SAND2017-12466C

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 conduct heat transport. This first part of the study concentrated on heat flow from a single waste package in an infinite medium. Of particular importance to this work is comparison of predictions of peak temperature at the drift wall using different solution methods. The simulation results show that the outputs of the different methods are very close.

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 protection against radioactive waste for people and for the environment. However, temperature increases due to the disposal of the heat-generating waste can lead to thermomechanical damage and to changes in the chemical constitution of the rock. This can have a negative impact on the ability of the host rock to enclose the waste. Therefore, temperature limits in the rock may be 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. In this study, the host rock of interest is bedded salt.

Prior to disposal, the configuration of the waste packages in the repository can be 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 the present study is to assess the validity of such codes used in Germany and the United States. To this effect, a US-German working group has been set up between DBE TECHNOLOGY GmbH and Sandia National Laboratories.

The qualification studies for this study are 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. Note that as described above heat transport by conduction only 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

An example case is presented for testing analytical thermal models. The example case represents thermal analysis of a generic repository in bedded salt at 500 m depth. For this study heat conduction from a single waste package at a center of a drift 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 the same material was assumed for the waste package, the backfilling material in the drift and the host rock. Thus, simulations were conducted with intact salt only. Table I provides material properties used in the 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 6.1m. For this study decay heat given in Figure 1 is used. Surface storage of 10 years was assumed.

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 x 10^{-6}
Crushed salt	0.57	2200	561.6	4.613 x 10^{-7}

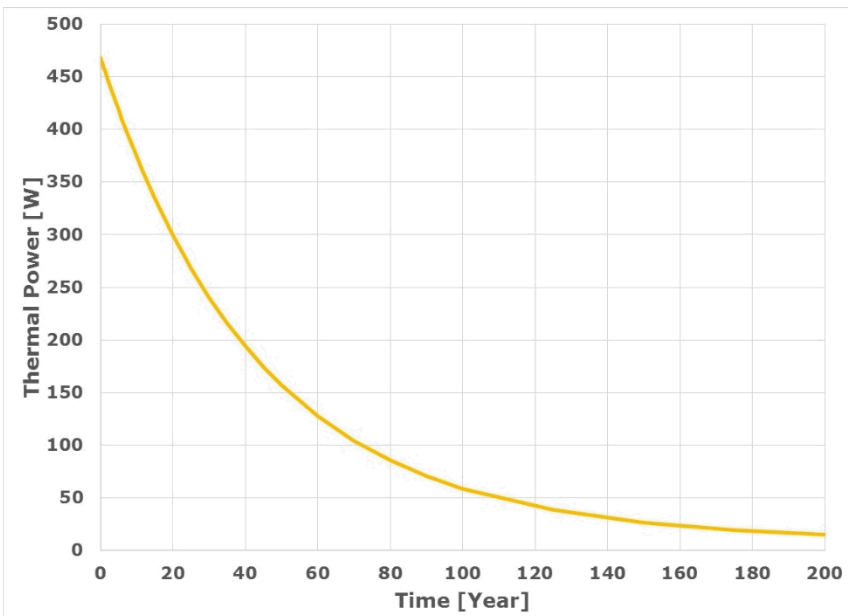

Figure 1. Thermal output of waste type considered.

The software used for the simulations are described below.

LinSour Software

LinSour or LINe SOURces is a computer code which has been developed to compensate the deficits of numerical codes when the thermal analysis of a whole repository with dimensions of up to several square kilometers over a time scale of millions of years have to be performed. It is the latest development of several researches 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, line shaped, 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]:

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

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 the thermal decay of the radioactive waste and is approximated in LinSour by a sum of exponential functions as follows:

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

$\Phi(t)$	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 the used coordinate system. In Addition, the time points at which the temperature has to be calculated must be specified.
2. LinSour calculates the distance between the line sources and the monitored points
3. In order 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 all time points. The temperature at such points will be set to a residual value
4. LinSour calculates the temperature at the monitored points at all time points through superposition of the temperature produced by all line sources. The temperature at each line source is calculated with the above equation. Only the monitored points which satisfy Step 3 will be considered in this operation.

The qualification model described in Section Model Setup has been simulated with LinSour. The results of these calculations are presented and compared to other codes in the Results and Discussion section.

Mathcad Based Thermal Analysis Software

A Mathcad-based semi-analytical thermal conduction model was also used for the analysis. The model is described in great detail in references [1,5]. The model considers thermal analysis of a central waste package together with contributions from adjacent waste packages, and waste packages in adjacent drifts. The model also includes radiation heat transfer, ventilation and other processes. Analytical solutions from different sources were utilized in developing the model. For the single waste package considered in this study the analytical solution of interest is finite line source in an infinite medium [6]. The finite line 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:

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

where,

T = temperature (initial or ambient temperature is added to get the final 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:

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

The Mathcad based model uses the finite line source solution (Eq. 3), the heat source given in Figure 1, and properties of the engineered barrier system to evaluate temperature at 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 in respect to time, temperature and pressure. Among the thermal conduction, other heat transport phenomena like conduction and radiation are also taking 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 qualification model will be calculated with 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 the numerical model which have been developed for the qualification problem described in the Model Setup section. The model is composed of the host rock where a drift is excavated. A cask is disposed in the drift which is backfilled by a crushed salt buffer. In the model, one can see the points where the temperature is monitored. The thermal decay described in Figure 1 is applied as volume specific heat-generating source in the cask.

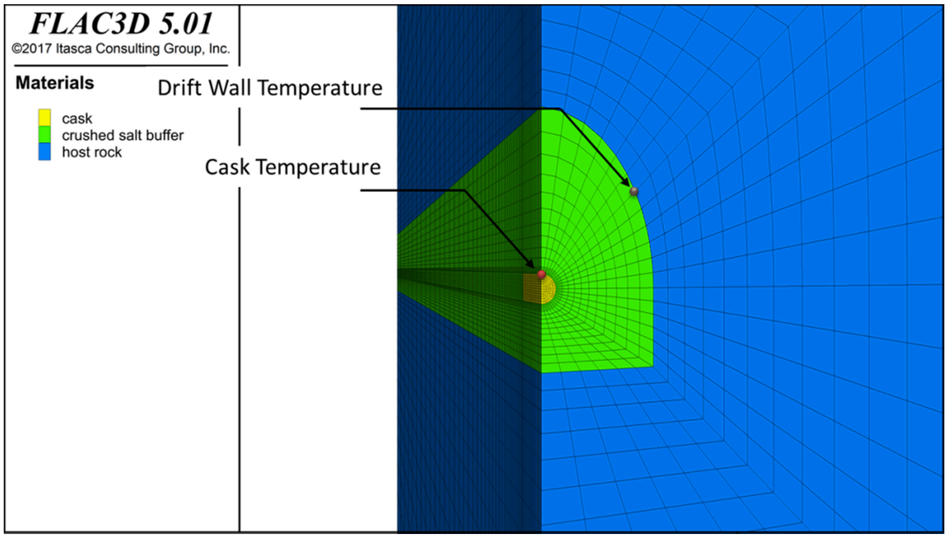

Figure 2. Numerical model of the qualification problem

The model is set up so that the initial and boundary conditions are identical to those of the semi-analytical codes. This insures a comparison of all codes under the same conditions. Therefore, Just the thermal process is considered in the simulation, i.e. the temperature dependence of rock salt and the pressure dependence of crushed salt is not taken into account. *Since the semi-analytical code LinSour can be used only for isotropic media*, further idealizations have to be considered in the numerical simulations: The same thermal material parameters are assigned to all materials (crushed salt, cask, rock salt) to establish isotropic conditions in the numerical model. With this approach, it is possible to determine the accuracy of the analytical codes in comparison to numerical code under identic conditions. Since the cask is embedded in the crushed salt buffer, on can expect that this material will have the highest influence on the temperature at near field. The thermal parameters of crushed salt have been therefore chosen for this simulation. A second simulation with properties of intact salt assigned to all materials was also conducted. The results of these simulations are presented and discussed below in the Results Discussion section.

RESULTS AND DISCUSSION

The results of the analysis of the qualification problem using the three codes LinSour, SANDIA Mathcad 14 and FLAC3D are presented in Figure 3. This case describe a model with intact salt material properties used everywhere. The curves in the Figure 3 represent the temperature at the monitored point at the drift wall over 100 years, see Figure 2.

In Figure 3, the maximum temperature in Mathcad (in green) is 29.87°C at 4 years. In FLAC3D (in red), a maximum of 29.76°C is reached at ca. 3.9 years which is mostly identic to the LinSour results (29.79°C at 4 years in blue). The maximum difference between the curves is less than 0.15°C which can be considered as negligible. Thus, the results obtained from all codes are very close. In addition, the shapes of the temperature curves are also identical over the simulation time. This proves that the physics of thermal conduction is well implemented in the semi-analytical codes.

The results show that under the same initial and boundary conditions the semi-analytical codes used in Germany and in the United States perform as well as a numerical code like FLAC3D. The comparison of the results described below in isotropic conditions using the intact salt material parameter shows a good accuracy even in realistic conditions. The results of the reference case are also close to those of other codes for the investigated problem. This does not mean that such a high accuracy will be reached for other different model setups with more complex geometry or with consideration of nonlinearities or at different locations for example. The results just show that under well-defined assumptions, semi-analytical codes can be used for thermal analysis in repository systems.

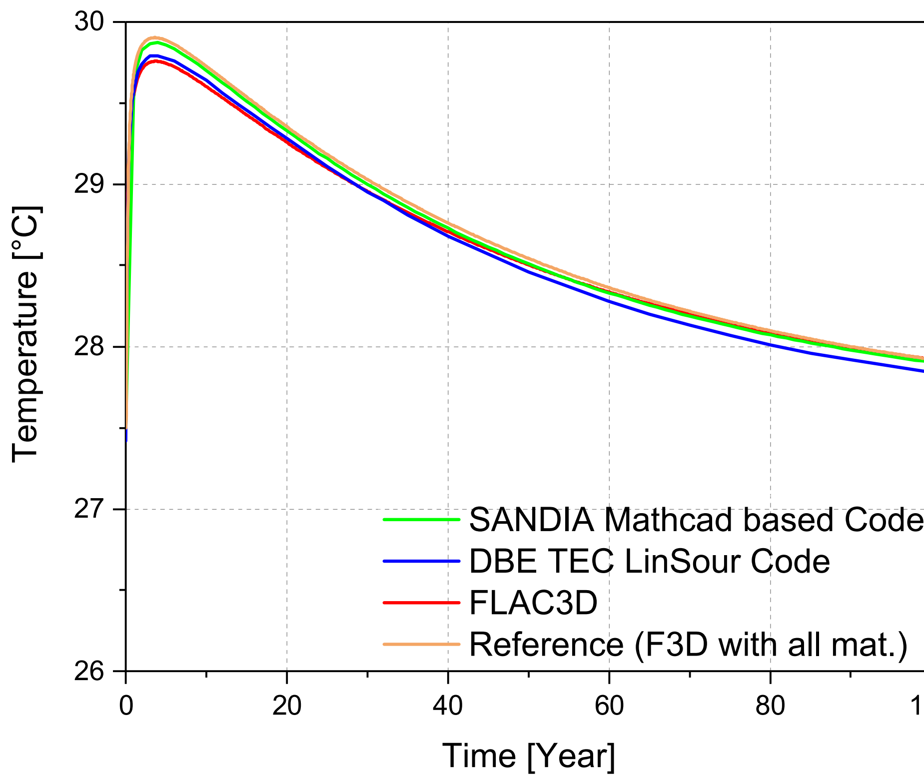

Figure 3. Temperature history prediction for the different methods for the case with intact salt material properties used everywhere, except for the reference case

CONCLUSIONS

Conduction-based thermal simulations of emplacement of a single waste package in a geological repository in bedded salt presented in this paper include use of two analytical codes and a numerical code. The different software were used to simulate thermal conditions at the drift wall as a function of time. As shown in the paper, all results of the different methods were very close. Comparison of simulation results of the different software and simulation methods provided a confidence building measure for further analyses. Further study will include simulations with addition of adjacent waste packages and drifts, and use of different materials. Future work will also include simulations for different repository waste emplacement layouts.

REFERENCES

1. E. Hardin, T. Hadgu, D. Clayton, R. Howard, H. Greenberg, J. Blink, M. Sharma, M. Sutton, J. Carter, M. Dupont, and P. Rodwell, “Disposal Concepts/Thermal Load Management (FY11/12 Summary Report)”, FCRD-UFD-2012-00219, Milestone: M3FT-12SN0804032, Work Package: FT-12SN080403, (2012).

2. H. Schmidt, Numerische Langzeitberechnungen instationärer Temperaturfelder mit diskreter Quellenverteilung unter Berücksichtigung temperatur- und ortabhängiger Stoffwerte,Dissertation, RWTH Aachen (1971)

3. P. Ploumen, G. Strickmann, Berechnungen der zeitlichen und räumlichen Temperaturverteilung bei der säkularen Lagerung hochradioaktiver Abfälle in Salzstöcken, Technical Report (1977)

4. K. Hahne, Vergleich von Methoden zur Berechnung der zeitabhängigen Temperaturverteilung in einem Endlager für radioaktive Abfälle, Dissertation (1988)

5. E. Hardin, J. Blink, H. Greenberg, M. Sutton, M. Fratoni, J. Carter, M. Dupont, and R. Howard, “Generic repository design Concepts and Thermal Analysis”, FCRD-USED-2011-000143, Rev. 0 (2011).

6. M. Sutton, J. A. Blink, M. Frantoni, H. R. Greenberg, W. G. Halsey, and T. J. Wolery, “Disposal System Evaluation Framework (DSEF) Version 1.0 – Progress report”, LLNL-TR-484011, Lawrence Livermore National laboratories, (2011).

ACKNOWLEDGEMENTS

DBE TECHNOLOGY GmbH is a wholly owned subsidiary of DBE - the German Company for Construction and Operation of Waste Repositories (a limited liability company) - which has been commissioned by the Federal Government to explore potential sites, and to design, construct, and operate the federal radioactive waste repositories.

This research work was supported by the German Federal Ministry for Economic Affairs and Energy (BMWi = Bundesministerium für Wirtschaft und Energie) represented by the Project Management Agency Karlsruhe (Karlsruhe Institute of Technology, KIT), under contract no. FKZ 02 E 1405A.

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