition that is a function of time or temperature can be described by either a piecewise linear curve or by a functional relationship defined in a user subprogram. Functions that are dependent upon both time and temperature must be defined by a user subprogram. The user supplied subroutine will also allow one to model chemical reaction kinetics and internal heat generation.

Computer Code Problems

TOPAZ3D is a powerful analytical tool which has many desirable features for EBS modelling. However, the version provided to the Center has a few discrepancies between the documentation and the program operation. The two major discrepancies found to date by the Center are listed below.

1. In specifying the material type on the material property data card No. 1, the manual defines the following material type codes:

   CODE = 1: isotropic material-define only K_1
   CODE = 2: isotropic temperature dependent
   CODE = 3: orthotropic-define K_1, K_2, and K_3
   CODE = 4: orthotropic temperature dependent.

   However, in the software the following material type codes are defined:

   CODE = 2: orthotropic-define K_1, K_2, K_3
   CODE = 3: isotropic temperature dependent.

   The correct material code definitions, shown above as the second set, were determined by closely examining the appropriate subroutines from a computer printout of the TOPAZ3D source code.

2. When one wants to import FACET-generated view factors into TOPAZ3D, one must place the numeral 3 in column 25 of the first TOPAZ3D control card. The August, 1985, TOPAZ3D manual indicates that this column is to be skipped. This fix was revealed only after a detailed discussion with Mr. Arthur B. Shapiro (TOPAZ3D developer) who provided the information necessary to solve this TOPAZ3D view factor import problem. The TOPAZ3D user's manual, provided to the Center by SSI, is dated August, 1985; perhaps the two discrepancies mentioned here have been corrected in an updated TOPAZ3D document.

Subsequent to completing the analysis, it was determined that the July, 1986, revision of the TOPAZ2D manual has the two discrepancies mentioned above defined correctly. TOPAZ2D requires the same input stream as TOPAZ3D.

Thermal Model Example Problem

This example analysis was designed to ascertain the suitability of the TOPAZ3D thermal code for inclusion into EBSPAC. The wall thickness of the waste package canister and the width of the air gap were chosen at the extremes of the design specifications [Refs. 3, 4] for these parameters in order to gain as much insight as possible into the behavior of the heat transfer mechanisms.

Half of a planar cross section through a single waste package, represented here as a section of a metal canister, and its surrounding features are shown schematically in Figure 1. The modelled canister has a radius of 33 cm. (12.99 in.), a uniform wall thickness of 3.0 cm. (1.18 in.), and a length of 460 cm. (181.1 in.). The 5.0 cm. (1.97 in.) gap between the canister and the rock medium is assumed uniform and air filled. The thermophysical properties for 304 stainless steel (Table 1) are used for the canister, while the thermophysical properties shown in Table 2 are used for the rock medium. The conductivity of steel is assumed to vary linearly between 100°C and 500°C. The nearest endpoint conductivity value is used for temperatures outside of this range where referenced data are not provided. The rock medium is assumed lithologically uniform and isotropic. All thermophysical properties are allowed to vary with temperature. No material phase change is considered in this example problem.

Analysis Model Definition

TOPAZ3D is a 3-dimensional heat transfer analysis computer code with an element library composed of 3-D solid elements. In order to simplify the analysis and to cut down on computer time, a subregion of the canister and the rock medium was modelled. The TOPAZ3D brick element was used to develop a finite element model of a subregion of the canister and 1 meter (3.28 ft.) of the rock medium. As measured from the center line of the canister, the subregion model subtends a 15 degree arc in the circumferential direction (Figure 2), extends 2.54 cm. (1.0 in.) in the axial direction and 1.41 meters (4.625 ft.) in the radial direction. The finite element model has 310 elements and 1248 nodes. In developing the above model, it is assumed that the temperature of the canister does not vary circumferentially or axially. The temperature is only allowed to vary in the radial direction from the inner canister surface outward.

Model Boundary Conditions

Three different test cases were developed and executed. All test cases allowed conductive heat transfer in the canister material and in the rock medium. The far field boundary of the rock (x=1.41 m.) is assumed insulated. The remaining boundary conditions for each test case are listed below.

1. The first test case accommodates heat flux input on the inner surface of the canister and radiative heat transfer between the canister and the rock medium.

2. The second test case uses temperature boundary conditions on the canister inner surface and radiative heat transfer between the canister and the rock medium.

3. The third test case is the same as the second test case with the exception that radiative and convective heat transfer is allowed between the canister and the rock medium.

Boundaries other than those specified above are considered insulated.

Limitations of Boundary Condition Modelling

In TOPAZ3D, the radiation model and the convection model have a constraint on how T_∞ in the temperature potential ($T - T_\infty$) can be defined. The T_∞ can be defined as a constant temperature or as a temperature which varies as a known function of time. However, in actuality, the T_∞ is not a known function of time and it is not a constant. Hence, the best way to analyze the actual problem using TOPAZ3D is through the user supplied subroutine. This capability allows one to prescribe the desired behavior of T_∞ as a function of time or temperature or both. Since implementing this capability requires time to code and test a subroutine and because the purpose of this analysis is to ascertain the suitability of TOPAZ3D for inclusion into EBSPAC and not develop thermal models, the user's supplied subroutine was not used in this analysis. It was decided that the radiation and the convection capabilities of TOPAZ3D can be ascertained by defining T_∞ as a constant. Even though this modelling approach limits the ability to completely describe the heat exchange between the canister and rock medium, it does allow one to examine the importance of certain heat exchange mechanisms.

Boundary Values and Initial Conditions

For the purpose of this analysis, the initial temperature of the canister metal is 148.9°C (300°F) and the initial temperature of the rock is 18.3°C (65°F). In the first test case, the heat flux applied to the canister inner surface is taken to be 322.8 W/m^2 (102.33 Btu/hr ft^2). The second and third test cases have a temperature boundary condition of 204.4°C (400°F) applied to the inner surface of the canister. On the boundaries (canister outer surface and bore hole wall) where radiative heat transfer is allowed, the emissivity of the steel was taken as 0.62 for temperatures up to 215.6°C (420°F) and was allowed to vary up to a value of 0.73 at 526.7°C (980°F). The emissivity of the rock was taken as 0.73 at a temperature of 15.6°C (60°F) and varied linearly to a value of 0.60 at a temperature of 626.7°C (1160°F). The emissivities for the rock are estimates based upon the behavior of emissivities of most nonmetals [Ref. 5]. In the third test case where convective heat transfer was also allowed, the transfer surfaces were modelled as vertical planes with free convection and laminar flow. The simplified equation for air [Ref. 6]:

$$h = 1.42(dt/L)^{0.25}\ W/m^2 \cdot C$$

or

$$h = 0.29(dt/L)^{0.25}\ Btu/hr\ ft^2 \cdot F,$$

was used to calculate these film coefficients. For the radiative and the convective boundary surfaces, the T_∞ is set equal to 148.9°C (300°F).

Analysis Results

Tabulated results of the thermal code check cases are presented in Tables 3, 4, and 5. These tables present transient and steady state temperature results for the modelled canister and the near rock region.

Table 3 shows the calculated results for the first test case which has heat flux on the inner surface of the canister and radiative heat transfer between the canister and the rock bore hole wall. The transient results are also shown in Figure 3. The initial conditions for this problem might crudely simulate the emplacement of a hot canister into an unheated bore hole. The temperature calculations show that the bore hole wall is heating up faster than the canister surface over the 0.03 hrs. of analysis simulated heat-up time. Also, at no time during this transient did the temperature gradient through the wall of the canister exceed 0.6°C (1°F). This small temperature gradient is due to the low rate of heat input by the heat flux applied at the canister inner surface. The steady state temperature gradient from the bore hole wall to 1 m. into the rock is 2.8°C (5.0°F). At these steady-state conditions, there is a 43.9°C (79°F) temperature drop across the air gap from the canister to the rock bore hole wall.

Table 4 shows the calculated results for the second test case which has a 204.4°C (400°F) temperature boundary condition applied to the inner surface of the canister and radiative heat transfer between the canister outer surface and the bore hole wall. This boundary condition imposes a 55.5°C (98.9°F) temperature gradient through the canister wall at the first time step. However, over the simulation time of 0.03 hours, the canister begins to heat up more uniformly and the temperature gradient through the canister wall drops to 21.1°C (38°F). Figure 4 shows the transient results. At steady state, the temperature gradient through the canister wall is 0.83°C (1.5°F) and the temperature drop across the air gap (from the canister outer surface to the bore hole wall) is calculated to be 63.7°C (114.7°F). This temperature drop across the air gap is larger than in the previous example because of the higher rate of heat input at the canister inner surface and the inability of the heat radiation model at the outer surface to transfer the added heat to the bore hole wall. The calculated steady-state temperature gradient from the bore hole wall to 1 m. into the rock is 2.8°C.

Table 5 shows the calculated results for the third model. The transient results are shown in Figure 5. This model has a 204.4°C (400°F) temperature boundary condition applied to the inner surface of the canister in conjunction with radiative and convective heat transfer between the outer surface of the canister and the bore hole wall. This model calculates the same temperature results for the canister as the previous model. However, with this model, more heat is transferred to the bore hole wall, thereby giving a slightly higher bore hole wall temperature. The steady-state temperature drop across the air gap is calculated to be 60°C (108°F).

Discussion

The analyses results presented above provide insight into the relative importance of certain heat transfer mechanisms on the heat exchange between the canister and the rock. The quality of the predictive model can be improved by better defining the heat transfer mechanisms between these surfaces and by developing for both materials a more complete data set of temperature dependent

emissivities and thermophysical material properties. Since the emissivity of a surface varies with the temperature of the surface, its degree of roughness, and, in metals, the degree of surface oxidation, it is understood that there are large variations possible in the data for each material.

In the above analyses, the model which allows radiative and convective heat transfer between the canister and the bore hole wall has a smaller steady-state temperature drop across the air gap than the model which allows only radiation in the air gap. These results imply that convection is a contributor to the heat transfer between these two surfaces and for completeness it should be included in the thermal analysis. Also, when one considers that for short distances transparent gases such as air may allow heat transfer by conduction, convection, and radiation [Ref. 7]; it follows that a more complete model would also contain conduction.

Strategy for Integration Into EBSPAC

For computational purposes, an EBSPAC simulation can be considered as a combination of modular simulation and cascade simulation. Modular simulation is when a process model is considered independent and needs no interaction with other process models in order to arrive at the needed results. The EBSPAC simulation becomes a cascade simulation when the results of one process module is input to another process module for purposes of recalculating, altering, or updating results previously calculated by the receiving process module. The TOPAZ3D thermal model code can be used for a modular thermal simulation of the waste package, air gap, and the near rock region. The resulting detailed temperature distributions may be input into other EBSPAC process models as an implicit or explicit function of time and do not need to be recalculated each time the receiving process module is activated. It is understood that this approach is conservative and that most processes that affect heat transfer tend to retard the heat transfer rate rather than accelerate it. Hence, recalculating the temperatures are only needed if one wants to model a process which significantly accelerates heat transfer. The timing and logic of the data transfers between these process modules can be controlled by a driver module.

Summary and Conclusions

The TOPAZ3D finite element heat transfer analysis code is a powerful analytical tool which has many positive features and strong points. The code can handle transient and steady-state heat transfer problems with temperature, flux, convection, and radiation boundary conditions. Example problems were developed and run using each of the aforementioned boundary condition types. These boundary conditions were found to be reasonably easy to implement. However, the user's manual is not very detailed and it assumes a level of subject knowledge that a novice user may not have. However, because TOPAZ3D has been benchmarked and verified [Ref. 4] and because the code allows a great deal of flexibility in boundary condition input, it is believed that the TOPAZ3D thermal models are adequate for a robust detailed finite element thermal analysis of the waste package canister and the near rock region.

TOPAZ3D allows the user to apply boundary conditions in functional form through user-supplied subroutines. This capability is an excellent way to implement refinements to the modelling of the heat transfer between the canister

and the bore hole wall without having to modify the basic computer code. This capability should be exploited when developing the thermal models for the EBS.

When complete axisymmetric models of the canister and the near rock region are required, the TOPAZ2D computer code (a 2-D version of TOPAZ3D) should be employed. It allows the modelling of axisymmetric structures without the use of the 3-D brick element required when using TOPAZ3D. This saves modelling time and computer time.

Table 1. 304 STAINLESS STEEL THERMAL PROPERTIES

Temperature		Thermal Conductivity		Specific Heat Capacity	
(°F)	(°C)	(W/mK)	*(Btu/hr ft R)	(J/cm^3K)	+(Btu/Lb R)
65	18.7	5.02	9.4	3.361	0.1025
212	100.3	5.02	9.4	3.712	0.1132
572	300.3	5.82	10.9	4.433	0.1352
932	500.3	6.62	12.4	4.295	0.1310
2012	1100.3	6.62	12.4	4.600	0.1403

Density = 7.833 g/cm^3

NOTE:

* Reference 5, Table A-4.

+ Reference 5, Table A-14: data for nickel.

Table 2. YUCCA MOUNTAIN ROCK THERMAL PROPERTIES

Temperature		Thermal Conductivity		Specific Heat Capacity	
(°F)	(°C)	+(W/mK)	(Btu/hr ft R)	+(J/cm^{3}K)	(Btu/Lb R)
65	18.7	1.80	3.371	2.480	0.2510
158	70.3	1.62	3.034	9.030	0.9140
212	100.3	1.62	3.034	8.658	0.8764
248	120.3	1.62	3.034	8.410	0.8513
3012	1656.9	1.44	2.696	1.860	0.1883

Density = 2.36 g/cm^3

NOTE:

+ Reference 8 and Reference 9

TABLE 3. HEAT FLUX - RADIATION BOUNDARY CONDITIONS

CANISTER				ROCK				TIME
INSIDE SURFACE		OUTSIDE SURFACE		*BORE HOLE WALL		FAR FIELD		HOURS
(°F)	(°C)	(°F)	(°C)	(°F)	(°C)	(°F)	(°C)	
300.0	148.9	300.0	148.9	65.0	18.3	65.0	18.3	0.00
300.2	149.0	300.0	148.9	66.1	18.9	65.0	18.3	0.002
300.4	149.1	300.0	148.9	66.7	19.3	65.0	18.3	0.006
300.5	149.2	300.0	148.9	67.2	19.6	65.0	18.3	0.010
300.6	149.2	300.1	148.9	67.6	19.8	65.0	18.3	0.014
300.6	149.2	300.2	149.0	67.9	19.9	65.0	18.3	0.018
300.7	149.3	300.2	149.0	68.3	20.2	65.0	18.3	0.022
300.8	149.3	300.3	149.1	68.5	20.3	65.0	18.3	0.026
300.9	149.4	300.4	149.1	68.7	20.4	65.0	18.3	0.030
363.7	184.3	362.7	183.7	283.8	139.9	278.8	137.1	STEADY STATE

NOTE: FAR FIELD = 1 METER FROM BORE WALL

* Reference temperature based on 148.9°C (300°F)

TABLE 4. TEMPERATURE - RADIATION BOUNDARY CONDITIONS

CANISTER				ROCK				TIME
INSIDE SURFACE		OUTSIDE SURFACE		*BORE HOLE WALL		FAR FIELD		HOURS
(°F)	(°C)	(°F)	(°C)	(°F)	(°C)	(°F)	(°C)	
300.0	148.9	300.0	148.9	65.0	18.3	65.0	18.3	0.00
400.0	204.4	300.1	148.9	66.1	18.9	65.0	18.3	0.002
400.0	204.4	303.5	150.8	66.7	19.3	65.0	18.3	0.006
400.0	204.4	314.4	156.9	67.2	19.6	65.0	18.3	0.010
400.0	204.4	326.7	163.7	67.6	19.8	65.0	18.3	0.014
400.0	204.4	337.7	169.8	67.9	19.9	65.0	18.3	0.018
400.0	204.4	347.1	175.1	68.3	20.2	65.0	18.3	0.022
400.0	204.4	355.0	179.4	68.5	20.3	65.0	18.3	0.026
400.0	204.4	361.7	183.2	68.7	20.4	65.0	18.3	0.030
400.0	204.4	398.5	203.6	283.8	139.9	278.8	137.1	STEADY STATE

NOTE: FAR FIELD = 1 METER FROM BORE WALL

* Reference temperature based on 148.9°C (300°F)

TABLE 5. TEMPERATURE - CONVECTION-RADIATION BOUNDARY CONDITIONS

CANISTER				ROCK				TIME
INSIDE SURFACE		OUTSIDE SURFACE		*BORE HOLE WALL		FAR FIELD		HOURS
(°F)	(°C)	(°F)	(°C)	(°F)	(°C)	(°F)	(°C)	
300.0	148.9	300.0	148.9	65.0	18.3	65.0	18.3	0.00
400.0	204.4	300.1	148.9	66.8	19.3	65.0	18.3	0.002
400.0	204.4	303.5	150.8	67.8	19.9	65.0	18.3	0.006
400.0	204.4	314.4	156.9	68.6	20.3	65.0	18.3	0.010
400.0	204.4	326.8	163.8	69.2	20.7	65.0	18.3	0.014
400.0	204.4	337.7	169.8	69.7	20.9	65.0	18.3	0.018
400.0	204.4	347.1	175.1	70.2	21.2	65.0	18.3	0.022
400.0	204.4	355.0	179.4	70.7	21.5	65.0	18.3	0.026
400.0	204.4	361.7	183.2	71.1	21.7	65.0	18.3	0.030
400.0	204.4	398.5	203.6	290.3	143.5	285.5	140.8	STEADY STATE

NOTE: FAR FIELD = 1 METER FROM BORE WALL

* Reference temperature based on 148.9° (300°F)

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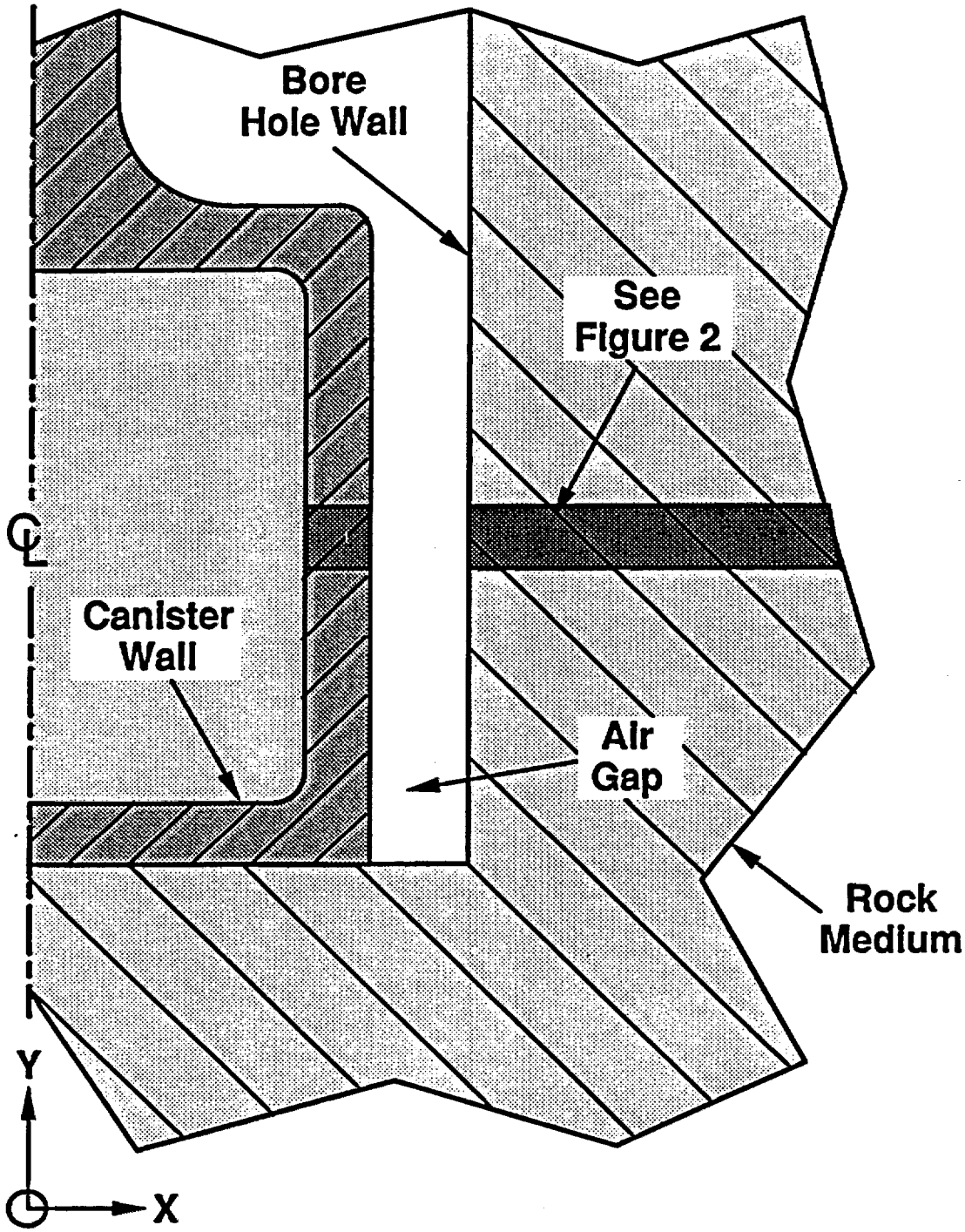

Figure 1.
Schematic of Half of a Planar Cross Section through a Waste Package Canister and Its Surrounding Features

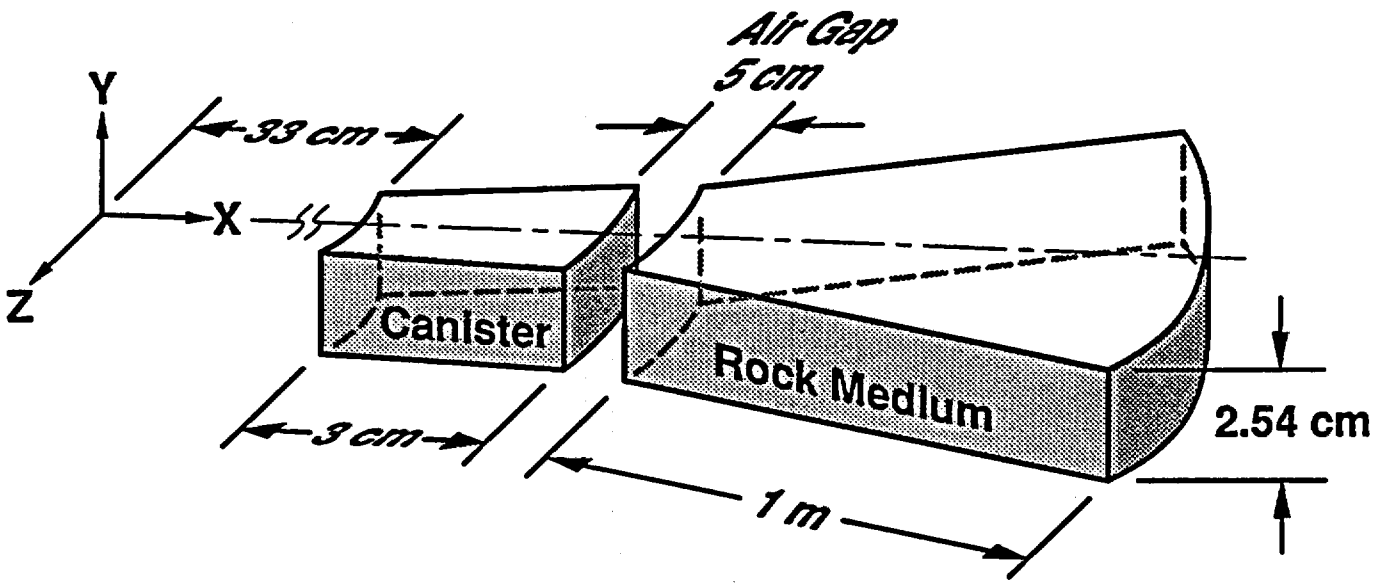

Figure 2.
Schematic Showing Analyzed Model of Canister and Near Rock Medium

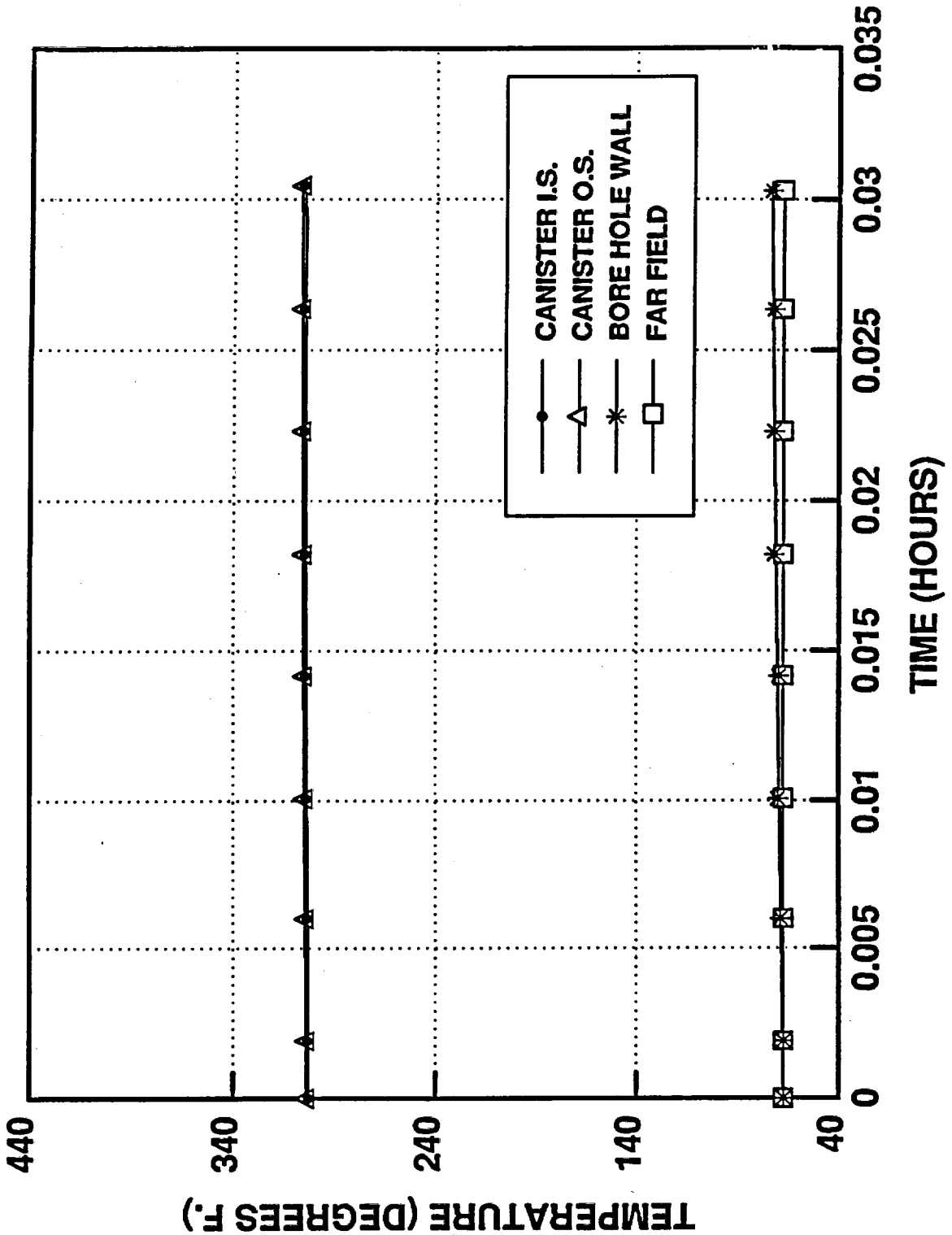

Figure 3.
Heat Flux - Radiation Boundary Conditions

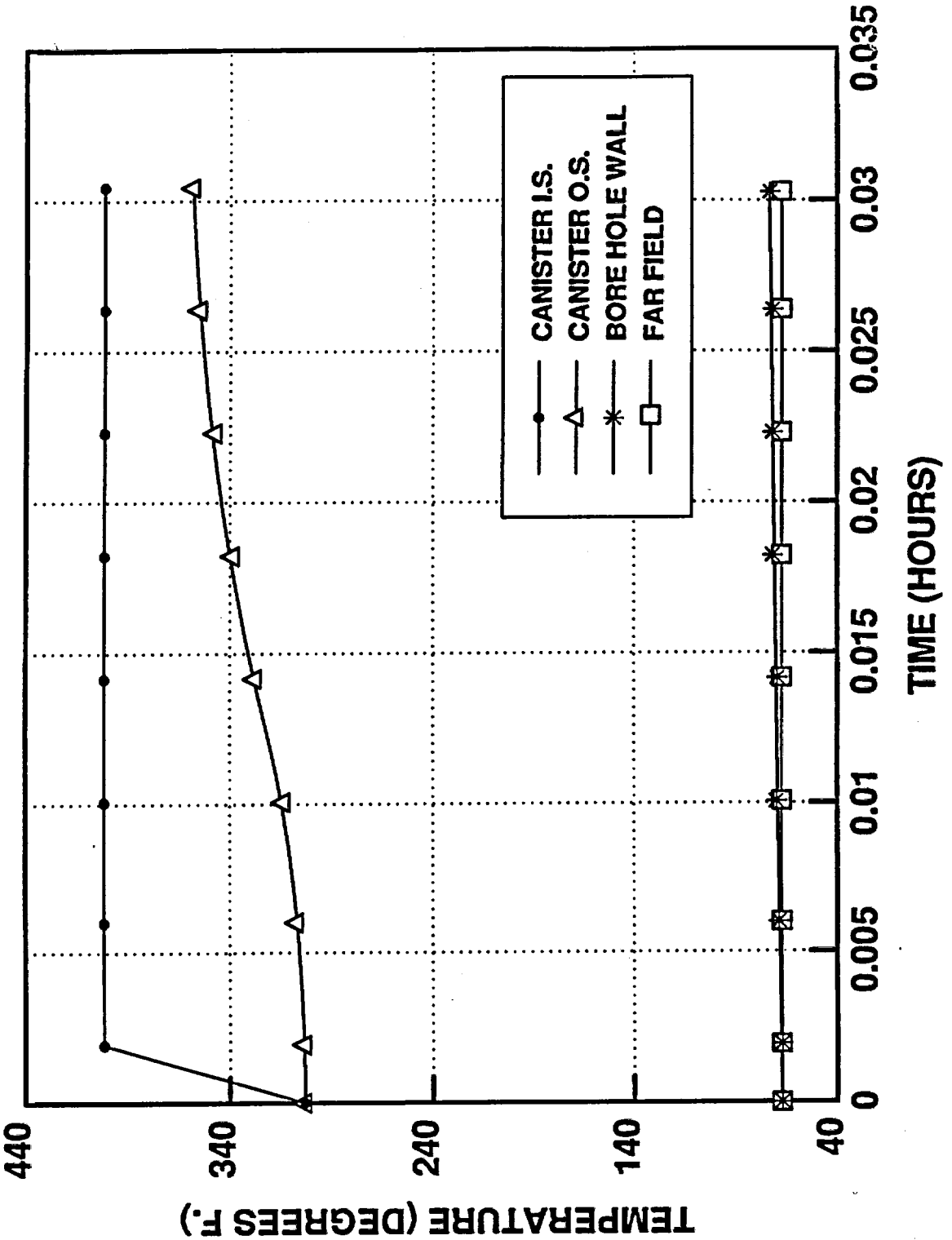

Figure 4.
Temperature - Radiation Boundary Conditions

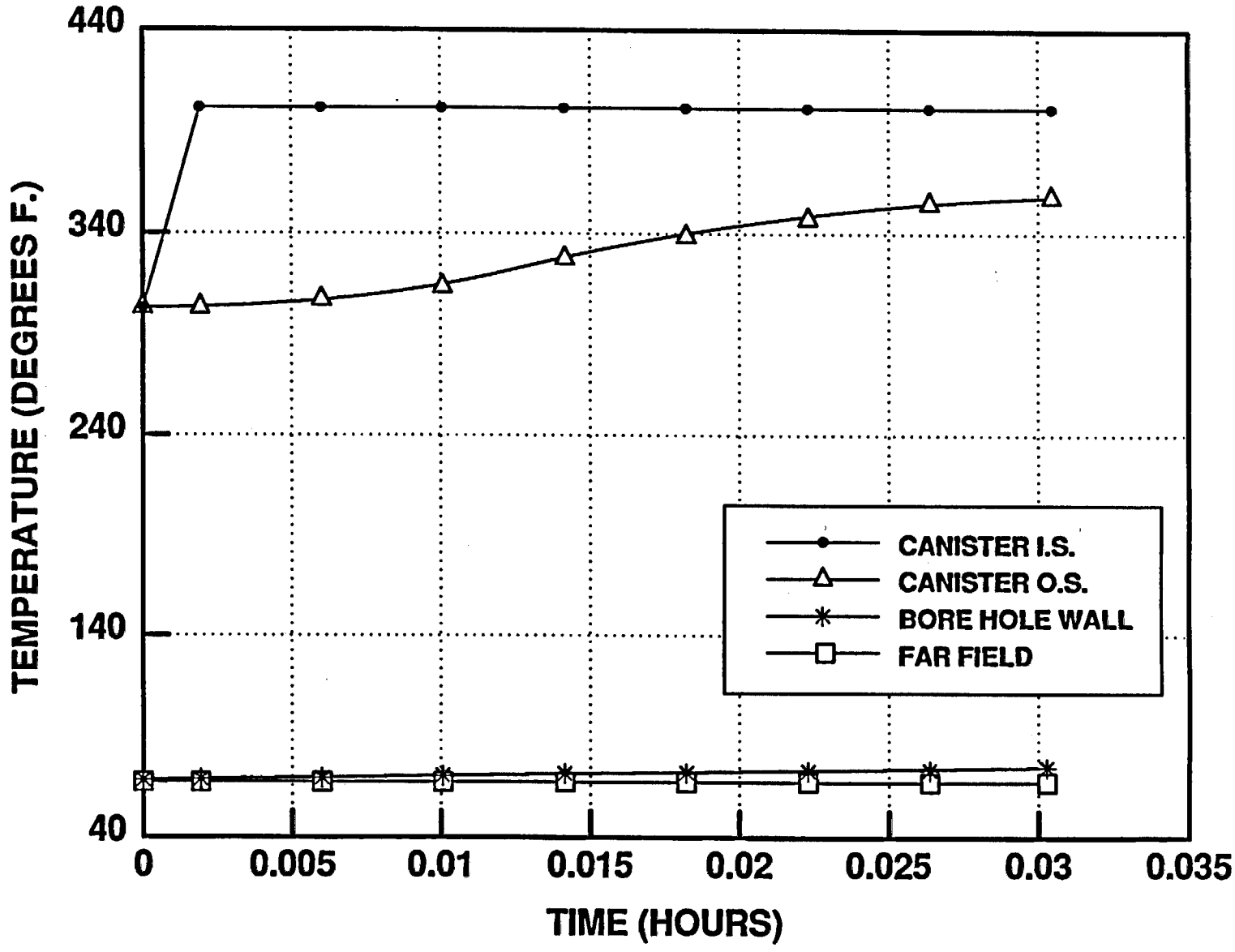

Figure 5.
Temperature - Convection-Radiation Boundary Conditions

APPENDIX A

Letter Report dated September 26, 1989
from
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to
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THERMAL MODEL COMPARISONS AND RECOMMENDATIONS

Introduction

This report presents a discussion of the characteristics of three thermal models which are candidates for use in modeling the proposed radioactive waste repository in Nevada. These models are, alphabetically, ANSYS, SINDA, and TOPAZ3D. They were selected, based on their overall capability, availability and utility, from the twenty-nine thermal models discussed in the referenced report.

The conclusions which are presented at the end of this report are based on the following general criteria:

1. Model capability for thorough analysis of the anticipated thermal environment.

2. Model maturity and validity.

3. Model utility, ease of use and technical support from developers.

4. Model compatibility with hardware.

5. Model acquisition and usage cost.

General

The following paragraphs contain general summary descriptions of the three thermal models under consideration.

ANSYS: This is a finite element model with extensive capabilities beyond thermal considerations. Its capabilities include dynamic analysis of structures, buckling and stability analysis, magnetic analysis, fluid flow and acoustic analysis, and coupled field analysis. It is available on a lease basis or under a time-share arrangement from nationwide vending services. The developers provide support, for a fee, in training, installation and operation. Source code is <u>not</u> accessible to the user. ANSYS can solve transient or steady-state, linear or non-linear heat problems involving conductive, convective (user-supplied coefficients) and radiative (in enclosures, say) thermal phenomena. Sensitivity analyses cannot be accomplished directly except by piecemeal variation of input parameters.

SINDA: This is a finite difference model which has fluid flow analysis capabilities as well as thermal. It is available on a lease basis. The developers offer training sessions and technical support for a fee. Source code is provided to the user. SINDA handles transient and steady-state, linear and non-linear heat transfer problems involving conductive, convective and radiative effects. Sensitivity analyses requires variation of input parameters.

TOPAZ3D: This is a finite element model for thermal analysis only. The software is sold outright and is available through the National Energy Software Center at Argonne National Lab. The NRC is a major supporter of NESC and has access to their software at no cost. The code developers provide training and installation/operation assistance for a fee. Source code is provided to the user for TOPAZ3D and the three ancillary codes it requires: INGRID, TAURUS and FACET. TOPAZ3D can solve transient and steady-state, linear and non-linear thermal problems involving conduction, convection (at boundaries) and radiation (enclosures). Sensitivity analysis is accomplished by input parameter variation.

Capabilities

Validation:

ANSYS: Extensively used in a wide range of applications by many customers, including David Sarnoff Labs and Bethlehem Steel. Many benchmark calculations made and compared with theoretic solutions. A formal Verification Manual is available from the developers.

SINDA: Developed with strong participation by NASA, who is currently the biggest user. Personnel at the Johnson Spaceflight Center in Houston have made use of SINDA in the thermal modeling of Space Station designs.

TOPAZ3D: Past and current users include Lawrence Livermore Laboratories (the developers), Lockheed, and others. Benchmark calculations have been made by Livermore, Lockheed and others, and compared to selected analytical results.

Machine:

ANSYS: Implemented on a wide range of mainframe systems, including VAX 11/780 and 8700, and IBM 4381 and 3090. A PC version of limited capability is also available. Source code is not accessible to the user.

SINDA: Implemented on a VAX 8650. Source code is available in FORTRAN 77 and is therefore transportable to most machines with some tailoring.

TOPAZ3D: Implemented on VAX 11 and IBM 3090 mainframe machines. Source code, in FORTRAN, is transportable.

Speed:

The speed with which calculations or runs can be made depends greatly on:

1. The size and complexity of the mesh or grid structure which is used to define the geometry and timing of the problem.

2. The complexity of the calculations required for each element or node.

3. The machine being used.

In the absence of data from all models on identical problems, it is not possible to compare model speeds. Approximate data do exist on the relative speeds, for a given model, on various machines. For example, run times on the VAX 8700 are comparable to run times on the IBM 4381, and are about one sixth as long as run times on the VAX 11/780.

Documentation:

ANSYS: Complete documentation is available, including a User's Manual, Examples Manual and Tutorials. The User's Manual is currently on backorder and could not be obtained for this study.

SINDA: A User's Manual is available; it was reviewed by the writer for this study. It is quite abstruse and considerable effort would be required to become proficient in program use.

TOPAZ3D: A User's Manual is available, reviewed by the writer for this study, which is written for the experienced engineer/programmer. Some effort would be required for proficiency. Similar technical documentation is available for the I/O and radiation routines.

Input:

All three models use input routines to define and structure the input data. All three models require the use of an ancillary routine to calculate the transfer characteristics for radiative heat transfer.

ANSYS: Input routines are included in the body of the main program. These routines are interactive and are reported to be fairly transparent and user-friendly. The routine RADFACT is used for addressing the radiative heat transfer geometric and physical considerations.

SINDA: Input routines are included as subroutines in the body of the main program. They are not interactive and are only partially automated. The user must rely on experience in the selection of appropriate routines. Not strongly user-friendly. TRASYS is used, as a separate routine, to calculate radiative interchange factors.

TOPAZ3D: The input routine INGRID is used to generate the mesh/grid structure. Input data handling routines are part of the main program. They are not interactive. Not strongly user-friendly. FACET is used, as a separate routine, to calculate radiation view factors.

Output:

ANSYS: The output formatting, graphing and printing routines are included in the main program and are manipulated in an interactive manner.

SINDA: The output processing routine, EXPLOT, is used for plotting data. An extensive library of output routines is available for data presentation. The user selects the routine(s) of choice with a CALL statement at the time of program submittal. No interaction.

TOPAZ3D: The post-processing routine TAURUS is used to format and present results of calculations. This is a separate program which accommodates plotting, contour mapping, etc. It is not an interactive program.

Technical Support:

ANSYS: The developers provide technical support, including debugging, for a fee, if the system is leased from them. If used on a time-share basis, the host company will, most likely, provide some assistance, again for a fee. The ANSYS developer is

Swanson Analysis Systems, Inc.
Johnson Road, PO Box 65
Houston PA 15342-0065.

A popular time-share service is

Solution Systems, Inc.
114 Forest Ave.
Narberth PA 19072.

SINDA: The code managers provide technical support for a fee. The code manager is

COSMIC
The University of Georgia
382 East Broad Street
Athens GA 30602.

TOPAZ3D: The developers of TOPAZ3D offer training and assistance in code usage and debugging on a fee basis. They are

Livermore Software Technology Corp.
2876 Waverly Way
Livermore CA 94550.

Cost:

The cost of acquiring and using the software is as follows:

ANSYS: Lease from developers: $1,000 per month (approx.) plus (for a VAX 8700) $0.034 per cpu second over 8.1 cpu hours per month of usage.

Time-share: Cost is (usually) based on usage only; no constant cost burden. The remote station equipment needed to access ANSYS on a time-share basis is not insignificant.

SINDA: $4,000 per 10 years to lease the package (one package per building). No cost for usage.

TOPAZ3D: Available from NESC. The NRC can provide their subcontractors with this software at no cost, since they are major contributors to NESC.

Conclusions and Recommendations:

The following conclusions are pertinent:

1. Any one of the three models discussed can perform the necessary thermal modeling.

2. A period of training and interaction with the developer will be necessary, whichever model is selected.

3. ANSYS:
   a. The lack of access to the source code is a significant drawback.

   b. The maturity of the model and the documentation and user interaction features are positive features.

   c. The costs of acquisition and usage are negative features.

4. SINDA:
   a. The access to the source code is a significant positive feature.

   b. The sketchy documentation and lack of user interaction are negative features.

   c. The low costs of acquisition and usage are positive features.

5. TOPAZ3D:
   a. The access to the source code is a significant positive feature.

   b. The sketchy documentation and lack of user interaction are negative features.

   c. The free acquisition and usage, via NRC, are significant positive features.

6. In the absence of user interaction for program input and control, as with SINDA and TOPAZ3D, it would be a straightforward matter to generate a user interface which would be tailored for the intended CNWRA application. This could be done very efficiently by Systems Support, Inc.

<u>RECOMMENDATION:</u>

Based on the above considerations, it is recommended that <u>TOPAZ3D</u> be used for the thermal analysis of the proposed radioactive waste repository.

REFERENCE:

Fuller, G.H., "Thermal Model Requirements and Survey", SYSTEMS SUPPORT, INC. Report to CNWRA, 28 February 1989.