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Qualification of Numerical and Semi-Analytical Modeling Codes for Thermal Design of HLW Repository-184550

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ABSTRACT

Disposal in a geological repository is a viable option for safely isolating high-level radioactive waste. Thermal processes induced by decay heat from the radioactive waste may impact the integrity of the engineered barrier system, and may lead to fluid flow and transport; and the associated migration of radionuclides. This study looks at an analysis of thermal conduction for the emplacement of high-level waste in a repository located in bedded salt. The simulations used analytical and numerical methods to study conductive heat transport in a repository. This study concentrated on heat flow in a central waste package with contributions from adjacent waste packages and drifts. Of particular importance to this work is comparison of predictions of peak temperature at the drift wall and at the waste package surface using different solution methods. Simulation results of analytical and numerical modeling methods are compared.

INTRODUCTION

Disposal of heat-generating radioactive waste and spent nuclear fuel in deep geological formations has been established as the preferred option to ensure the long-term isolation of radioactive waste is achieved. However, temperature increases due to the disposal of the heat-generating waste may lead to thermomechanical damage and to changes in the chemical constitution of the host rock. This can have a negative impact on the long-term isolation of the waste within the host rock. Therefore, temperature limits in the rock are defined during the design of a disposal layout for a high-level waste repository. These limits vary depending on the type of host rock and on the national legislation in place. For this study, the host rock of interest is bedded salt, which has a thermal limit of about 200°C, to avoid reaching the decrepitation temperature of salt.

Prior to disposal, the configuration of the waste packages in the repository is optimized under the requirement that the maximum temperature in the repository is below the temperature limit of the host rock. Several methods are available to perform this thermal analysis. The methods include simpler semi-analytical codes that provide quick analysis of heat transport, and the more complex numerical methods that provide distributions of heat, often coupled to mechanical phenomena and fluid flow transport. The aim of this present study is to assess the validity of such codes used by researchers in Germany and the United States. To this end, a US-German working group has been set up between DBE TECHNOLOGY GmbH and Sandia National Laboratories.

The comparative benchmark in this study is based on a US disposal layout from Sandia National Laboratories. Conduction-only thermal analysis was carried out at Sandia National Laboratories using the semi-analytical method implemented using Mathcad 14. Thermal analysis of this example was also done by DBE TECHNOLOGY GmbH with the codes FLAC3D and LinSour. The thermal simulations at both DBE TECHNOLOGY GmbH and Sandia National Laboratories used the same original input parameters. The studies include comparisons of results, which will be used to assess and improve the performance of the codes. As described above, only conductive heat transport was considered, neglecting convection and thermal radiation. These simplifications are reasonable for low permeability media (such as bedded salt) and enclosed emplacement modes [1].

MODEL DESCRIPTION

A base case test problem is presented for testing the different analytical thermal models used in this study. This case represents thermal analysis of a generic repository in bedded salt at 500 m depth. Heat conduction of a central waste package at a center of a drift with contributions from adjacent waste packages and drifts is considered. The intact salt beyond the drift was assumed to be an infinite medium. The space between the waste package and the drift was assumed to be backfilled with crushed salt. To simplify the simulation for the base case the same material was assumed for the waste package, the backfilling material in the drift and the host rock (case #1). Thus, simulations were conducted with the thermal conductivity of crushed salt and the heat capacity of intact salt. This follows the assumption that the heat propagation in the near field is mostly dominated by transport through the crushed salt buffer, whereas transport through the intact salt dominates heat transport in the far field. To quantify the effect of using the same material properties in the base case, a separate simulation was done with a numerical simulator using representative properties for each material (Case #2). Table I provides material properties used in all simulations.

Ambient average ground surface temperature of 15°C; and a natural geothermal gradient of 25°C/km, were assumed to calculate temperature at the near field. The waste package has a diameter of 0.61 m and is 3.05 m long. The drift diameter is 6.1 m. The decay heat curve for the waste package type is shown in Figure 1. Each waste package in the study generates heat according to this heat decay curve. Surface storage of 10 years was assumed.

The heat transport and the resulting maximum temperature in the repository are the result of the heat generation from each waste package and the superposition of the heat from all waste packages. Therefore, the example case will be analyzed in two different surface layout configurations. In the first configuration, a single waste package in the repository is considered. This allows the simulation of the thermal propagation of a single heat source, with no contribution from other sources. In the second configuration, the repository setup with multiple drifts and waste packages, with a drift spacing of 20 m and a waste package spacing of 10 m was simulated. The second configuration calculates the superposition of the heat output produced by multiple waste packages.

TABLE I. Material properties

Material	Thermal Conductivity (W/m/K)	Density (kg/m^3)	Heat Capacity (J/kg/K)	Thermal Diffusivity (m^2/s)
Intact salt	3.20	2200	931	1.562×10^{-6}
Crushed salt	0.57	2200	561.6	4.613×10^{-7}

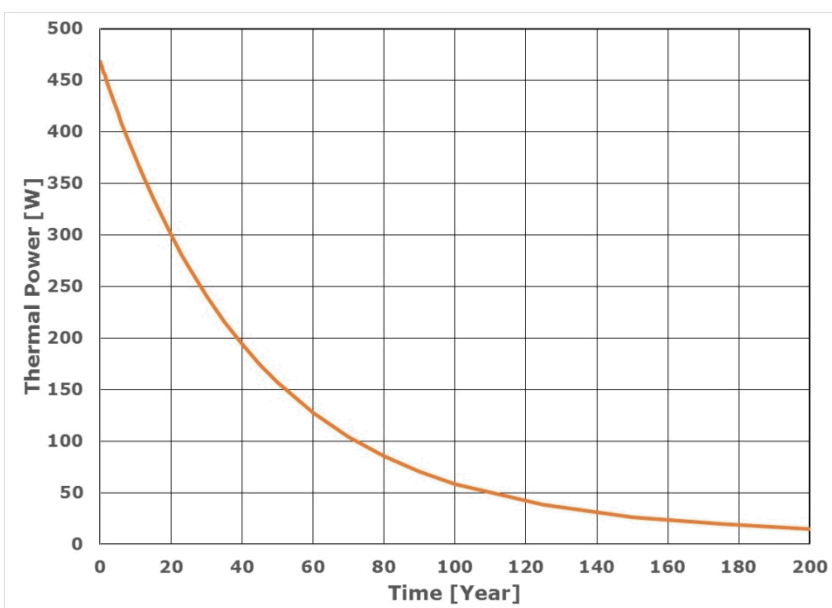

Figure 1. Thermal output of waste type considered.

The software used for the simulations are described below.

LinSour Software

LinSour or LINe SOURces is a computer code which has been developed to manage the complexity that arises in numerical codes when the thermal analysis is performed on an entire repository with large dimensions (up to several km^2) and over a time scale of 10^6 years. It is the latest development of several research studies on the development of analytical solutions for thermal analysis in repository systems in Germany [2, 3].

LinSour relies on the analytical solution of the heat transfer differential equation for a finite, linear, stationary heat source emplaced in an infinite, homogeneous and isotropic medium with constant material data. With respect to the linearity of the differential equation LinSour uses superposition to model the temperature field of more than one source. The differential equation solved numerically in LinSour for each line source is displayed below [3,4]:

$$\vartheta(t,R,z) = \frac{1}{8\rho c_p(\pi a)^{3/2}}\left[\int_0^t \frac{\Phi(t')}{(t-t')^{3/2}}\int_{-h}^{h} e^{-\frac{R^2+(z-z')^2}{4a(t-t')}}dz'\right]dt' + \vartheta_0 \qquad \text{(Eq. 1)}$$

where,

ϑ	Temperature
ϑ_0	Initial temperature
$\Phi(t)$	Time dependent thermal heat per meter
t	Time
ρc_p	Volumetric specific thermal capacity
a	Thermal diffusivity: $a = \frac{\lambda}{\rho c_p}$
λ	Thermal conductivity
R	Radial distance of the monitored point to the line source
z	Axial distance of the line source
h	Half length of the line source

The time dependent thermal heat represents, t, the thermal decay of the radioactive waste and is approximated in LinSour by a sum of exponential functions as follows:

$$\Phi(t) = \sum_{i=1}^{m}\{a_i \cdot e^{-b_i t}\} \qquad \text{(Eq. 2)}$$

Where;

$\Phi(t)$	Thermal heat at time t
a_i, b_i	Coefficients
m	Number of approximation functions

The analytical solution is a mathematical integral. The integration is achieved using the trapezoidal rule with increasing step size. The trapezoidal rule denotes an A-stable second order method. The temperature distribution in the repository is calculated in LinSour according to the following steps:

1. Input by the user of the coordinates of the line sources and the points where the temperature will be calculated according to a selected coordinate system. In addition, the times at which the temperature is calculated must be specified.

2. LinSour calculates the distance between the line sources and monitored points
3. To increase the numerical efficiency, LinSour calculates the distance between the monitored points and the line sources with a temperature increase of less than 0.1 K/W at selected times. The temperature at such points will be set to a residual value.
4. LinSour calculates the temperature at the monitored points at all selected times through superposition of the temperature produced by all line sources. The temperature at each line source is calculated with Eqns. 1 and 2. Only the monitored points which satisfy Step 3 will be considered in this operation.

The benchmark example problem for the base case described above has been simulated with LinSour. The results of these calculations are presented and compared to the other codes in the "Results and Discussion" Section below

Mathcad-Based Thermal Analysis Software

A Mathcad-based semi-analytical transient thermal model was also used for the analysis. The model is described further by Hardin et al. in references [1,5]. The model calculates the heat distribution produced by a central waste package including contributions from adjacent waste packages, as well as from waste packages in adjacent drifts. The model also includes convection, radiant heat transfer, ventilation and other processes. Analytical solutions from different sources were utilized in developing the model.

For this study, a backfilled repository in a salt host is assumed. Thus, the analysis will be conduction dominated and other processes (e. g., convection) are excluded on the basis that their contribution to the heat distribution will be negligible in the absence of large, open voids in the repository. The thermal conduction solution is a superposition of three components that represent contributions from the different sources. They include:

- a finite line source representing a central waste package of interest.
- infinite line sources representing laterally spaced adjacent drifts. This is represented by 8 adjacent drifts (four on each side of the central drift).
- Infinite point sources representing adjacent waste packages in the same drift aligned axially with the central waste package. This is represented by 8 adjacent waste packages (four on each side of the central waste package).

The analytical solution representing the central waste package is a finite line source in an infinite medium [6]. The finite line source solution is derived from the point source solution as shown in [6]. The integral form of the finite line source solution in the form of the error function in Cartesian coordinates is given by:

$$T_{central-line}(t,x,y,z) = \frac{1}{8\pi k}\int_0^t \frac{q_L(t')}{t-t'} e^{\frac{-(x^2+z^2)}{4\alpha(t-t')}} \left[erf\left[\frac{1}{2}\frac{\left(y+\frac{L}{2}\right)}{\sqrt{\alpha(t-t')}}\right] - erf\left[\frac{1}{2}\frac{\left(y-\frac{L}{2}\right)}{\sqrt{\alpha(t-t')}}\right]\right] dt' + T_0 \qquad \text{(Eq. 3)}$$

where,

T = temperature

T_0 = initial or ambient temperature

L = characteristic length (waste package length)
k = thermal conductivity of medium
τ = dimensionless time (Fourier number) = $(\alpha \cdot t)/L^2$

$q_L(t)$ = continuous line heat source (heat load of a single waste package divided by its length)

If radial distances are desired, Cartesian coordinates can be converted to radial coordinates using:

$$r^2=(x-x0)^2+(y-y0)^2+(z-z0)^2 \quad \text{(Eq. 4)}$$

where the source is located at (x0, y0, z0);

The contribution of adjacent drifts is represented by the infinite line source equation. The solution to the equation is given in [6, 7]. Considering two sets of four drifts on both sides of the central waste package, with given drift spacing and waste package spacing, the solution can be represented as:

$$T_{adjacent-drifts}(t,x,y,z) = 2\left[\sum_{id=1}^{N_{drifts}} \frac{1}{4\pi k}\int_0^t \frac{q_L(t')\cdot\frac{L}{wps}}{t-t'} e^{\frac{-[(x^2+z^2)+(id\cdot ds)^2]}{4\alpha(t-t')}} dt'\right] \quad \text{(Eq. 5)}$$

where;

$T_{adjacent-drifts}$ = temperature contribution of waste packages in adjacent drifts

N_{drifts} = number of adjacent drifts on each side of the central waste package (=4)

wps = waste package center to center spacing
ds = drift center to center spacing

The contribution of adjacent waste packages is represented by the infinite point source equation. The solution to the transient point source equation is provided by Carslaw and Jaeger [7]. Considering two sets of four waste packages on both sides of the central waste package aligned axially, with given waste package spacing, the solution can be represented as:

$$T_{adjacent-waste\ packages}(t,x,y,z) = 2\left[\sum_{ip=1}^{N_{wps}} \frac{1}{8\pi k\sqrt{\alpha}\pi^{1.5}}\int_0^t \frac{q(t')}{(t-t')^{1.5}} e^{\frac{-[(x^2+z^2)+((ip\cdot wps)^2)]}{4\alpha(t-t')}} dt'\right] \quad \text{(Eq. 6)}$$

where,

$T_{adjacent-waste\ packages}$ = temperature contribution of adjacent waste packages in the same drift

N_{wps} = number of adjacent waste packages on each side of the central waste package (=4)

q(t) = continuous line heat source

The Mathcad-based model uses Eqns. 3 through 6, the heat source given in Figure 1, and properties of the engineered barrier system to evaluate temperature at the waste package surface and the drift wall as a function of time.

FLAC3D Numerical Code

A repository for radioactive waste is characterized by its complex geometry, heterogeneous materials whose parameters can be nonlinear with respect to time, temperature and pressure. In addition to thermal conduction, other heat transport phenomena such as convection and radiation also take place in a repository. In such conditions, the thermal analysis of heat distribution in a repository system is usually accurately performed with numerical codes. For this reason, the example problem was also solved using the finite difference code FLAC3D. FLAC3D (Fast Lagrangian Analysis of Continua in 3 Dimensions) is a numerical modeling software developed by Itasca Inc. for geotechnical analyses of soil, rock, groundwater, constructs, and ground support. FLAC3D has a thermal option for analyzing both conduction and advection in materials for nuclear waste disposal and cement hydration and a creep option for analyzing time-dependent material behavior, for excavations in salt or potash, for example.

Figure 2 shows a representation of the repository setup used for the numerical model that was developed for the model comparison example problem described above. This figure shows an illustration of the host rock with an excavated drift. A waste package is disposed in the drift and is backfilled with crushed salt buffer. Figure 2 also shows two observation points (at the drift wall and at the waste package surface). For the numerical simulations, the thermal decay curve shown in Figure 1 was applied as volume specific heat-generating source in the cask.

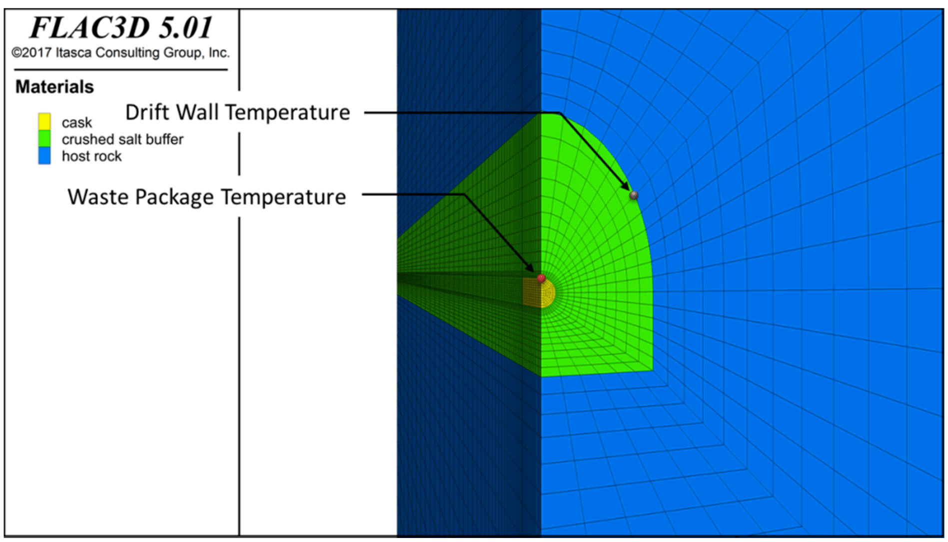

Figure 2. Representation of the repository setup for the numerical model used in the example problem

The numerical model is set up so that the initial and boundary conditions are identical to those of the semi-analytical codes. This insures a basis for comparison between all codes under the same conditions. Because of the limitations of the semi-analytical codes thermal conduction only is considered in the simulation. Thus, processes such as the temperature-dependent properties of rock salt and the pressure-dependent properties of crushed salt are not taken into account. Since the semi-analytical code LinSour can be used only for isotropic media, further adjustments were made in the numerical simulations: For Case #1, the same thermal material parameters are assigned to all materials (crushed salt, cask, rock salt) to establish isotropic conditions in the numerical model. This approach made it possible to determine the accuracy of the analytical codes in comparison to the numerical code under identical input conditions. A second separate numerical simulation with properties of each material according to Table 1 was also conducted (Case #2). For this case, the waste package was represented by a thermal conductivity of 1 W/m·K and thermal capacity of 800 J/kg·K. The results of all simulations are presented and discussed below for the two configurations.

RESULTS AND DISCUSSION

The results of the analysis using the three codes LinSour, SANDIA Mathcad 14 and FLAC3D are presented in Figure 3 for Configuration 1 and in Figure 4 for Configuration 2. Configuration 1 represents the case of a single waste package placement while Configuration 2 is a representative repository layout with given drift and waste package spacing. The plots in Figures 3 and 4 represent the simulated temperature values at the monitoring points at the drift wall (left) and the waste package surface (right) over a simulation period of 100 years using parameters according to case #1. The results of the numerical simulation with FLAC3D using corresponding properties for each material are also presented in Figures 3 and 4 for both configurations (Case #2). Note that semi-analytical codes can be considered as accurate when their results are comparable to those of the numerical code FLAC3D (i.e. Temperature vs. Time plots have overlay or nearly overlay at the observation points, see Figure 3 and Figure 4).

For the case of a single, isolated waste package emplacement (Configuration 1), the temperature results calculated with the two analytical codes and the numerical code FLAC3D, using the same material parameter values, are almost identical (Figure 3). The maximum temperature predicted by FLAC3D at the drift wall is equal to 39.1°C. This is very close to the maximum temperature of 38.8°C and 38.7 calculated with SANDIA Mathcad 14 and with LinSour, respectively. Similar results were also obtained at the waste package surface where maximum temperatures of 96.3°C, 96.8°C and 96.7°Cwere calculated with FLAC3D, SANDIA Mathcad 14 and LinSour, respectively, using the same parameter values. In addition, the shapes of the temperature curves are also identical over the simulation period. This indicates that the implementation of thermal conduction in the semi-analytical codes produces heat distribution calculations that are comparable to the analytic solution, and thus the physics of thermal conduction is well-captured by the semi-analytic model.

Figure 4 shows the temperature results at the observation points for Configuration 2 (which simulates multiple waste packages). Predictions of temperature with SANDIA Mathcad 14 and LinSour are almost identical to those of FLAC3D at the drift wall (48.6°C for Mathcad 14, 49.1°C for LinSour vs 48.9°C for FLAC3D) as well as at the waste package surface (98.4°C for Mathcad14, 98.4°C for LinSour vs 98.0°C for FLAC3D).Even after 100 years the predicted temperature decay predicted by the semi analytical codes compared to FLAC3D results remain small. One can conclude that both semi-analytical codes are able to calculate the thermal superposition of contributions of adjacent drifts and waste packages with accuracy.

As discussed above a separate second set of simulations were carried out with FLAC3D. In these simulations, realistic representative parameter values for each material were used (Table I). This analysis was conducted to investigate the effect of the assumption of using the invariant material properties for all materials adopted in the base case. Results of the second separate numerical simulations show that the assumed constant parameter values in the analytical codes for Case #1 lead to an overestimation of the temperature at the drift wall and at the waste package surface for both configurations. According to the second FLAC3D simulations, maximum simulated temperatures at the drift wall and the waste package surface are 29.9°C and 89.9°C respectively, for Configuration 1. This means a discrepancy of around 10°C at the drift wall and 6°C at the waste package surface compared to the semi-analytical results of the base case. For Configuration 2, the discrepancy in drift wall temperature prediction is equal to 12°C when compared to SANDIA Mathcad 14, and almost 13°C compared to LinSour. At the waste package surface, one can measure a difference of 9°C when compared with both semi-analytical codes. These results show that choosing the same material parameter values as used in Case #1 would result in conservative results. Therefore, the thermal design of a repository using a semi-analytical code leads to conservative drift and waste package spacings. However, this approach allows use of simpler and quick simulations using semi-analytical codes to ensure that the temperature limit in rock salt is met.

The accuracy of the semi-analytical codes can be improved for the realistic case (Case #2) by performing a parameter calibration on a representative numerical model where nonlinear material behavior and geometrical heterogeneities are taking into account. This method is usually used for LinSour. The Mathcad 14 based code is able to model multiple materials and can consider non-constant material properties which increase its accuracy under realistic conditions.

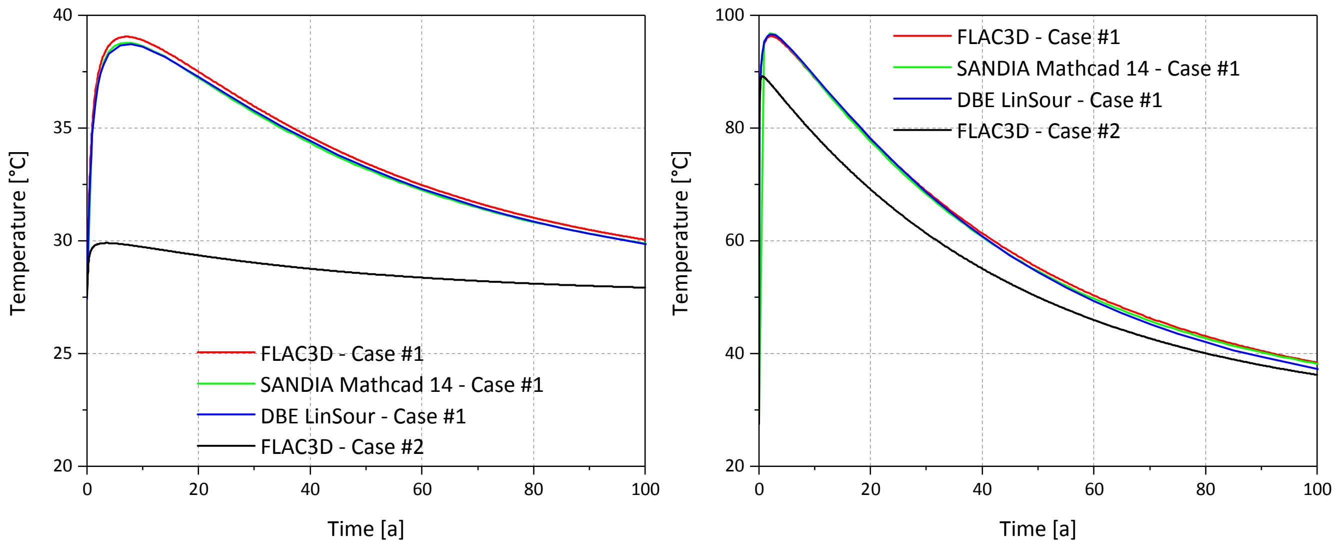

Figure 3: Prediction of temperature history at the drift wall (left) and the waste package surface (right) for Configuration 1

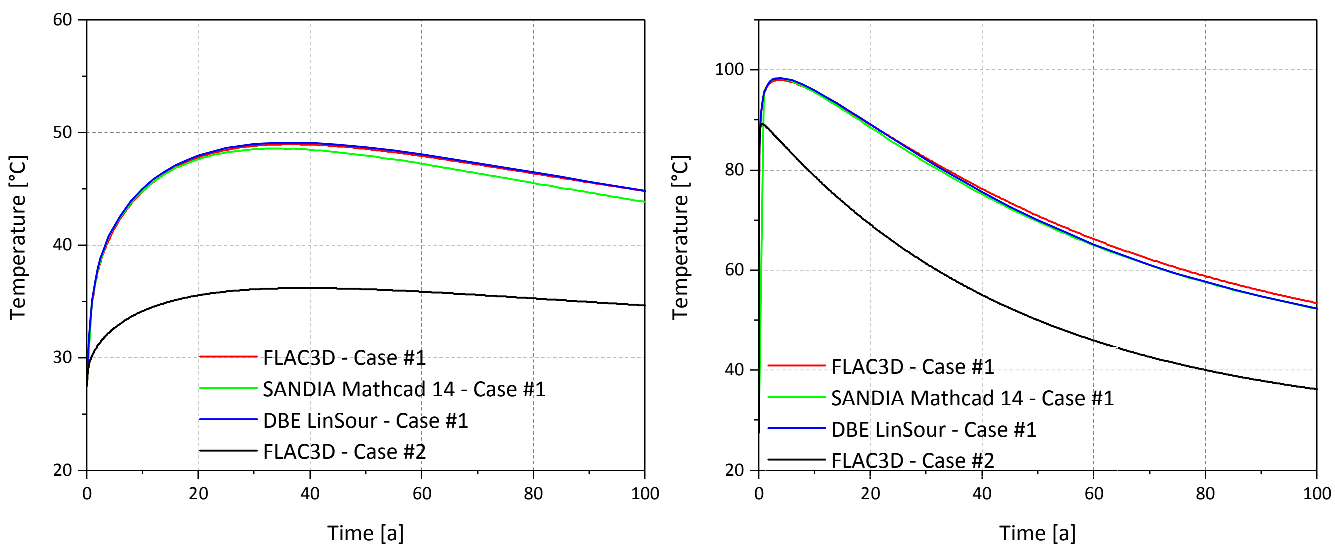

Figure 4: Prediction of temperature history at the drift wall (left) and the waste package surface (right) for Configuration 2

CONCLUSIONS

This paper presents conduction-based thermal simulations for the emplacement of nuclear waste in a geological repository in bedded salt. Benchmark simulations were conducted to assess the validity of semi-analytical codes to perform thermal simulations. Two waste package configurations were analyzed with the same parameter values applied to all materials. The first configuration involves a single waste package emplaced in an infinite medium.

The second configuration represents a repository layout with arrays of waste packages in different drifts. The investigation included use of the semi-analytical code LinSour used at DBE Technology in Germany, a Mathcad 14-based semi-analytical code used at Sandia National Laboratories, and the numerical code FLAC3D. These codes were used to calculate the temperature at the drift wall and waste package surface as a function of time for the two configurations. The results show that predictions of the three codes for Configurations 1 and 2 were comparable under identical initial and boundary conditions. Comparison of simulation results of the different software and simulation methods provided a confidence building measure for further analyses.

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