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April 15, 1986

Mr. John Peshel Engineering Branch Division of Waste Management U.S. Nuclear Regulatory Commission 7915 Eastern Avenue Silver Spring, MD 20910

Dear Mr. Peshel:

The enclosed monthly report summarizes the activities during the month of March for FIN A-1755.

If you have any questions, please feel free to contact me at FTS 844-8368 or E. J. Bonano at FTS 844-5303.

Sincerely,

Robert M. Cranwell

R. M. Cranwell Supervisor Waste Management Systems Division 6431

RMC:6431:jm

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Enclosure

Copy to: Office of the Director, NMSS Attn: Program Support Branch 6400 R. C. Cochrell 6430 N. R. Ortiz 6431 R. M. Cranwell 6431 E. J. Bonano 6431 K. K. Wahi 6431 L. R. Shipers

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To provide technical assistance to NRC in the assessment of coupled thermal-hydrological-mechanical phenomena and site characterization activities for high-level waste repositories.

ACTIVITIES DURING MARCH 1986

Activities and Accomplishments

During the month of March, substantial effort was devoted to the CorStar Benchmarking Project. The computational mesh was generated and the input data deck prepared for the STEALTH formulation of Problem 5.2. Occasional consultation with SAIC was necessary due to the incomplete documentation of input instructions for some of the newer capabilities of STEALTH. In attempting to model Problem 5.2, two "bugs" were found in the STEALTH code by K. Wahi. These were reported to SAIC and appropriate corrections were made. In addition, Fortran logic had to be developed at SNLA to approximate convective losses since the standard waste isolation version of STEALTH does not have this capability. A sample 10-cycle computer run of Problem 5.2 has been made and the results are currently being analyzed. In the current STEALTH formulation of problem 5.2. a severe time-step restriction exists in order for the thermal response calculation to be stable. In order to increase the time-step size, gross modifications of the source geometry and mesh resulting in a coarse spatial resolution will be necessary. Through discussion with Dr. D. Vogt, an agreement has been reached on how to resolve this problem. The STEALTH input files for the salt and basalt problems will be sent to Dr. D. Vogt in the near future.

K. Wahi and L. Shipers travelled to Silver Spring, Mayland for NRC meetings on March 24 and 25 to discuss issues related to the BWIP exploratory shaft test plan and review the SCP. The meeting was chaired by Mr. J. Buckley, and NRC staff and other consultants were present. A trip report will be prepared and attached to the April monthly report.

A written review of an NRC draft working paper on thermal considerations for waste package emplacement was prepared at Dr. Pearring's request. A copy of the draft comments was given to Dr. Pearring. Following SNLA management approval of the written review, finalized comments will be sent to the NRC.

The report on the computer code USRC3D was completed. As discussed in previous monthly reports, this code is a 3-dimensional thermal model of a conducting medium with an embedded finite volume heat source. A draft of the report and a floppy disc containing the Fortran source code, the executable file, and the input and output data files for the sample problems discussed in the report is included in this monthly report.

Travel

K. Wahi and L. Shipers travelled to Silver Spring. Maryland on March 24 and 25, 1986, to attend NRC meetings.

Problems Encountered

None.

VSRC3D: A 3-Dimensional Thermal Model of a Conducting Medium with an Embedded Finite Volume Heat Source

by

L. R. Shipers

and

K. K. Wahi

Abstract

A computer code to based on an analytical solution calculate the temperature distribution resulting from a transient finite volume heat source embedded in a conducting medium is presented. A 3-dimensional model is used to simulate either a semi-infinite or an infinite conducting medium. Either constant temperature or constant flux boundary condition may be specified for the semiinfinite case. The infinite medium may be composed of either a single material or a two material composite medium with a planar contact. All thermal properties must remain constant; i.e., they cannot be a function of temperature. The analytical solutions, computational implementation, input data description, and sample problems are included in this report.

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1. Introduction

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This work was undertaken in an effort to produce a small scale, efficient computer code to simulate a conducting medium with a finite volume embedded transient heat source. The effort centered on generating a code that would run on a personal computer in a reasonable period of time yet retain enough complexity to realistically simulate a physical situation. It was also desired that the input data required to run the code remain as uncomplicated as possible so that the amount of time required to "learn" the code would be minimized. The VSRC3D computer code presented here satisfies these requirements.

The VSRC3D computer code uses a 3-dimensional model to generate the temperature distribution resulting from a finite heat source embedded in either a semi-infinite or infinite region. In the case of a semi-infinite region, either a constant temperature or a constant flux condition may be specified on the plane surface boundary. The infinite region solution may be calculated for either a single material or a two material composite region with a planar interface. In all cases considered, constant properties are required. The thermal output is currently specified by a piecewise linear function, but any function of time may be supplied by the user by modification of the heat source subroutine.

In Chapter 2 the analytical solutions used by the VSRC3D computer code are presented. Chapter 3 describes the implementation of these analytical solutions and the structure of the code. The subroutines and necessary input data are also discussed in detail in this chapter. Three sample problems that illustrate the applications and use of the code are presented in Chapter 4.

2. Analytical Solution

analytical solution for the temperature distribution in a conducting medium due to an embedded finite volume heat source was developed for three geometries: an infinite region, a semiinfinite region with specified temperature or flux boundary conditions, and an infinite composite medium. In all cases, the specific heat, density, and thermal conductivity of the conducting medium were assumed to be constant. It was also assumed that the conducting medium was initially at thermal equilibrium and that the transient thermal output of the embedded heat source was known. The physical situation considered is
shown in Figure 1. The heat source was assumed to be a 3-The heat source was assumed to be a 3 dimensional slab located a distance d below a reference plane. The x_2 , y_2 and z dimensions of the heat source were given, respectively, by a, b, and c. The origin of a Cartesian coordinate system was located on the reference plane above the center of the heat source. This reference plane is the boundary for a semi-infinite medium or the plane of contact for the composite medium.

Figure 1. Physical Situation

2.1 Infinite Region

 $\frac{1}{2}$

For the case of an infinite medium, the governing differential equation for temperature is expressed as

$$
\frac{\partial \mathcal{Z}}{\partial x^2} + \frac{\partial \mathcal{Z}}{\partial y^2} + \frac{\partial \mathcal{Z}}{\partial z^2} + \frac{1}{\kappa} g_{\mathbf{S}}(x, y, z, t) = \frac{1}{\alpha} \frac{\partial T}{\partial t}
$$
 (1)

where the thermal diffusivity, α , is given by

$$
\alpha = \frac{E}{F(C)} \tag{2}
$$

and ϵ , ϵ , and C are, respectively, density, thermal conductivity, and specific heat. The initial condition is

$$
T(x,y,z,0) = T_{f_1}(z)
$$
 (3)

and the domain is infinite. The thermal output of the heat source is defined as

$$
g_{\frac{1}{2}}(x,y,z,t) = g(t) [u(x + \frac{a}{2}) - u(x - \frac{a}{2})] [u(y + \frac{b}{2})
$$

- u(y - \frac{b}{2})] [u(z + \frac{c}{2}) - u(z - \frac{c}{2})] (4)

where $u(T)$ in the unit step function defined by

$$
u(\tau) = \begin{cases} 0, & \tau < 0 \\ 1, & \tau > 0 \end{cases}
$$
 (5)

Eq. (1) was solved by applying the Green's function method. From [1], the solution may be expressed as

$$
T(x,y,z,t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(x,y,z,t|x',y',z',0)T_0(z')dx'dy'dz'
$$

+ $\frac{\alpha}{\pi} \int_{0}^{t} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(x,y,z,t|x',y',z',\tau)g_{s}(x',y',z',\tau)dx'dy'dz'd:(6)$

where $G(x,y,z,t/x',y',z',T)$ represents the solution of the analogous homogeneously problem with a zero initial condition and an impulse point heat source of strength unity located at x' , y' , z' that instantaneously releases its heat at time τ . The first integral term in Eq. (6) represents the change in temperature due to a non-uniform initial temperature profile. Since it is desired to examine only the effect of the heat generation, this term was replaced by the initial temperature profile given in Eq. (3), resulting in

$$
T(x,y,z,t) = T_0(z) + \frac{C}{E} \int_0^t \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(x,y,z,t|x',y',z',\tau)
$$

• $g_2(x',y',z',\tau)dx'dy'dz'd\tau$ (7)

Note that this is consistent with the assumption that the conducting medium was initially at an equilibrium state since, at large times, the solution will approach the initially specified temperature profile rather than the uniform profile normally associated with an infinite medium.

The 1-dimensional Green's function for an infinite conducting medium is (see E1l)

$$
G(x, t|x^*, \tau) = \frac{1}{\sqrt{4\pi\omega(t-\tau)}} \exp \frac{-(x-x^*)^2}{4\omega(t-\tau)}
$$
(8)

Since the heat source given in Eq. (4) can be expressed as a product of functions x, y, and z, a product solution may be used to express the 3-dimensional Green's function in an infinite medium as

$$
G(x,y,z,t|x',y',z',\tau) = \frac{1}{t4\pi\epsilon(t-\tau)1^{\alpha/2}} \exp \frac{-(x-x')^{\alpha}}{4\epsilon(t-\tau)}
$$

4

 $\mathbf{v} = (v_1, v_2, \ldots, v_{N-1})$

o exp
$$
\frac{-(y - y^{*})^2}{4\omega(t - \tau)}
$$
 exp $\frac{-(z - z^{*})^2}{4\omega(t - \tau)}$ (9)

 $\varphi_{\rm{max}}$ and $\varphi_{\rm{max}}$. As in

When Eqs. (3) and (9) are substituted into Eq. (6) and the definition of the unit step function, Eq. (5), is utilized, the temperature distribution in the infinite conducting medium becomes

$$
T(x,y,z,t) = \frac{\alpha}{E} \int_0^t \frac{g(\tau)}{14\pi\alpha(t-\tau)} \exp\left[\frac{e^{+d}}{c}\right]_0^{b/2} e^{a/2} \exp\left[\frac{-(x-x^2)^2}{4\alpha(t-\tau)}\right]
$$

$$
\text{o exp } \frac{-(y - y^2)^2}{4\alpha(t - \tau)} \text{ exp } \frac{-(z - z^2)^2}{4\alpha(t - \tau)} \, dx' \, dy' \, dz' \, d\tau + T_0(z) \tag{10}
$$

By introducing the definition of the error function

$$
erf(\tau) = \frac{2}{\pi} \int_{0}^{\tau} exp(-\tau)^{2} d\tau
$$
 (11)

Eq. (10) may be expressed as

 \sim .

$$
T(x,y,z,t) = T_0(z) + \frac{1}{8} \frac{\alpha}{E} \int_0^t g(\tau) \left(erf \frac{(x + \frac{a}{2})}{\tau_{4\alpha}(t - \tau)}\right)
$$

$$
- erf \frac{(x - \frac{a}{2})}{\tau_{4\alpha}(t - \tau)} \left(erf \frac{(y + \frac{b}{2})}{\tau_{4\alpha}(t - \tau)} - erf \frac{(y - \frac{b}{2})}{\tau_{4\alpha}(t - \tau)}\right)
$$

$$
e \left(erf \frac{(z - d)}{\tau_{4\alpha}(t - \tau)} - erf \frac{(z - c - d)}{\tau_{4\alpha}(t - \tau)}\right) d\tau
$$
 (12)

2.2 Semi-infinite Region

In the case of a semi-infinite region, the domain was limited to the half-space below the reference plane where $z \geq 0$ (see Figure 1). The governing equation, Eq. (1), initial condition, Eq. (3), and the thermal output from the heat source, Eq. (4), remain unchanged from that given in the case of the infinite region but, it is necessary to specify a boundary condition on the reference plane in the case of the semi-infinite region. The option to specify either a constant temperature boundary condition, Eq. (13a),

$$
T(x,y,0,t) = T_{\text{c}}
$$
 (13a)

or a constant flux boundary condition, Eq. (13b),

 $\omega = \omega$.

$$
Q_{\rm s} = - \kappa \left. \frac{\partial T}{\partial z} \right|_{z=0} \tag{13b}
$$

is included in the analysis. The temperature distribution may again be expressed in terms of Green's functions as

$$
T(x,y,z,t) = T_0(z) + \alpha F(z,t)
$$

$$
+\sum_{k=0}^{\infty}\int_{0}^{t}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}G(x,y,z,t1x^2,y^2,z^2,\nabla)g_{s}(x^2,y^2,z^2,\nabla)dx^2dy^2dz^2d\mathbb{E}^{(14)}
$$

where the additional term, introduced by the non-homogeneous boundary conditions, is given by

$$
F(z,t) = \begin{cases} \int_0^t \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [T_s - T_0(0)] \frac{\partial G}{\partial z}, \Big|_{z^2=0} dx'dy'dT \text{ for Eq. (13a)} \\ \int_0^t \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{E} Q_s G(x,y,z,t/x',y',0,\text{and}x'dy'dT \text{ for Eq. (13b)} \end{cases}
$$

As before, the first integral term was replaced with the specified initial temperature.

The 1-dimensional Green's function for a semi-infinite medium is

$$
G(z,t|z',\tau) = \frac{1}{\sqrt{4\pi\omega(t-\tau)}} \left(exp \frac{-(z-z')^2}{4\omega(t-\tau)} \pm exp \frac{-(z+z')^2}{4\pi(t-\tau)} \right) \qquad (16)
$$

where the minus sign is used when the reference plane temperature is specified and the plus sign is used when the flux is specified as the boundary condition. A product solution may again be used to express the 3-dimensional Green's function in a half space as

G(x,y,z,t1x',y',z',t) =
$$
\frac{1}{[4\pi\omega(t-\tau)]^{3/2}} \exp \frac{-(x-x')^{2}}{4\omega(t-\tau)}
$$

• exp
$$
\frac{-(y-y')^{2}}{4\omega(t-\tau)} \left(exp \frac{-(z-z')^{2}}{4\omega(t-\tau)} \pm exp \frac{-(z+z')^{2}}{4\omega(t-\tau)} \right)
$$
 (17)

with the appropriate sign chosen for the desired boundary condition. When Eqs. t4) and (17) are substituted into Eqs. (14) and (15), the integrals are evaluated, and the error function, Eq. (11) , is introduced, the temperature distribution in a semiinfinite medium may be expressed as

$$
T(x,y,z,t) = T_0(z) + \frac{1}{8} \frac{\alpha}{E} \int_0^t g(\tau) \left(erf \frac{(x + \frac{a}{2})}{\sqrt{4\alpha(t - \tau)}} - erf \frac{(x - \frac{a}{2})}{\sqrt{4\alpha(t - \tau)}} \right)
$$

 $\sim 10^{11}$

 ~ 1000 m $^{-1}$.

 $\sim 10^7$

 \sim \sim

 $\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$

 $\Delta\sim 10^{-1}$ km

$$
\mathbf{e}\left(\text{erf }\frac{(y+\frac{b}{2})}{4\omega(t-\tau)}-\text{erf }\frac{(y-\frac{b}{2})}{4\omega(t-\tau)}\right)\left[\text{erf }\frac{(z-d)}{4\omega(t-\tau)}\right]
$$
\n
$$
-\text{erf }\frac{(z-c-d)}{4\omega(t-\tau)}\pm\left(\text{erf }\frac{(z+d)}{4\omega(t-\tau)}-\text{erf }\frac{(z+c+d)}{4\omega(t-\tau)}\right)\right]d\tau
$$
\n
$$
+\left\{\begin{array}{l}\text{LT}_{s}-\text{T}_{0}(0) \text{ orfc }\frac{z}{4\omega t} \text{ for Eq. (13a)} \\ \frac{a}{\omega}\left[\left(\frac{4\omega t}{\pi}\right)^{1/2} \text{ exp }\frac{-z^{2}}{4\omega t}-\text{erfc }\frac{z}{4\omega t}\right] \text{ for Eq. (13b)}\end{array}\right.
$$
\n(18)

where the minus sign is chosen for the case of a constant temperature boundary condition and the plus sign is used for a constant flux boundary condition. The complimentary error function is defined as

$$
erfc(T) = 1 - erf(T)
$$
 (19)

2.3 Infinite Composite Medium

<u>mmuk</u>

 ~ 100 km s $^{-1}$

The reference plane was specified as the dividing plane between the two different materials considered in the study of the infinite composite medium. This analysis required the solution of a pair of coupled partial differential equations used to describe the temperature in the conducting medium. For the region below the reference plane $(z \ge 0)$ the governing differential equation for the temperature is

$$
\frac{\partial \mathbb{E}[T]}{\partial x^2}1 + \frac{\partial \mathbb{E}[T]}{\partial y^2}1 + \frac{\partial \mathbb{E}[T]}{\partial z^2}1 + \frac{1}{E_1}g_S(x,y,z,t) = \frac{1}{\alpha_1}\frac{\partial T}{\partial t}1
$$
 (20)

with the initial condition

$$
T_{n}(x,y,z,0) = T_{n}(z)
$$
 (21)

where the subscript denotes the temperature and material properties of this region. The thermal output defined in Eq. (4) was again used to describe the heat source that exists in this region. Above the reference plane $(z \le 0)$ the governing differential equation and initial condition are

$$
\frac{\partial^2 T}{\partial x^2} z + \frac{\partial^2 T}{\partial y^2} z + \frac{\partial^2 T}{\partial z^2} z = \frac{1}{\alpha} \frac{\partial T}{\partial t} z
$$
 (22)

$$
T_p(x, y, z, 0) = T_q(z)
$$
 (23)

where the subscript again represents the temperature and material properties in this region. These two differential equations are

7

coupled with compatibility conditions requiring the temperature and the flux to be continuous at the reference plane. These two conditions are given by

$$
T_1(x,y,0,t) = T_2(x,y,0,t)
$$

\n
$$
K_1 \frac{\partial T}{\partial z}i\Big|_{z=0} = K_2 \frac{\partial T}{\partial z}\Big|_{z=0}
$$
 (24)

 \mathbf{A}^{max} and \mathbf{A}^{max}

In order to solve these coupled partial differential equations, first consider the case of the analogous 1-dimensional problem given by

$$
\frac{\partial \mathbb{S}^4}{\partial z \cdot \mathbb{S}} \mathbf{1} + \frac{1}{E} \mathbb{S}(t) \mathbb{S}(z - z') = \frac{1}{E} \frac{\partial \phi}{\partial t} \mathbf{1} \qquad z \ge 0
$$
 (25a)

$$
\frac{\partial^2 \Phi}{\partial z^2} z = \frac{1}{\alpha} \frac{\partial \Phi}{\partial t} z \qquad z \leq 0 \tag{25b}
$$

$$
\begin{aligned}\n\phi_1(z,0) &= \phi_2(z,0) = 0 \\
\phi_1(0,t) &= \phi_2(0,t) \\
\phi_1 \frac{\partial \phi_1}{\partial z}1\Big|_{z=0} &= \mathbb{E}_2 \left[\frac{\partial \phi_2}{\partial z}\right]_{z=0}\n\end{aligned}
$$
\n(25c)

where $\varepsilon(\tau)$ is the Dirac delta function defined by

 $E(T) = \begin{cases} 0, & T \neq 0 \\ 1, & T = 0 \end{cases}$ (26)

Note that the first equation of this system includes a source term of unit strength located at z' that instantaneously releases all its heat at time zero. It is this type of source term that is used to develop the Green's function for a given differential equation E1l. Paralleling a procedure presented in [2), this system of partial differential equations was transformed into a system of ordinary differential equations by defining the Laplace transform as

$$
\mathbb{E}_{\mathbf{i}}(z,\mathbf{s}) = \int_0^\infty \phi_{\mathbf{i}}(z,\mathbf{t}) e^{-\mathbf{st}} d\mathbf{t}
$$
 (27)

Applying this definition to Eqs. (25a), (25b) and (25c) results in

$$
\frac{d^{2\frac{\pi}{2}}}{dz^{2}}1 - \frac{5}{\alpha_{1}}\bar{x}_{1}(z_{1}s) = -\frac{1}{\kappa_{1}}\mathcal{E}(z - z^{*}) \qquad z \geq 0 \qquad (28a)
$$

 $\omega = 1/\sqrt{2}$

 $\omega_{\rm{eff}}$, $\omega_{\rm{eff}}$,

$$
\frac{d\mathbb{Z}\bar{z}}{dz\bar{z}}z = \frac{5}{\alpha_{\bar{z}}}\bar{z}_{\bar{z}}(z,s) = 0 \quad z \leq 0 \quad (28b)
$$

 $\mathbb{E}_1(0, s) = \mathbb{E}_2(0, s)$ (28c) $K_1 \left. \frac{d\tilde{z}}{dz} \right|_{z=0} = K_2 \left. \frac{d\tilde{z}}{dz} \right|_{z=0}$

The homogeneous solution to this system of differential equations has the form

$$
\mathbb{E}_{i}(z,s) = A_{i} \exp(-\gamma_{i} z) + B_{i} \exp(\gamma_{i} z)
$$
 (29)

where

 $\frac{1}{4}$.

$$
r_{\mathbf{i}} = \left(\frac{5}{\alpha_{\mathbf{i}}}\right)^{1/2} \tag{30}
$$

In order for $\mathbb{F}_q(z, s)$ to remain bounded as z approaches infinity B, must be zero. Similarly, A₂ must be zero so that \mathbb{F}_2 (2,5) remains bounded as z approaches negative infinity. Next, the particular solution of the differential equation for \tilde{x} , (z,s) must

be determined and added to its corresponding homogeneous solution. Since the non-homogeneity in this equation is the result of a source term of the same type as is used to develop the Green's function C11, it was assumed that the particular solution had the same form as the 1-dimensional Green's function for an infinite medium. Applying the definition of the Laplace transform to the functional form for this Green's function given in Eq. (8) and adding the result to the remaining portion of the homogeneous solution of \mathbb{F}_q (z,s) results in

$$
\mathbb{E}_{1}(z, s) = A_{i} \exp(-\gamma_{i} z) + \frac{1}{2\kappa_{i}\gamma_{j}} \exp(-\gamma_{i} z - z'1) \quad z \ge 0 \quad (32a)
$$

$$
\mathbb{E}_{\gamma}(z,\mathsf{s}) = \mathsf{B}_{\gamma}\mathsf{exp}(\gamma_{\gamma}z) \quad z \leq 0 \tag{32b}
$$

The two remaining constants in Eqs. (32a) and (32b) are evaluated using the compatibility conditions in Eq. (28c), resulting in

$$
\mathbb{E}_{1}(z, s) = \frac{1}{2\mathbb{E}_{1}\mathbb{Y}_{1}} \exp(-\mathbb{Y}_{1}|z - z'|)
$$

+
$$
\frac{\mathbb{E}_{1} - 1}{\mathbb{E}_{1} + 1} \exp(-\mathbb{Y}_{1}(z + z')) \qquad z \ge 0
$$
 (33a)

$$
\mathbb{E}_{\mathbb{S}}(z, s) = \frac{1}{E_{\mathbb{S}^{\mathbb{V}_{\mathbb{S}}}(1 + \mathbb{S})}} \exp(\gamma_{\mathbb{S}^{\mathbb{Z}}} - \gamma_{1} z^{\prime}) \quad z \leq 0 \quad (33b)
$$

where

 $\frac{1}{2} \frac{1}{2}$

 $\chi^2 \to 0$

 $\overline{N_{\rm eff}}$, and $\overline{N_{\rm eff}}$, and

$$
\mathbb{P} = \frac{\mathbb{E}}{\mathbb{E}\left\{ \frac{\alpha}{\alpha} z \right\}}^{1/2} \tag{34}
$$

The inverse Laplace transform of Eqs. (33a) and (32b) is

$$
\begin{aligned}\n\phi_1(z,t) &= \frac{c_0}{E_1} \frac{1}{\sqrt{4\pi c_1 t}} \left(\exp\left(\frac{-(z-z^*)}{4c_1 t} \right) \right. \\
&\left. + \frac{z-1}{z+1} \exp\left(\frac{-(z+z^*)}{4c_1 t} \right) \right) \quad z \ge 0\n\end{aligned}
$$
\n(35a)

$$
\phi_{2}(z,t) = \frac{\alpha_{2}}{E_{3} \sqrt{\frac{2}{4\pi\alpha_{2}t}}} \frac{1}{E+1} \exp \frac{-(z-\alpha_{2})^{2}}{4\alpha_{3}t} \qquad z \leq 0 \qquad (35b)
$$

where

$$
\sigma = \left(\frac{\alpha}{\alpha_1}\right)^{1/2} \tag{36}
$$

The functional form of Eqs. (35a) and (35b) is the same as the previously presented infinite medium Green's functions, so that these two solutions can be thought of as two separate infinite medium problems with appropriately located heat sources. As such, the product solution should apply for the consideration of the associated 3-dimensional problem. Thus for a unit point heat source located at $x = x'$, $y = y'$, $z = z'$, $(z' > 0)$ that instantaneously releases all of its energy at $t = 0$, the temperature distribution can be expressed as

$$
\phi_1(x,y,z,t) = \frac{c_1}{E_1} \frac{1}{(4\pi c_1 t)} \sigma_{/2} exp \left[\frac{(x-x^2)^2}{4c_1 t} exp \left(\frac{y-y^2}{4c_1 t} \right) \right]
$$

\n•
$$
\left(exp \left(\frac{-(z-z^2)^2}{4c_1 t} + \frac{p-1}{p+1} exp \left(\frac{-(z+z^2)}{4c_1 t} \right) \right) = z \ge 0
$$
 (37a)
\n
$$
\phi_2(x,y,z,t) = \frac{c_2}{E_2} \frac{2}{(4\pi c_2 t)^3} \sigma_{/2} \frac{1}{1+E} exp \left(\frac{-(x-x^2)^2}{4c_2 t} \right)
$$

$$
\exp \left(-\frac{(\gamma - \gamma^*)^2}{4\omega_{2}t} \exp \left(-\frac{(\gamma - \gamma^*)^2}{4\omega_{2}t}\right)\right)^2 \qquad z \leq 0 \qquad (37b)
$$

by employing the functional form of the 1-dimensional Green's function given in Eq. (8). When the heat source becomes a function of both space and time, the solution may be expressed in terms of a sum of point heat sources by integration as follows

$$
\frac{d}{dt}(x,y,z,t) = \frac{a_1}{E_1} \int_0^t \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{g_s(x,y,z,z',\tau)}{[4\pi a_1(t-\tau)]} d\tau \frac{dx-y'}{[4\pi a_1(t-\tau)]}
$$

\n
$$
= x p \frac{-(y-y')^2}{4a_1(t-\tau)} \left(\exp \frac{-(z-z')^2}{4a_1(t-\tau)} \right)
$$

$$
+\sum_{i=1}^{\infty}\frac{-1}{i} \exp \frac{-(z+z^*)^2}{4\pi i (t-\tau)}dx'dy'dz'd\tau
$$
 (38)

for $z \ge 0$ and

 $\mathbf{v}=(\mathbf{v}_1,\ldots,\mathbf{v}_N,\mathbf{v}_N)$, \mathbf{v}_N

$$
\Phi_{\otimes}(x,y,z,t) = \frac{\sigma_{\otimes}}{\pi_{\otimes}} \int_{0}^{t} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{q_{\mathsf{S}}(x^{\prime},y^{\prime},z^{\prime},t)}{[4\pi\sigma_{\otimes}(t-\pi)]^{\alpha/2}} \frac{z}{1+\sigma}
$$

$$
\exp \frac{-(x-x^*)^2}{4\alpha_0 (t-\tau)} \exp \frac{-(y-y^*)^2}{4\alpha_0 (t-\tau)} \exp \frac{-(z-\alpha z^*)^2}{4\alpha_0 (t-\tau)} dx'dy'dz'd\tau
$$
 (39)

for $z \leq 0$ where $g(x', y', z', \tau)$ represents the thermal output of the heat source. Eqs. (36) and (39) are, respectively, the solutions to Eqs. (20) and (22) for the case of homogeneous initial conditions. Since the system was assumed to be initially in thermal equilibrium, superposition can be used to include the nonzero initial conditions given in Eqs. (21) and (23). Using this, along with the expression for the thermal output of the heat source given in Eq. (4), the temperature distribution in the infinite composite medium can be expressed as

$$
T_1(x,y,z,t) = T_0(z) + \frac{1}{8} \frac{\alpha}{8} i \int_0^t g(\tau) \left(e^{\frac{t}{8} \tau} \frac{(x + \frac{a}{2})}{4\alpha} \right)
$$

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$$
= erf \frac{(x - \frac{a}{2})}{\sqrt{4\alpha_1(t - \tau)}} \bigg) \bigg(erf \frac{(y + \frac{b}{2})}{\sqrt{4\alpha_1(t - \tau)}} - erf \frac{(y - \frac{b}{2})}{\sqrt{4\alpha_1(t - \tau)}} \bigg)
$$

$$
\int \text{erf } \frac{(z-d)}{4\omega_1(t-\tau)} - \text{erf } \frac{(z-c-d)}{4\omega_1(t-\tau)} - \frac{\beta-1}{\beta+1} \text{erf } \frac{(z+d)}{4\omega_1(t-\tau)}
$$

$$
= \text{erf } \frac{(z+c+d)}{4\omega_1(t-\tau)} \bigg) \bigg] d\tau \qquad z \ge 0 \qquad (40)
$$

$$
T_{\alpha}(x,y,z,t) = T_{\alpha}(z) + \frac{1}{4} \sum_{k=2}^{\infty} \int_{0}^{t} \frac{q(\tau)}{\sigma(1+\epsilon)} \left(erf \frac{(x+\frac{a}{\rho})}{4\pi \epsilon_{\alpha}(t-\tau)} \right)
$$

$$
= erf \frac{(x - \frac{a}{2})}{\sqrt{4\alpha_{\mathbb{S}}(t - \tau)}} \bigg(erf \frac{(y + \frac{b}{2})}{\sqrt{4\alpha_{\mathbb{S}}(t - \tau)}} = erf \frac{(y - \frac{b}{2})}{\sqrt{4\alpha_{\mathbb{S}}(t - \tau)}} \bigg)
$$

$$
\mathbf{e} \left(\operatorname{erf} \frac{(z - \alpha d)}{4\alpha_{\underline{\alpha}}(t - \tau)} - \operatorname{erf} \frac{(z - \alpha(c + d))}{4\alpha_{\underline{\alpha}}(t - \tau)} \right) d\tau \qquad z \leq 0 \qquad (41)
$$

after the integration is performed and the definition of the error function is introduced. It should be noted that when the same material is specified above and below the reference plane (i.e. $\beta = \sigma = 1$, $\alpha_{1} = \alpha_{2}$, $\kappa_{1} = \kappa_{3}$) Eqs. (40) and (41) reduce to the solution presented in Eq. (12) for an infinite medium.

3. Computational Formulation

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In an effort to more readily implement the results presented in the previous chapter, the analytical solutions for the temperature distributions below the reference plane (z \geq 0) were combined into a single expression of the form

$$
T_1(x,y,z,t) = T_0(z) + \frac{1}{8} \frac{\omega}{h} \int_0^t g(\tau) \left(erf \frac{(x + \frac{a}{\epsilon})}{4\omega_1(t - \tau)} \right)
$$

\n- erf $\frac{(x - \frac{a}{\epsilon})}{4\omega_1(t - \tau)}$ $\left(erf \frac{(y + \frac{b}{\epsilon})}{4\omega_1(t - \tau)} - erf \frac{(y - \frac{b}{\epsilon})}{4\omega_1(t - \tau)} \right)$
\n• $\left(erf \frac{(z - d)}{4\omega_1(t - \tau)} - erf \frac{(z - c - d)}{4\omega_1(t - \tau)} - a_1 \left(erf \frac{(z + d)}{4\omega_1(t - \tau)} \right) \right)$
\ner $f \frac{(z + c + d)}{4\omega_1(t - \tau)}$ $\left(1 - erf \frac{z}{4\omega_1 t} \right) + a_0 \left(\tau \exp \frac{-z^2}{4\omega_1 t} \right)$ (42)

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|--|--|-----|--|--|--|
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Coefficients for Eq. (42)

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where the values of a_1 , a_4 , and a_5 are given in Table I for the cases considered. Recall that a solution for the case of a single material infinite medium will result if the composite medium solution is used in conjunction with the requirement that the same material properties are specified above and below the reference plane. In the cases where applicable, the temperature distribution above the reference plane ($z \leq 0$) was evaluated using Eq. (41).

In order to numerically evaluate the integrals in Eqs. (41) and (42) it is necessary to specify the functional form of the time dependence of the thermal output of the heat source. A piecewise linear function of the form

> g(t) = \circ m_{γ} t m_{ϕ} ${\bf t}$ $\mathsf{m}_{\mathsf{k}}^{\vphantom{\dag}}$ t 0 $+ b$ + b + b $t + t_{\alpha}$ \mathbf{t}_{α} < \mathbf{t} < **t. <** t < \mathfrak{r}_{k-1} ζ $t \rightarrow t_{k}$ (43) t. t, ζ t

was used. The computer code currently allows the thermal output to be specified at a maximum of 40 points in time. As a result of this, the heat source thermal output can be constructed of a maximum of 39 linear segments. It should be noted that the structure of the computer code will allow any functional form for

the thermal output of the heat source by modifying the function subprogram QHT(T), which evaluates this function.

The algorithm developed to numerically evaluate the integrals in Eqs. (41) and (42) employs Gaussian quadrature based upon Legendre Polynomials. This numerical procedure allows up to 40 quadrature points with valid numbers of quadrature points being 2, 3, 4, 5, 6, 10, 15, 20, and 40. The default number of quadrature points, which is set when an invalid number is specified, is 6. When the number of quadrature points is increased, the accuracy of the numerical integration is increased but the computational time required to evaluate the integral also increases. The functional form of the transient thermal output of the heat source may be used to help determine the number of quadrature points to specify. The smoother this functional form becomes, the fewer quadrature points that will be necessary to generate an accurate solution. In general, if it is desired to evaluate the temperature at only a few points in time and space, large number of quadrature points may be specified without strongly effecting the required computational time. For a large number of temperature evaluations, a smaller number of quadrature points should be initially specified in an effort to avoid excessive computational times. The effects on the solution of the number of quadrature points used should be explored. While the analytical solution developed in the previous chapter allows a z-direction dependence of the initial temperature, the computer code requires that this quantity be a constant. This was done in order to simplify the input data for the code.

The flow chart for the computer code VSRC3D is shown in Figure 2. All data input and output is performed in the main program using the default input (keyboard) and output (screen) devices. While specific data files could have been used for input and output, this is not necessary for IBM personal computers since the input and output data can be easily routed to the appropriate files by redirection of the standard input and output devices. This is accomplished by appending the appropriate file names to the execution command (see £3)). It should be noted that the loop for temperature evaluation at multiple times is within the loop for evaluation at multiple spatial locations. This was done so that the integrand arguments, with the exception of the time dependence, would be evaluated only once for a given spatial location in an effort to minimize the computational time of the code. The locations and times for temperature evaluation may be specified in any arbitrary order because the individual calculations for a given time and spatial location are independent of one another.

3.1 Computer Code

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The computer code is composed of the main program, VSRC3D, three subroutines: GLQUAD, HTSC, XYZV; and three function subprograms: ERF(X), FNCT(T), QHT(T). A description of each of these follows. The subroutine structure of the computer code is shown in Figure 3.

Figure 2. Flow Chart of VSRC3D

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Figure 3. Subroutine Flow Chart

Main program: VSRC3D

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calls: GLQUAD, HTSC, XYZV

The main program performs all data input and output using the default input (keyboard) and output (screen) devices. Programming loops have been included that allow the temperature to be evaluated at multiple spatial locations and times.

Subroutine: GLQUAD

called from: VSRC3D

calls: FNCT(T)

GLQUAD performs a Gaussian-Legendre numerical integration allowing a maximum of 40 quadrature points. Valid numbers of quadrature points are 2, 3, 4, 5, 6, 10, 15, 20, and 40. The default number of quadrature points, which results when an invalid number is specified, is 6. Recall that when the number

of quadrature points specified increases the computational time also increases.

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Subroutine: HTSC

called from: VSRC3D

HTSC calculates the slopes and intercepts of the piecewise continuous time dependent thermal output of the heat source. If an alternate function of time is used for the thermal output of the heat source, this subroutine may not be necessary or may require modification.

Subroutine: XYZV

called from: VSRC3D

XYZV evaluates the spatial location arguments of the integrand and specifies the coefficients of Eq. (42). This subroutine is called each time a new spatial location is specified. The same argument values are used for temperature evaluation at multiple times at a fixed spatial location.

Function subprogram: ERF(X)

called from: FNCT(T)

ERF(X) evaluates the error function of X. A fifth order rational expansion from [4], accurate to within 1.5×10^{-7} , was used to evaluate the error function.

Function subprogram: FNCT(T)

called from: GLQUAD

calls: ERF(X), QHT(T)

FNCT(T) evaluates the integrand of either Eq. (41) or Eq.(42).

Function subprogram: OHT(T)

called from: FNCT(T)

QHT(T) evaluates the thermal output of the heat source at time T. While a piecewise continuous time dependence is currently used, any functional form may be used by modifying this function subprogram. If an alternate functional form is used, the thermal output at time T should be assigned to the variable QHT in this function.

3.2 User Input Data

This section contains a description of the input data used in VSRC3D. The data set is composed of three blocks of "cards" or lines and is listed in the order of occurence. Variable names and input formats are included in this description. All input data should be right justified within the specified card column
field. The computer code contains no specified dimensional The computer code contains no specified dimensional constants, so that any consistent set of units (or dimensionless parameters) may be used.

Block 1 - region type and thermal properties

Card 1 (110,2F10.0)

Permissible values of IBC are defined in terms of the region type and the type of boundary condition in Table II. ZBC is the numerical value of the appropriate specified boundary condition (temperature or flux) at the reference plane $(z = 0)$.

Card 2 (6F10.0)

When a semi-infinite region is specified (IBC = 1 or 2) only the first three entries on this card are necessary. For the case of an infinite region (IBC = 3) all six entries are required. Recall, a single material infinite region solution will be generated by specifying the same thermal properties above and below the reference plane.

Region Type Specification

Block 2 - heat source data

Card 1 (110)

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A minimum of 2 and a maximum of 40 data points may be used to describe the piecewise linear thermal output of the heat source.

Card 2 thru NQ + 1 (2F10.0)

Card NQ + 2 (4F10.0)

Note that these quantities are labeled in Figure 1 as a, b, c, and d.

$$
Card NO + 3 (110)
$$

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The following data block must be repeated in order to specify multiple spatial locations.

Block 3 - spatial location and time data

Card 1 (3F10.0)

The origin of the rectangular coordinate system is located above the center of the heat source on the reference plane (see Figure 1). ZZ must be greater than zero unless the case of an infinite region (IBC = 3) is specified.

Card 2 (110)

Card 3 thru NT **+** 1 (Il0,F10.0)

Valid values of M are 2, 3, 4, 5, 6, 10, 15, 20, and 40. The default value, which results when an invalid value is specified, is 6. The temperature in the entire region is assumed to be initially at the ambient temperature at time zero. Note, the cards in Block 3 must be repeated for each spatial location specified (NL times).

4. Sample Problems

Three sample problems will be presented in an effort to illustrate the input specification and applicability of the VSRC3D computer code. The problems considered here have application to the methodology for assessing the risk from the geologic disposal of radioactive waste being developed by the Waste Management Systems Division of Sandia National Laboratories, Albuquerque. Specifically, a hypothetical waste repository in bedded salt discussed in detail elsewhere [5] will be considered.

4.1 Sample Problem 1

Sample Problem 1 is a 3-dimensional formulation of Sample Problem 2 presented in the DNET computer code user's manual [5]. In this problem, a 1100 acre high-level waste repository was assumed to be located in a layer of bedded salt at a height of 2814.81 ft. above datum. In order to be consistent with the problem statement in [5), a semi-infinite region with a specified temperature boundary condition (IBC = 1) was used to model the thermal medium. The reference plane was located at a height of 3363.06 ft above datum so that the repository is located a distance of 548.25 ft. below the reference plane. The temperature specified on this boundary was set equal to the assumed ambient

temperature of 110^{\degree} F. The repository was assigned a unit thickness and a square cross-section $(AA = BB = 6912.0 ft. for$ 1100 acres). The heat capacity, density, and thermal

conductivity of salt were specified as 0.27 BTU/lb $\mathrm{^{^{13}F}}$, 134.0

lb/ft³, and 21915.0 BTU/yr ft ⁸F, respectively. The 11 points used to describe the thermal output of the repository are the same as those used in [5] and are given in Table III. The temperature was evaluated at two locations above the center of the repository $(XX = YY = 0)$. The first point was located at the upper repository surface $(ZZ = 548.25$ ft) and the second point was located 200 ft below the reference plane $(22 = 200 \text{ ft})$. At both these spatial locations the temperature was evaluated at 5 year intervals for the first 100 years, 20 year intervals for the next 400 years, 50 year intervals for the following 500 years, and 100 year intervals for the last 1000 years. This resulted in the temperature being evaluated at 50 points in time over a period of 2000 years. In all cases, 40 quadrature points were used to evaluate the integrals given in Eq. (42). The input data for Sample Problem 1 is given in Appendix A.

Thermal Output Data Points

The output of Sample Problem 1 is given in Appendix B. In an effort to verify the VSRC3D code, a similar calculation was performed using both the 1- and 2-dimensional models currently available in the DNET computer code. In the 1-dimensional DNET computer code thermal model, an infinite planar heat source was located at the repository elevation. The DNET 2-dimensional model is formulated in a cylindrical coordinate system and uses a planar disc located at the repository horizon as the heat source. For purposes of comparison, this planar disc was specified to have the same effective cross sectional area (1100 acres) as the 3-dimensional model in VSRC3D. The results of these calculations at the two previously specified spatial locations are given in Table IV. Recall that the ambient temperature in all cases

considered was 110 ^CF. As can be seen, the agreement of the results for the points considered is quite good. The geometry of the systems considered is such that the results of the $2-$ and 3 dimensional models should approach those of the 1-dimensional model due to the large cross-sectional area of the heat source and the spatial locations considered. The slightly lower temperatures calculated from the VSRC3D computer code are a result of the truly 3-dimensional nature of the model.

In order to compare the computational time required to generate a temperature history, driver main programs were written for the 1- and 2-dimensional thermal calculation subroutines in the DNET computer codes. Using these computationally equivalent codes, the calculations in Table IV were repeated and the required computational times were compared with those of the VSRC3D code. Using the computational time of the simple 1 dimensional model as a base, the 2-dimensional DNET model required almost 40 times as much computational time to generate

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Table IV

Comparison of VSRC3D and DNET Results

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the results in Table IV while the 3-dimensional VSRC3D model required approximately 6 times as much computational time. While the more general 3-dimensional model does require more computational time than the 1-dimensional model, this increase in computational time is significantly less than a previously developed 2-dimensional model.

4.2 Sample Problem 2

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Sample Problem 2 is a three part extension of the previous sample problem that illustrates the different boundary condition and region type options of the VSRC3D code. In Part A, a constant flux boundary condition will be specified at the reference plane. This modification of the problem requires that only the first two entries on the first input data card be changed. The first entry (IBC) must be changed to 2 in order to specify a flux type boundary condition. Since it was desired to specify the reference plane as an insulated boundary, the flux at the boundary was specified as zero. This was accomplished by specifying the second entry on the first input data card (7BC) as zero.

In Part B, the temperature in an infinite salt medium is calculated. This problem modification requires that the first two cards in the input data file from Sample Problem 2A be changed. The first entry on the first card (IBC) should be set to a value of 3 in order to specify a solution in an infinite medium. The second value on this card (ZBC) is not used for an infinite medium solution and can assume any value. The second card contains material property data. For an infinite medium, six entries are required on this card. The first three entries represent the properties of the material below the reference plane and should remain unchanged from the values previously
specified. The three additional entries on the second card are, The three additional entries on the second card are, in order, the specific heat capacity, density, and thermal conductivity of the material above the reference plane. In the case of a single material infinite medium the first three entries are repeated.

An infinite composite medium was considered in Part C of this sample problem. A semi-infinite layer of salt was assumed to be capped by a layer of shale. The only modification necessary to the input data used in Sample Problem 2B is to change the properties of the material above the reference plane. To accomplish this the last three entries on the second data input card should be changed, respectively, to the specific heat capacity $(0.19$ BTU/lb ^OF), density (137.3 lb/ft³), and thermal conductivity (5568.0 BTU/yr ft $^{\circ}$ F) of shale.

The temperature histories at the two previously specified spatial locations resulting from Sample Problems 1, 2A, 2B, and 2C are shown in Figures 4 and 5. As can be seen from the figures, the choice of the boundary condition and/or the region type has no effect on the resulting calculated temperature for early times, but as time increases a significant difference results due the the choice of model type. Note that the

insulated boundary condition, allowing no heat loss across the reference plane, results in the highest temperatures at longer times, while the specified temperature boundary condition resulted in the lowest temperatures. The two infinite medium cases resulted in temperature histories between the two semiinfinite medium cases. The composite medium case, where the shale with its lower thermal conductivity acts as an insulator, resulted in higher temperatures at a given location at longer times than the infinite salt medium. Note also that that magnitude of the peak temperatures at a point away from the repository surface depends upon the model type. Again, an insulated boundary results in the maximum peak temperature.

It has been shown in this sample problem that the assumptions embedded in the models used for the thermal analysis of a geologic repository for radioactive waste can have significant effects on the resulting time dependent temperature distribution. While a period of time exists when the different models seem to predict the same temperature distribution, the length of this time period depends upon both the physical characteristics of the system and the distance from the repository. The resulting peak temperature at a point away from the repository boundary are also significantly affected by the assumptions of the thermal analysis.

4.3 Sample Problem 3

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The third sample problem is verification exercise for the composite medium portion of the VSRC3D computer code. The results generated by the VSRC3D computer code were compared to those generated from a 2-dimensional version of the STEALTH computer code (6]. As in Sample Problem 2C, the repository was assumed to be located in a layer of salt bounded above by a layer of shale. The salt and shale properties were the same as those presented in the previous example. The ambient temperature was set to zero in this case so that the temperature rise could be easily examined. A constant heat source was applied to the

system by specifying a thermal output of 2000 BTU/yr ^OF at two points in time (0 and 10 years). The repository was assumed to be located 50 ft below the reference plane and to have a thickness of 20 ft. An x-dimension of 200 ft was specified for the repository. The y-dimension of the repository in VSRC3D was specified an order of magnitude larger than the x-dimension (2000 ft) so that the 3-dimensional VSRC3D solution on a plane perpendicular to the y-axis near the repository center would approach a 2-dimensional solution. The temperature was evaluated at a total of 50 spatial locations so that both a vertical and a horizontal temperature profile could be examined. The vertical profile was located along the line where $X = 5$ ft, $Y = 0$ and temperatures were evaluated at 5 ft intervals from 45 ft above the reference plane to 55 ft below the reference plane. The horizontal temperature profile was evaluated at 5 ft intervals from the repository center to a distance of 145 ft along the line $Y = 0$, $Z = 55$ ft. The 5 ft shift from the repository center was

necessary because STEALTH evaluates temperatures at block centers rather than nodal locations. At each spatial location the temperature was evaluated at 1 year intervals for a period of 8 years. In all cases, 40 quadrature points were used to evaluate the time integrals. The VSRC3D input data for Sample Problem 3 is given in Appendix C and the VSRC3D output is given in Appendix D.

The version of STEALTH used in this comparison applied a 2 dimensional explicit finite difference method to generate the desired thermal solution. This numerical method requires that the region of analysis have finite spatial dimensions. To satisfy this requirement, an insulated (symmetry) boundary was specified through the repository center and the remaining boundaries were specified to be at a constant temperature of zero degrees. These constant temperature boundaries were located 50 ft above the salt/shale interface, 150 ft from the symmetry boundary and 150 ft below the repository. A uniform nodal spacing of 10 ft was used within this specified computational region.

The comparison of the VSRC3D and STEALTH results is shown in Figures 6 and 7. Figure 6 is a vertical temperature profile through the shale and salt layers along a line very near the center of the repository. Recall that since STEALTH calculates temperatures at block centers rather than nodal locations and since a vertical plane of symmetry was placed at the repository, it was necessary to shift the the line of the temperature profile 5 ft. In Figure 6, the reference plane is located at the zero value of the abscissa. Negative values of the abscissa represent the shale layer and positive values represent the salt layer. The upper edge of the repository was located at an abscissa value of 50 ft. At early times the agreement between the two solutions is quite good. As time increases the difference between the temperatures in the shale layer increases. This is due to the effect of modeling an infinite region with a finite computational region in the STEALTH computer code. Recall that the upper boundary of the computational region in the STEALTH simulation was located 50 ft above the reference plane (-50 ft) and a constant temperature of zero degrees was specified on this boundary. This has the effect of increasing the heat loss through the upper boundary as the temperature front approaches this boundary. The resulting effect is a lower temperature in the vicinity of this boundary.

Figure 7 represents a horizontal temperature profile across the salt layer at the repository level. Recall that the upper boundary of the repository was located 50 ft below the reference plane $(Z = 50 ft)$. In this figure, the repository extends from an abscissa value of zero to a value of 100 ft since in the STEALTH simulation a plane of symmetry was placed at the repository center. The zero degree fixed temperature boundary for the STEALTH simulation was located at an abscissa value of 150 ft. As before, the agreement is good at early times, but as time is increased the effects of the fixed temperature boundary become more pronounced. In all cases examined, the temperature calculated by the VSRC3D computer code was slightly below that

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calculated by the STEALTH code. This was due to the 3 dimensional versus 2-dimensional character of the models. The VSRC3D computer code, being a 3-dimensional model, allows a heat loss in a plane perpendicular to the repository cross section while the STEALTH code, with its 2-dimensional formulation, does not. In conclusion, for the case considered and within the limitations of the computer codes considered the agreement between the VSRC3D and STEALTH computer codes is quite good.

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Appendix **A**

VSRC3D Input Data for Sample Problem 1

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Appendix B

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VSRC3D Output from Sample Problem 1

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Appendix ^C

VSRC3D Input Data for Sample Problem 3

 $\label{eq:2.1} \mathcal{F}^{(2)}_{\mathcal{F}}(x) = \mathcal{F}^{(2)}_{\mathcal{F}}(x) \mathcal{F}^{(2)}_{\mathcal{F}}(x)$

 $\label{eq:2} \begin{split} \mathcal{F}^{(1)}_{\text{max}}(\mathbf{x}) &= \mathcal{F}^{(1)}_{\text{max}}(\mathbf{x}) \\ &= \mathcal{F}^{(1)}_{\text{max}}(\mathbf{x}) + \mathcal{F}^{(2)}_{\text{max}}(\mathbf{x}) \end{split}$

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 $\label{eq:1} \mathcal{L}_{\mathcal{A}}(\mathbf{x},\mathbf{y})=\mathcal{L}_{\mathcal{A}}(\mathbf{x},\mathbf{y})=\mathcal{L}_{\mathcal{A}}(\mathbf{x},\mathbf{y})=\mathcal{L}_{\mathcal{A}}(\mathbf{x},\mathbf{y})=\mathcal{L}_{\mathcal{A}}(\mathbf{x},\mathbf{y})$

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 $\epsilon_{\rm{max}} = \sqrt{2\pi m_{\rm{max}}}$ \mathcal{L}_{max} and \mathcal{L}_{max}

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 $\label{eq:1} \frac{1}{\sqrt{2}}\int_{0}^{2\pi} \frac{d\mu}{\lambda} \frac{$

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 $\label{eq:2.1} \frac{1}{\sqrt{2}}\int_{\mathbb{R}^{2}}\left|\frac{d\mathbf{x}}{d\mathbf{x}}\right|^{2}d\mathbf{x}^{2}d\mathbf{x}^{2}d\mathbf{x}^{2}d\mathbf{x}^{2}d\mathbf{x}^{2}d\mathbf{x}^{2}d\mathbf{x}^{2}d\mathbf{x}^{2}d\mathbf{x}^{2}d\mathbf{x}^{2}d\mathbf{x}^{2}d\mathbf{x}^{2}d\mathbf{x}^{2}d\mathbf{x}^{2}d\mathbf{x}^{2}d\mathbf{x}^{2}d\mathbf{x}^{2}d\mathbf{x}^{2}d\math$

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 $\label{eq:2.1} \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\right)^2\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\right)^2.$

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 $\sigma_{\rm{eff}}=2.0$ \mathcal{L}_{max} and \mathcal{L}_{max}

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 $\mathcal{L}(\mathbf{z})$

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 $\label{eq:2} \frac{d\mathbf{r}}{d\mathbf{x}} = \frac{1}{2} \sum_{\mathbf{r} \in \mathcal{R}^{(n)}} \mathbf{r} \mathbf{r}^{\mathbf{r}} \mathbf{r}^{\mathbf{r}}$

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 $\label{eq:2.1} \mathcal{L}(\mathcal{L}^{\mathcal{L}}_{\mathcal{L}}(\mathcal{L}^{\mathcal{L}}_{\mathcal{L}})) = \mathcal{L}(\mathcal{L}^{\mathcal{L}}_{\mathcal{L}}(\mathcal{L}^{\mathcal{L}}_{\mathcal{L}})) = \mathcal{L}(\mathcal{L}^{\mathcal{L}}_{\mathcal{L}}(\mathcal{L}^{\mathcal{L}}_{\mathcal{L}}))$

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Appendix D

VSRC3D Output for Sample Problem 3

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 $\label{eq:2.1} \frac{1}{\sqrt{2}}\int_{\mathbb{R}^3}\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\right)^2\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\right)^2\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\right)^2\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\right)^2.$

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 $\label{eq:2.1} \Psi_{\rm{eff}} = \frac{1}{2} \left(\frac{1}{2} \right)^{2} \left(\frac{1}{2} \right)^{2}$ $\frac{1}{2}$.

 $\label{eq:2.1} \frac{1}{\sqrt{2}}\int_{\mathbb{R}^3}\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\right)^2\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\right)^2\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\right)^2.$

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 $\label{eq:2.1} \frac{1}{\sqrt{2}}\int_{\mathbb{R}^3}\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\right)^2\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\right)^2\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\right)^2.$

 $\mathcal{L}^{\text{max}}_{\text{max}}$ and $\mathcal{L}^{\text{max}}_{\text{max}}$

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 $\mathcal{F}_{\text{max}}(\mathbf{x})$ $\Delta \phi = 0.000$

 $\lambda_{\rm{max}}=2.5$ $\mathbf{q}^{(1)}$

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TIME 0.100000E+01 0.200000E+01 0.300000E+01 0.400000E+01 0.500000E+01 0.600000E+01 o.700000E+01 0.800000E+01 x y 2 TEMPERATURE 0.500000E+01 0.500000E+01 0.500000E+01 0.500000E+01 0.500000E+01 0.500000E+01 0.500000E+01 0.500000E+01 O.OOOOOOE+00 **O.OOOOOOE+00 O.OOOOOOE+00** O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.202392E+02 0.304721E+02 0.382339E+02 0.446375E+02 0.501306E+02 0.549542E+02 0.592591E+02 0.631483E+02 TIME 0.100000E+01 O.200000E+01 0.300000E+01 0.400000E+01 0.500000E+01 0.600000E+01 0.700000E+01 0.800000E+01 x y z TEMPERATURE 0.500000E+01 0.500000E+0l 0.500000E+01 0.500000E+01 **0.500000E+01** 0.500000E+01 0.500000E+01 0.500000E+01 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.202392E+02 0.304721E+02 0.382339E+02 0.446375E+02 0.501306E+02 0.549542E+02 0.592591E+02 0.631483E+02 TIME 0.100000E+01 0.200000E+01 0.300000E+01 0.400000E+0l 0.500000E+01 0.600000E+01 0.700000E+01 0.800000E+01 x y 2 TEMPERATURE 0.100000E+02 0.100000E+02 0.100000E+02 0.100000E+02 0.100000E+02 0.100000E+02 0.100000E+02 0.100000E+02 O.OOOOOOE+OO O.OOOOOOE+OO O.OOOOOOE+OO 0.000000E+00 O.OOOOOOE+OO O.OOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+OO 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.202355E+02 0.304439E+02 0.381773E+02 0. 445566E+02 0.500299E+02 0.548374E-02 0.591292E+02 0.630075E+02 TIME x Y Z TEMPERATURE

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TEMPERATURE

0.198618E+02 0.290841E+02 0.358960E+02 0.415229E+02 0.463911E+02 0.507080E+02 0.545963E+02 0.58e132E+02

TEMPERATURE

0.196890E+02 C.286541E+02 0. 352645E+02 0.407339E+02 0.454768E+02 0.496922E+02 0.534970E+02 0. 569690E+02

TEMPERATURE

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 $\label{eq:2.1} \frac{1}{2} \sum_{i=1}^n \frac{1}{2} \sum_{j=1}^n \frac{$ $\label{eq:1} \frac{1}{\sqrt{2}}\sum_{i=1}^n\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\sum_{i=1}^n\frac{1}{\sqrt{2}}\sum_{i=1}^n\frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}}\sum_{i=1}^n\frac{1}{\sqrt{2}}\sum_{i=1}^n\frac{1}{\sqrt{2}}\right).$

TIME 0.100000E+01 0.200000E+01 0.300000E+01 0.400000E+01 O.500000E+01 0.600000E+01 o.700000E+01 0.800000E+0l x Y z 0.125000E+03 0.125000E+03 0.125000E+03 0.125000E+03 0.125000E+03 0.125000E+03 0.125000E+03 0.125000E+03 O.OOOOOOE+00 O.OOOOOOE+00 **O.OOOOOOE+00** O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 0.550000E+02 0.217732E+01 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 TEMPERATURE 0.504418E+01 0.774382E+01 0.103025E+02 0.127415E+02 0.150722E+02 0.173019E+02 0.194366E+02 TIME 0.100000E+01 0,200000E+0l 0.300000E+Ol 0.400000E+0l 0.500000E+01 0.600000E+o1 0.700000E+01 0.800000E+0l X X Y X Z TEMPERATURE 0.130000E+03 0.130000E+03 0.130000E+03 0.130000E+03 0.130000E+03 0.130000E+03 0.130000E+03 0.130000E+03 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+O0 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.157553E+Ol 0.404252E+01 0.647414E+01 0.882781E+01 0.111002E+02 0.132909E+02 0.154008E+02 0.174314E+02 TIME 0.100000E+01 0.200000E+01 0.300000E+01 0.400000E+01 0.500000E+01 0.600000E+01 0.700000E+01 0.800000E+01 x x y x z TEMPERATURE 0.135000E+03 0.135000E+03 0.135000E+03 0.135000E+03 0.135000E+03 0.135000E+03 0.135000E+03 0.135000E+03 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.112877E+O'I 0. 322960E+0 1 0.540644E+01 0.756219E+01 0.96721eE+01 0.117257E402 0.137174E*02 0.156451E+02 TIME 0.100000E+01 0.200000E+01 0.300000E+01 0.400000E+01 0.500000E+01 0.600000E+0l 0.700000E+01 0.800000E+01 x y z 0.140000E+03 0.140000E+03 0.140000E+03 0.140000E+03 0.140000E+03 0.140000E+03 0.140000E+03 0.140000E+03 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 TEMPERATURE 0. 799825E+00 0.257012E+01 0.450678E+01 0.647264E+01 0.842522E+Cli 0.103447E+02 0.122204E+02 0.140465E+02 TIME 0.lOOOOOE+01 0.200000E+01 0.300000E+01 0.400000E+01 O.500000E+01 0.600000E+01 0.700000E+01 0.800000E+01 x y z 0.145000E+03 0.145000E+03 0.145000E+03 0.145000E+03 0.145000E+03 0.145000E+03 0.145000E+03 0.145000E+03 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 O.OOOOOOE+00 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 0.550000E+02 TEMPERATURE 0.560039E+OO 0.203614E+01 0.374828E+01 0.553303E+01 0.733374E+01 0.912291E+01 0.108851E+02 0.126112E+02

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A-1755 1628.010 March 1986

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THIS IS AN ESTIMATE ONLY AND MAY NOT MATCH THE INVOICES SENT TO NRC BY SANDIA'S ACCOUNTING DEPARTMENT.

Other = rounding approximation by computer

III. Funding Status

