Numerical Calibration of an Analytical Generic Nuclear Repository Heat Transfer Model

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INTRODUCTION

This work describes a benchmarking effort conducted to determine the accuracy of a new generic geology thermal repository model relative to more traditional techniques and proposes a physically plausible auxiliary thermal resistance component to improve their agreement.

The analytic model to be calibrated was developed at Lawrence Livermore National Laboratory (LLNL) [1, 2, 3] and calculates the superposition of line and point source solutions representing a generic geology nuclear repository. It was benchmarked and calibrated against a numeric model that utilizes a geometrically-explicit lumped-parameter modeling approach developed over several years at Argonne National Laboratory (ANL) using the Systems Improved Numerical Differencing Analyzer (SINDA) thermal modeling code [4, 5]. Application of this approach to underground storage of heat generating nuclear waste streams within the proposed Yucca Mountain Repository Site (YMR) site has been widely reported [6].

The auxiliary thermal resistance component improves the accuracy of the rapid analytic model by calibration against the numeric model. Specifically, it improves estimations of the peak repository temperature as well as the timing of the peak temperature.

BACKGROUND: NUMERICAL SINDA/G MODEL

The numeric heat transport model created by the Used Fuel Disposition (UFD) team at ANL using the SINDA/G heat transport framework employs detailed finite-difference numeric models describing two distinct geometric arrangements: a single storage drift and an infinite array of identical, uniformly spaced storage drifts. For a given waste stream, tunnel radius, and geologic parameters (i.e. thermal conductivity, density, and specific heat capacity), the model is able to compute the temperature field surrounding the tunnel wall and beyond.

Calculation Method

The SINDA/G calculation engine uses a lumped parameter numeric model. Originally created for optimal waste loading analysis of the YMR, the model for an array of drifts is geometrically adjustable, as illustrated in Figure 1.

The SINDA/G lumped capacitance tool solves a thermal circuit, for which conducting nodes may be of four types corresponding to the four modes of heat transfer. Nodes are connected by conduction, convection, radiation, and mass flow heat transfer links. In the SINDA/G engine, these are represented by

$$ R_{\text{rad}} = \frac{1}{\sigma F_{ij} A [T_i + T_A + T_j + T_A] [(T_i + T_A)^2 + (T_j + T_A)^2]} $$

$$ R_{\text{cond}} = \frac{L}{K_{th} A}, \quad R_{\text{conv}} = \frac{1}{h A}, \quad \text{and} \quad R_{mf} = \frac{1}{\dot{m} c_p} \quad (1) $$

where

- $K_{th}$ = thermal conductivity [$W \cdot m^{-1} \cdot K^{-1}]$
- $A$ = area [$m^2$]
- $c_p$ = specific heat capacity [$J \cdot K^{-1}]$
- $h$ = heat transfer coefficient [$W \cdot m^{-1} \cdot K^{-1}]$
- $\dot{m}$ = mass transfer rate [$kg \cdot s^{-1}]$
- $T_i$ = lump temperature [$^\circ C$]
- $T_A$ = absolute temperature [$^\circ C$]
- $F_{ij}$ = radiation interchange factor [-]

Two SINDA/G model geometries have been used in this benchmark.
Single Drift

In the single drift geometry, there is a distant fixed boundary condition and one waste tunnel is modeled with a continuous, cylindrical heat source of infinite length. The linear heat source in \( \left[ \frac{W}{m} \right] \) is modeled as if it is spread azimuthally over the surface of the drift tunnel.

Multiple Drift

As illustrated in Figure 1, an infinite array of identical single-drift heat sources is modeled, by assuming one-half of a storage tunnel with a reflective boundary condition at a vertical plane midway between drifts.

BACKGROUND: ANALYTICAL MATHCAD MODEL

The analytic model, created at LLNL for the UFD campaign seeks to inform heat limited waste capacity calculations for each lithology, for many waste package loading densities, and for many fuel cycle options [1, 2, 3]. It employs an analytic model from Carslaw and Jaeger and is implemented in MathCAD [7, 8]. The integral solver in the MathCAD toolset is the primary calculation engine for the analytic MathCAD thermal model, which relies on superposition of integral solutions.

Calculation Method

The model consists of two conceptual regions, an external region representing the host rock and an internal region representing the waste form, package, and buffer Engineered Barrier System (EBS) within the disposal tunnel wall. The first region is taken to be a transient calculation unit. Since the thermal mass of the EBS is small in comparison to the thermal mass of the host rock, the internal region may be treated as quasi-steady state. The transient state of the temperature at the calculation radius is found with a convolution of the transient external solution with the steady state internal solution. The process is then iterated with a one year resolution in order to arrive at a temperature evolution over the lifetime of the repository.

The geometric layout of the analytic LLNL model in Figure 2 shows that the central package is represented by the finite line solution

\[
T_{\text{line}}(t, x, y, z) = \frac{1}{8\pi K_h \sqrt{\alpha \pi}} \int_{t_0}^{t} \frac{q_L(t') \cdot \left( x^2 + z^2 \right)}{t - t'} e^{-\frac{(x^2 + z^2)}{4\alpha(t-t')}} \, dt',
\]

\[
\cdot \left[ \text{erf} \left( \frac{1}{2} \sqrt{\frac{y + \frac{1}{2}}{\alpha(t-t')}} \right) - \text{erf} \left( \frac{1}{2} \sqrt{\frac{y - \frac{1}{2}}{\alpha(t-t')}} \right) \right], \quad (2)
\]

adjacent packages within the central tunnel are represented by the point source solution

\[
T_{\text{point}}(t, r) = \frac{1}{8K_h \sqrt{\alpha \pi}} \int_{t_0}^{t} \frac{q(t')}{(t-t')} e^{-\frac{r^2}{4\alpha(t-t')}} \, dt', \quad (3)
\]

and adjacent disposal tunnels are represented by infinite line source solutions

\[
T_{\text{line}}(t, x, z) = \frac{1}{4\pi K_h} \int_{t_0}^{t} \frac{q_L(t') \cdot \left( x^2 + z^2 \right)}{t - t'} e^{-\frac{(x^2 + z^2)}{4\alpha(t-t')}} \, dt', \quad (4)
\]

in infinite homogeneous media, where

\[\alpha = \text{thermal diffusivity} \left[ m^2 \cdot s^{-1} \right] \]

\[q(t) = \text{point heat source} [W] \]

and

\[q_L(t) = \text{linear heat source} [W \cdot m^{-1}] \]

Superimposed point and line source solutions allow for a notion of the repository layout to be modeled in the host rock.

RESULTS OF COMPARATIVE ANALYSES

Benchmarking

Benchmarking results shown in Tables 2 and 1 below effort between the analytic LLNL model and the numeric SINDA/G ANL models illustrate the degree of agreement between analytic and numeric models. In particular, the analytic model
would seem well-suited for purposes of rapid evaluation of
generic geologic repository configurations.

Specifically, for the single drift geometry benchmark, the
analytic model gave peak temperatures for all cases run which
agreed with the numeric model within 4°C and, for calculation
cross radii less than 5 meters, consistently reported peak temperature
timing within 11 years of the ANL numeric model. For the
multiple drift case, in which the numeric model approximated
an infinite array of drifts and the analytic approach modeled
101, the differences between models were slightly greater. The
benchmarking cases run in this validation effort are listed in
Table 1 and for the simplified single drift and in Table 2 for the
multiple drift case.

In light of the magnitude of uncertainties involved in generi-
cally modeling a non-site-specific geologic repository, this suf-

The benchmark revealed a notable discrepancy between the
two models, however. The time of peak heat arrived consist-
ently sooner and the value of the peak temperature was con-
sistently lower in the homogeneous medium analytic model
than in the numeric model.

Calibration

The goal of the calibration effort is accurate estimation of
temperature fields in geologic repositories both across large
expanse of host rock over long time spans using the analytic
model and locally, over much shorter time spans within the en-
gineered barrier systems using the numeric model. Physically,
it would be expected that the analytic line source model pro-
vides accurate temperatures across large spans of a repository
over large spans of time in regions far enough from storage
units that heat generated in the repository would be accurately
described as line sources. It is also possible the model’s accu-

It is assumed that EBS components within the disposal tun-
else only a small volume fraction of the rock and Due to the
high heat conductivity materials in the EBS it can be assumed
that in reality, the temperature field in the EBS responds to
changes in the waste package decay heat more rapidly than the
field in the surrounding host rock. This behavior is not taken
into account in the analytic model, but is explicitly accounted
for in the numeric model. The following simple empirical ex-
pression is plausibly added to the analytic model to more accu-

The difference in temperature due to the instantaneous tran-
sient response in the tunnel is here modeled as \( \Delta T \),

\[
\Delta T(t) = C q_L(t) \frac{1}{K_{th} D_d} \frac{1}{2} \left( \frac{D_d}{2} \right) 
\]

where

\[
D_d = \text{Distance between drifts}[m] \\
r_t = \text{Tunnel wall radius, calculation radius}[m] \\
K_{th} = \text{thermal conductivity coeficient} \\
C = \text{A coefficient derived from fitting}[m].
\]

This allows the capacitive behavior of the model to remain
entirely in the analytic model, and embeds the resistive behav-
ior in a purely algebraic calibration. The calibration is valid
for all repository configurations which share a tunnel diameter,
tunnel spacing, and host rock material.

### Table 1: Benchmarking Results for Single Drift Scenario

<table>
<thead>
<tr>
<th>Material</th>
<th>( K_{th} )</th>
<th>( \alpha )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clay</td>
<td>2.5</td>
<td>1.13 \times 10^{-6}</td>
</tr>
<tr>
<td>Salt</td>
<td>4.2</td>
<td>2.07 \times 10^{-6}</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Years Cooling</th>
<th>10</th>
<th>25</th>
<th>50</th>
</tr>
</thead>
<tbody>
<tr>
<td>R=0.35m</td>
<td>3.0</td>
<td>2.3</td>
<td>1.6</td>
</tr>
<tr>
<td>R=0.69m</td>
<td>3.1</td>
<td>2.4</td>
<td>1.6</td>
</tr>
<tr>
<td>R=3.46m</td>
<td>2.1</td>
<td>1.9</td>
<td>1.5</td>
</tr>
<tr>
<td>R=7.04m</td>
<td>3.1</td>
<td>2.4</td>
<td>1.8</td>
</tr>
<tr>
<td>R=14.32m</td>
<td>3.6</td>
<td>2.9</td>
<td>2.1</td>
</tr>
</tbody>
</table>

### Table 2: Benchmarking Results for 101 Drift Scenario

<table>
<thead>
<tr>
<th>Material</th>
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<th>( \alpha )</th>
</tr>
</thead>
<tbody>
<tr>
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<td>2.5</td>
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</thead>
<tbody>
<tr>
<td>R=0.35m</td>
<td>7</td>
<td>4.6</td>
<td>2.1</td>
</tr>
<tr>
<td>R=0.35m</td>
<td>-13.5</td>
<td>2</td>
<td>-6</td>
</tr>
</tbody>
</table>
A fitting coefficient of $C = 0.0265m$ improves agreement for the clay case with a $0.7m$ tunnel diameter and multiple drifts. The success of the fit decreases for longer cooling times.

For a clay repository $(K_{th} = 2.5|W \cdot m^{-1} \cdot K^{-1}, \alpha = 1.13 \times 10^{-6}[m^2 \cdot s^{-1}])$, with a tunnel diameter of $0.7m$, the calibration was completed using a fit between a 101 drift analytic scenario and the numeric model with an infinite number of drifts. $D_d$, the drift spacing, was $30m$ in each case. The results are shown in Figure 3.

**CONCLUSIONS**

The result of this work is a procedure for calibration of a rapid analytic heat transport model which improves peak temperature value and timing agreement with a more detailed, but more time intensive heat transport model. With a single calibration, it is possible for the disagreement between the two models to be alleviated for many configurations. Further work toward developing a dimensionally appropriate theoretical dependence for the coefficient is forthcoming. However, we recommend that for this and other analytic models which neglect rapid heat transport in engineered components near the calculation radius, the additional step will improve results near the area of interest.

**REFERENCES**

5. “SINDAG,” Network Analysis Inc., Tempe, AZ.