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 auxillary 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 calulates the superposition of line and point source solutions representing a generic geology nuclear repository. It was benchmarked and calibrated against a numeric thermal 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\Gaski (SINDA\G) 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 auxillary thermal resistance component improves the accuracy of the rapid analytic model by calibration against the numeric model. Specificially, 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

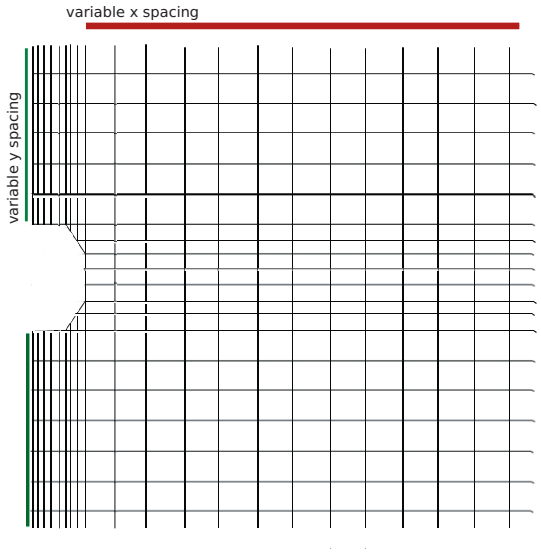

Fig. 1: The geometry of the 2D thermal model can be adjusted by altering tunnel diameter, tunnel spacing, and the vertical distance below the surface.

$$R_{rad} = \frac{1}{\sigma F_{ij} A \left[T_i + T_A + T_j + T_A\right]\left[(T_i + T_A)^2 + (T_j + T_A)^2\right]}$$
$$R_{cond} = \frac{L}{K_{th} A}, R_{conv} = \frac{1}{hA}, \text{ and } R_{mf} = \frac{1}{\dot{m} c_p} \quad (1)$$

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 $[\frac{W}{m}]$ is modeled as if it is spread azimuthally over the surface of the drift tunnel.

Multiple Drift

As llustrated 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 buff 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

$$T_{line}(t,x,y,z) = \frac{1}{8\pi K_{th}} \int_0^t \frac{q_L(t')}{t-t'} e^{\frac{-\left(x^2+z^2\right)}{4\alpha(t-t')}} \cdot \left[\operatorname{erf}\left[\frac{1}{2} \frac{\left(y+\frac{L}{2}\right)}{\sqrt{\alpha(t-t')}} \right] - \operatorname{erf}\left[\frac{1}{2} \frac{\left(y-\frac{L}{2}\right)}{\sqrt{\alpha(t-t')}} \right] \right] \mathrm{dt}', \tag{2}$$

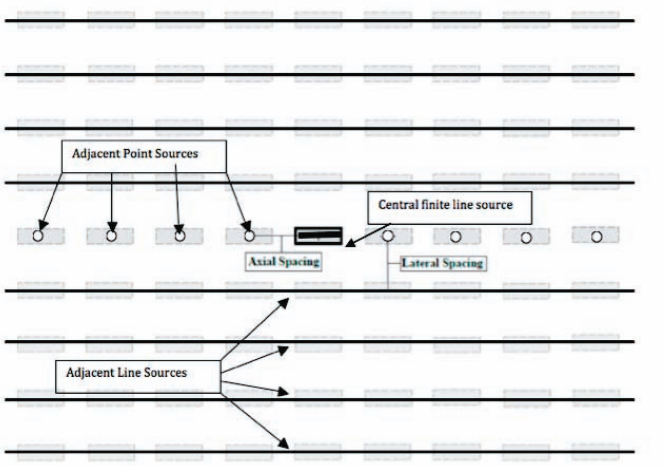

Fig. 2: The central package is represented by a finite line source, adjacent packages in the central drift are represented as points, and adjacent disposal tunnes are represented as infinite lines. [2].

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

$$T_{point}(t,r) = \frac{1}{8K_{th}\sqrt{\alpha}\pi^{\frac{3}{2}}} \int_0^{-t} \frac{q(t')}{(t-t')^{\frac{3}{2}}} e^{\frac{-r^2}{4\alpha(t-t')}} \mathrm{dt}', \tag{3}$$

and adjacent disposal tunnels are represented by infinite line source solutions

$$T_{\infty line}(t,x,z) = \frac{1}{4\pi K_{th}} \int_0^t \frac{q_L(t')}{t-t'} e^{\frac{-\left(x^2+z^2\right)}{4\alpha(t-t')}} \tag{4}$$

in infinite homogeneous media, where

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

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

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

Benchmarking Results for Single Drift Scenario

	Peak Temperature Discrepancy $T_{peak,num} - T_{peak,an}$ [°C]					
Material	Clay $K_{th} = 2.5$ $\alpha = 1.13 \times 10^{-6}$			Salt $K_{th} = 4.2$ $\alpha = 2.07 \times 10^{-6}$		
Years Cooling	10	25	50	10	25	50
R=0.35m	3.0	2.3	1.6	2.0	1.7	1.2
R=0.69m	3.1	2.4	1.6	2.2	1.8	1.3
R=3.46m	2.1	1.9	1.5	2.2	1.7	1.3
R=7.04m	3.1	2.4	1.8	2.5	2.1	2.2
R=14.32m	3.6	2.9	2.1	2.8	2.6	3.7
	Peak Heat Timing Discrepancy $t_{peak,num} - t_{peak,an}$ [yr]					
Material	Clay $K_{th} = 2.5$ $\alpha = 1.13 \times 10^{-6}$			Salt $K_{th} = 4.2$ $\alpha = 2.07 \times 10^{-6}$		
Years Cooling	10	25	50	10	25	50
R=0.35m	1	1	1	1	1	3
R=0.69m	2	2	1	2	3	4
R=3.46m	9	7	6	4	2	11
R=7.04m	4	13	10	11	10	288
R=14.32m	16	14	21	17	285	282

TABLE 1: Benchmarking in the single drift case showed that the peak heat was calculated to be lower and arrived consistently sooner in the analytic (an) model than in the numeric (num) 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 radii less than 5 meters, consistently reported peak temperature timing within 11 years of the ANL numeric model. For the multiiple 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 generically modeling a non-site-specific geologic repository, this sufficiently validated the analytic LLNL model with respect to its goals.

The benchmark revealed a notable discrepancy between the two models, however. The time of peak heat arrived consistently sooner and the value of the peak temperature was consistently 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 expanses of host rock over long time spans using the analytic model and locally, over much shorter time spans within the engineered barrier systems using the numeric model. Physically, it would be expected that the analytic line source model provides 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 accuracy in the vicinity of tunnel walls or waste package configurations can be improved by "calibration" against the SINDAG models discussed can be expected to accurately model temperatures close in to engineered storage units and in shorter time frames.

Benchmarking Results for 101 Drift Scenario

Material	Clay $K_{th} = 2.5$ $\alpha = 1.13 \times 10^{-6}$		
	Peak Temperature Discrepancy $T_{peak,num} - T_{peak,an}$ [°C]		
Years Cooling	10	25	50
R=0.35m	7	4.6	2.1
	Peak Heat Timing Discrepancy $t_{peak,num} - t_{peak,an}$ [yr]		
R=0.35m	-13.5	2	-6

TABLE 2: Benchmarking in the multiple drift case showed that the peak heat was calculated to be consistently lower in the analytic (an) model and deviated further from the numeric (num) model than did the single drift case.

It is assumed that EBS compenents within the disposal tunnel are 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 expression is plausibly added to the analytic model to more accurately estimate temperatures at locations within storage drifts.

The difference in temperature due to the instantaneous transient response in the tunnel is here modeled as ΔT,

$$\Delta T(t) = T_{numeric}(r_t) - T_{analytic}(\frac{D_d}{2}) \quad (5)$$

$$\Delta T(t) = C q_L(t) \frac{1}{K_{th}} \frac{1}{D_d} \quad (6)$$

where

$$D_d = \text{Distance between drifts}[m]$$
$$r_t = \text{Tunnel wall radius, calculation radius}[m]$$

and

$$C = \text{A coefficient derived from fitting}[m].$$

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

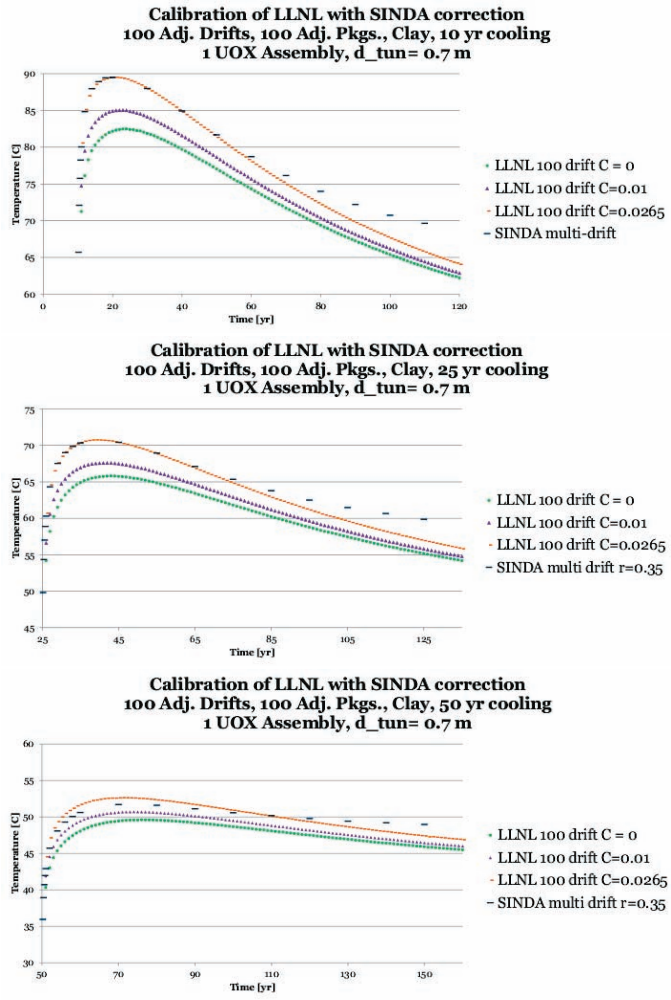

Fig. 3: A fitting coefficient of $C = 0.0265m$ improves agreement for the clay case with a $0.7m$ tunnel diameter and multiple drifts. The success of the fit decreases for longer cooling times.

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 aleviated 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.

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