



Thermal dimensioning to determine acceptable waste package loading and spatial configurations of heat-generating waste packages

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ABSTRACT

Heat-generating waste provides a number of additional technical challenges over and above those associated with the disposal of ILW. A priority area of work for Radioactive Waste Management (RWM) concerns the effect of heat on the engineered barrier system, and how this may be mitigated through the management of heat (thermal dimensioning) in a UK Geological Disposal Facility (GDF). The objective of thermal dimensioning is to provide a strategy to enable acceptable waste package loading and spatial configurations of the packages to be determined in order to enable high-heat generating waste to be successfully disposed in a GDF. An early focus of the work has been to develop a thermal modelling tool to support analyses of different combinations of package assumptions and other GDF factors, such as spacing of those packages, to assess the compliance with thermal limits. The approach has a capability to investigate quickly and efficiently the implications of a wide range of disposal concepts for the storage of spent fuel/HLW and the dimensions of a GDF. This study describes the approach taken to undertaking this work, which has included a robust appraisal of the key data (and the associated uncertainty); recent thermal dimensioning analysis has been performed to identify constraints on those disposal concepts.

KEYWORDS: thermal dimensioning, waste packages, heat-generating waste, Geological Disposal Facility, GDF.

Introduction

THE disposal of high-heat-generating wastes in a Geological Disposal Facility (GDF) creates a number of technical questions that need to be addressed in order that a safe disposal solution can be developed. Project Ankhiale has been established by Radioactive Waste Management Limited specifically to address these questions. The project aims to enhance the understanding of the factors affecting geological disposal of high-heat generating wastes

with a view to supporting the development of the disposal system specification for these wastes (i.e. the disposal system requirements) and spent fuel life cycle options (e.g. supporting the development of packaging solutions). A full description of the scope of work being undertaken is provided in the project roadmap (Holton *et al.*, 2012).

The wastes for geological disposal are referred to as higher activity wastes and comprise all radioactive material that has no further use and that cannot be managed under the Policy for the Long-term Management of Solid Low Level Radioactive Waste in the United Kingdom (DEFRA, 2007) through, for example, emplacement in the Low-level Waste Repository (LLWR). Included in these

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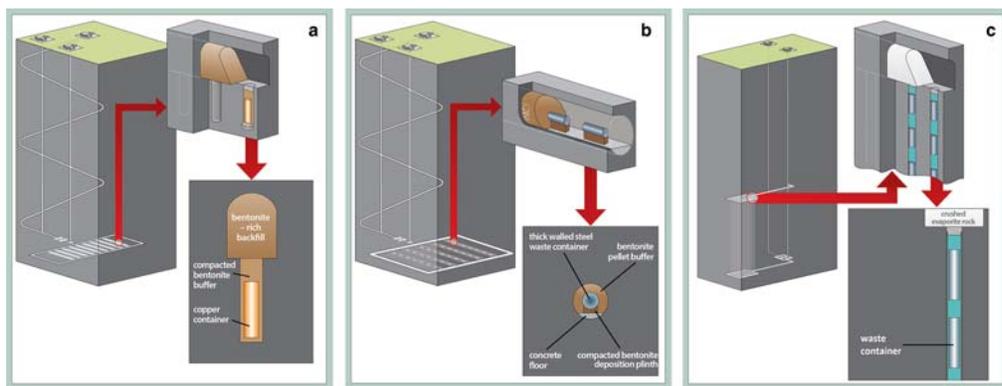


FIG. 1. (a) Concept A1, (b) Concept A2, (c) Concept A3. Figure published with permission of the NDA.

higher activity wastes are a number of high-heat generating wastes and nuclear materials (spent fuel, uranium and plutonium) that are subject to government policy decisions and nuclear plant operating decisions, and therefore may be declared as wastes in the future.

One important aspect of Project Ankhiale is to develop further the understanding of constraints placed on various Engineered Barrier System (EBS) materials by the disposal of high-heat generating waste. One such constraint is to ensure the temperature of the buffer material is within limits such that its safety functions are not unduly impaired. The process of spacing out the heat generating waste to ensure these limits are not exceeded is called thermal dimensioning.

Thermal Dimensioning Tool

The Project Ankhiale Thermal Dimensioning Tool (TDT) has been developed to explore, for a series of disposal concepts, the impact of a range of key physical parameters and engineering decisions on the temperature in the EBS (Myers *et al.*, 2014).

Requirements on the Thermal Dimensioning Tool are that:

- (1) It has the ability to efficiently perform thermal dimensioning for the range of disposal concepts for heat generating waste.
- (2) It uses analytical and semi-analytical expressions to solve the relevant heat conduction problem to take full advantage of speed and ‘accuracy’ inherent in these approximations, when allied to simple geometrical configurations of the waste.
- (3) It can model the consequences of parametric uncertainty.

(4) It supports the project principle of quality assurance of data, reinforcing the basic principles of verification and data management.

(5) It has a simple, clear user interface to help the user construct a model.

Disposal concepts

The TDT can perform thermal dimensioning on five illustrative disposal concepts (NDA RWMD, 2010):

(1) Concept A1 (Fig. 1a). Concept A1 describes the emplacement of copper disposal containers in vertical deposition holes. The disposal containers are surrounded by a compacted bentonite buffer. The compacted bentonite buffer leaves small gaps (a few millimetres to a centimetre) at the interfaces between the disposal container and buffer, and between the buffer and host rock. It is assumed that the innermost gap is open at the time of emplacement, and that the outermost gap is filled with bentonite pellets. A higher-strength host rock is assumed.

(2) Concept A2 (Fig. 1b). Concept A2 describes the emplacement of carbon-steel disposal containers horizontally along the centre of emplacement tunnels. A pelleted bentonite backfill is assumed, and a cementitious tunnel lining may be specified. It is assumed this is applicable to a lower-strength sedimentary host rock.

(3) Concept A3 (Fig. 1c). Concept A3 describes the emplacement of disposal containers vertically in a mined borehole matrix of deposition holes. The disposal containers are of smaller diameter than the standardized designs, for consistency with international precedents for this concept. A number of disposal containers are emplaced in each deposition

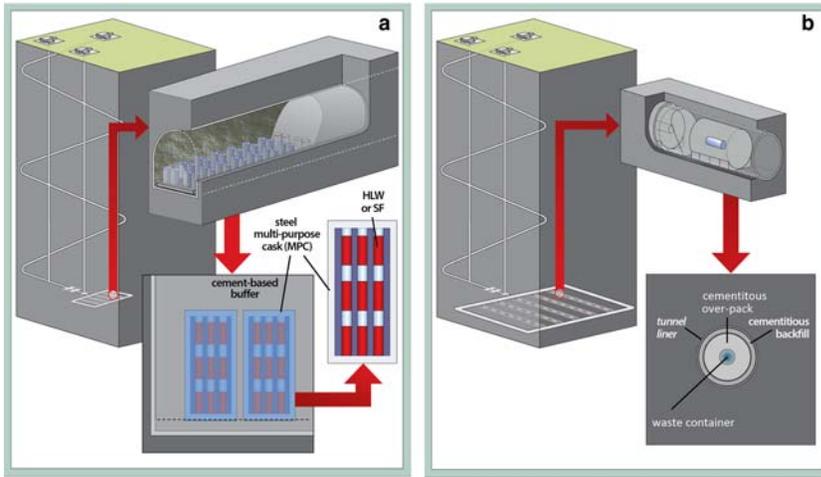


Fig. 2. (a) Concept B, (b) Concept C. Figure published with permission of the NDA.

hole, separated from each other. The assumed host rock is an evaporite. A backfill of crushed host rock would be used.

(4) Concept B (Fig. 2a). Concept B describes the emplacement of rows of multi-purpose containers standing vertically in a disposal vault. A cementitious backfill and higher-strength host rock have been assumed.

(5) Concept C (Fig. 2b). Concept C describes the emplacement of pre-fabricated engineered modules ('super-containers') horizontally along emplacement tunnels. The pre-fabricated engineered modules incorporate a carbon steel disposal container within a cementitious over-pack. Any remaining volume in the emplacement tunnels is backfilled with cement. A cementitious tunnel lining may be specified. A lower-strength sedimentary host rock is assumed.

Methods

There are two possible approaches to calculating the temperature in the vicinity of a disposal container for either high-level waste or spent fuel. The first is based on semi-analytical models and the second is based on numerical models (e.g. a finite-element model) implemented in a computer program. Both approaches have advantages and disadvantages. The use of a semi-analytical approach is capable of giving more insight into the key parameters influencing the temperature rise and is numerically efficient, but may require simplifications to the geometry and assumptions

about the properties of the host rock (e.g. the thermal conductivity is homogenous). Conversely, although a numerical approach can represent the geometry and thermal properties accurately, it is computationally intensive.

Currently, RWM does not have a site for the disposal of radioactive wastes, and is still evaluating a number of disposal concepts. Given the generic nature of this current work, the semi-analytical approach is most appropriate for thermal modelling, and has been used in the TDT. However, a limited set of detailed numerical calculations will be run to verify the TDT.

The TDT makes use of a number of modelling assumptions to represent heat generated from a GDF in a computationally efficient way. This involves the superposition of the heat contribution at a point of interest from each of the heat sources in the GDF. The main region of interest within a GDF is the temperature in the EBS surrounding the hottest disposal container. Within the TDT, a GDF is split into three regions: The 'detail window' within the local module, surrounding the point of interest where the temperature is calculated and a detailed description of the near field is required; the rest of the local module; and distant modules. Figure 3 describes the layout for a typical Concept A1 representation. The size of the detailed window would depend on the disposal concept and the separation between each waste container: typically this could be of the order of several tens to a hundred metres.

The nearest containers to the point of interest are represented as compound line sources (with the

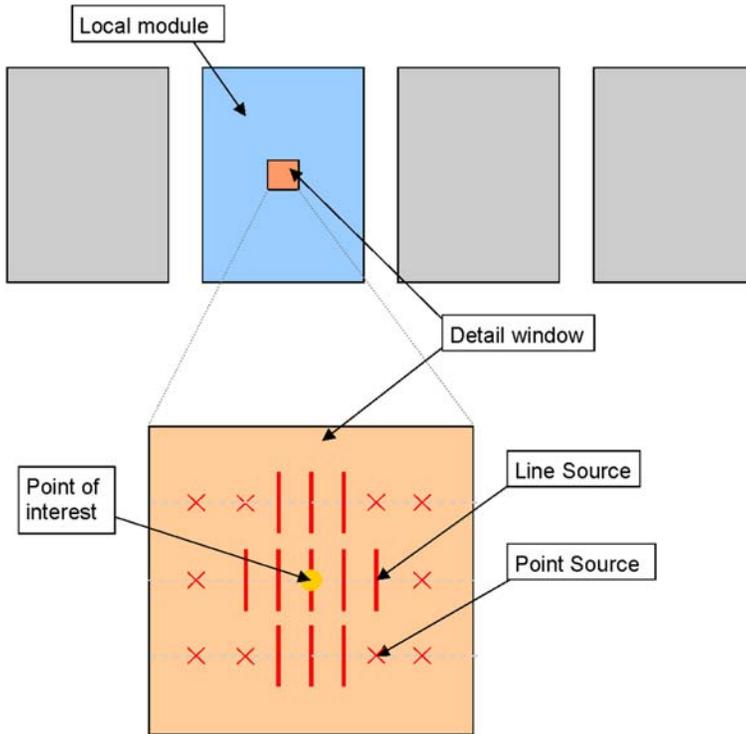


FIG. 3. Concept A1 as modelled by the TDT, showing how different types of source are arranged. The local module is shown in blue, and the detail window is in orange. The distant modules are grey. Figure published with permission of the NDA.

main body of the container treated as a line source, and the flat ends treated as point sources), with the line contribution given by equation 1 (Carslaw and Jaeger, 1959; Hökmark *et al.*, 2009):

$$T_p(r, z; t) = \frac{1}{\rho c 4 \pi a} \int_0^t \frac{Q(t')}{H_c \sqrt{t-t'}} e^{-\frac{r^2}{4a(t-t')}} \times \frac{1}{2} \left(\operatorname{erf} \left(\frac{H_c + z}{\sqrt{4a(t-t')}} \right) + \operatorname{erf} \left(\frac{H_c - z}{\sqrt{4a(t-t')}} \right) \right) dt' \quad (1)$$

where H_c is half the height of the line source, r is radial distance, z is axial distance, t is time, a is thermal diffusivity of host rock, given by $a = k/(\rho c)$, k is the (effective) thermal conductivity of the host rock, c is the specific heat capacity of the host rock, and ρ is the density of the host rock.

More distant containers, still within the detail window are represented as point sources (Carslaw

and Jaeger, 1959; Hökmark *et al.*, 2009):

$$T_p(r; t) = \frac{1}{\rho c (\sqrt{4 \pi a})^3} \int_0^t \frac{Q(t')}{(\sqrt{t-t'})^3} e^{-\frac{r^2}{4a(t-t')}} dt' \quad (2)$$

The rest of the local module, and each distant module, are represented as extended plane sources, whose contribution is described by (Carslaw and Jaeger, 1959):

$$f = \frac{1}{\rho c \sqrt{4 \pi a} (t-t')} \left(e^{-\frac{z^2}{4a(t-t')}} - e^{-\frac{(z-2H)^2}{4a(t-t')}} \right) \quad (3)$$

$$h = \frac{1}{4} \left(\operatorname{erf} \left(\frac{L_x + x}{\sqrt{4a(t-t')}} \right) + \operatorname{erf} \left(\frac{L_x - x}{\sqrt{4a(t-t')}} \right) \right) \left(\operatorname{erf} \left(\frac{L_y + y}{\sqrt{4a(t-t')}} \right) + \operatorname{erf} \left(\frac{L_y - y}{\sqrt{4a(t-t')}} \right) \right) \quad (4)$$

$$T_p(x, y, z; t) = \int_0^t \frac{Q(t')}{p_x p_y} f h dt' \quad (5)$$

where H is the distance between the GDF, which is

assumed to be located at $z = 0$, and ground level, L_x is half the length of the rectangular plane in the x direction (i.e. along the tunnels) and L_y is half the width in the y direction (i.e. across the tunnels). The second exponential term in equation 3 accounts for the 'negative mirror' source used to implement the top surface boundary condition. p_x and p_y are the container separations in the x - and y -directions. This approach allows fast computation of the heat contribution from effectively many thousands of disposal containers.

It is worth noting that a line heat source is an excellent approximation of a cylindrical canister, when temperature is measured at a distance. However, the heat flux from a real cylindrical canister is not uniformly distributed along its length.

TDT inputs

The TDT interfaces with the Project Ankhiale Database, which acts as a repository for the carefully identified data (and parametric uncertainty) associated with each disposal concept. These data are loaded when a disposal concept is chosen. With the additional specification of one or multiple disposal container inventories per GDF, the thermal dimensioning assessment can be performed. Inventories are generated by the Project Ankhiale inventory tool. Figure 4 describes the relationship between the Inventory Tool, the Project Ankhiale database and the TDT. Categories of input include: (1) disposal container inventory; (2) disposal container design; (3) repository design;

(4) EBS thermal properties; (5) geosphere thermal properties; and (6) GDF layout.

The inventory is input as a list of 229 activities associated with relevant radionuclides. Each reaction sequence (involving decay or neutron capture) of each radionuclide will generate heat. The thermal power curve takes account of all of the relevant radionuclides. A series of 15 exponentials is fitted to the power curve to give an efficient evaluation of the power output at a given time.

Example outputs

The TDT runs a series of calculations, to determine the expected temperature of the EBS based on the reference case parameters, and a range of temperatures based on the uncertainty ranges in the supplied data. The graphs in Fig. 5 show typical outputs from a TDT run. The standard outputs are intended to allow the assessment of which parameters have a large impact on the EBS temperature.

The TDT also allows the specification of iteration loops over the specified ranges for various parameters (e.g. disposal container separation, host rock thermal conductivity).

Verification and testing

A series of 2D and 3D calculations were completed to both confirm and demonstrate an understanding of the approximations made as part of semi-analytical analysis in the TDT. In particular, a comparison was made between the line source approximation and

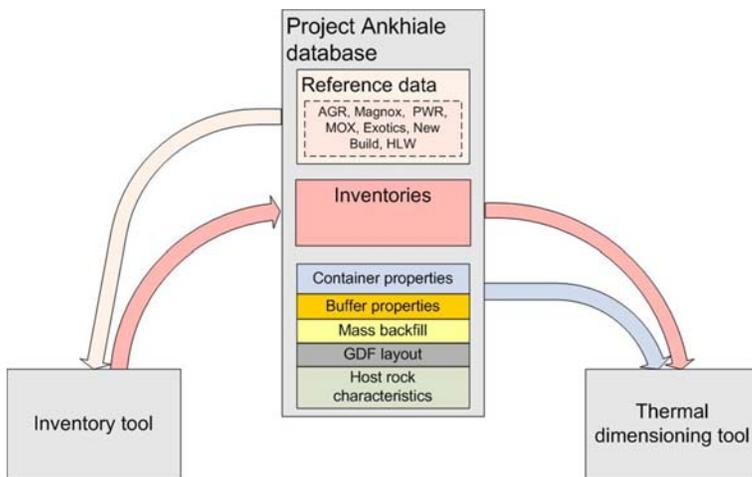


FIG. 4. Relationship between the Inventory Tool, the Thermal Dimensioning Tool and the Project Ankhiale database. Figure published with permission of the NDA.

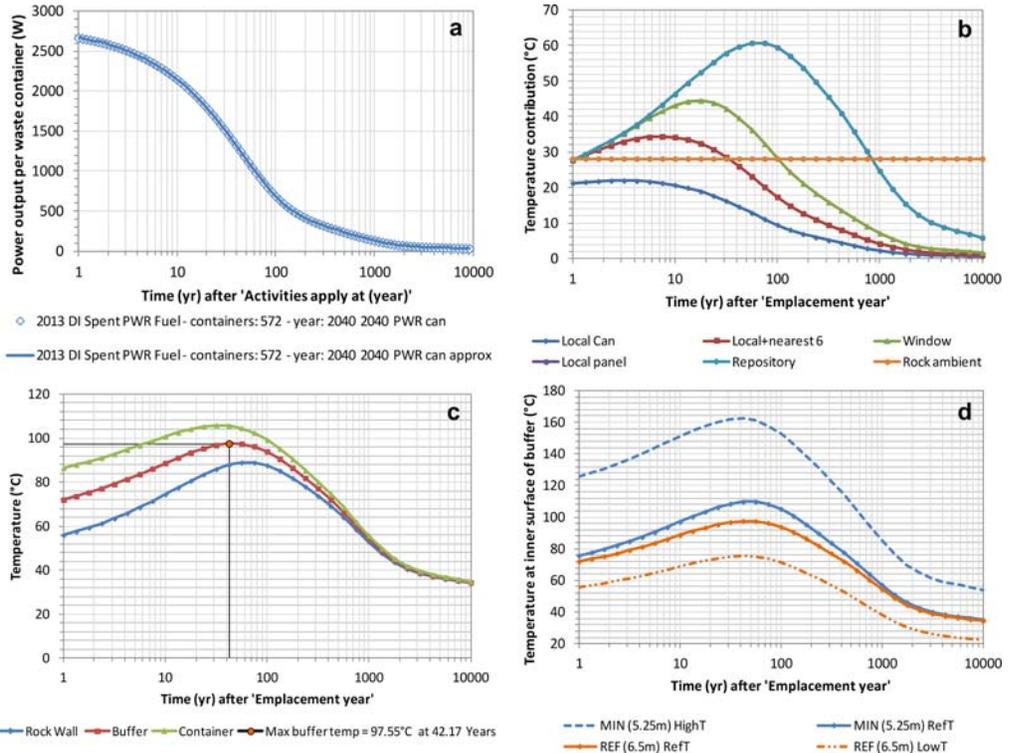


FIG. 5. (a) The power curve from an illustrative inventory of spent PWR fuel; (b) The contribution to the temperature of the rock adjacent to the buffer in contact with a container from all of heat-generating waste containers at different distances (*Local Can* is the contribution to the temperature from the local canister/container; *Local + nearest 6* is the contribution from the local container and the next 6 nearest containers; *Window* is the contribution from a wider collection of containers; both *Local panel* and *Repository* is the contribution from all of the containers for this illustrative model); (c) This shows the evolution of the *Container* temperature, the *Buffer* temperature, and temperature of the rock adjacent to the buffer; (d) This shows the effect of changing both the host rock and buffer material properties to reflect the reference values and the range of these parameters, at this generic stage. *RefT* corresponds to the reference parameters (at different package spacing). *HighT* corresponds to the combination of parameters providing the highest temperature; *LowT* corresponds to the combination of parameters providing the lowest temperature. Figure published with permission of the NDA.

numerical calculations in which the full geometry of the container was considered. It is recognized that the cases considered did not cover all eventualities, but did provide adequate reassurance of the validity of the approximations over a suitable range.

The main modelling stage concerned calculations at the container scale. This is the most important scale for the assessment of the maximum buffer temperature. These activities were undertaken to determine (confirm) the adequacy of the modelling assumptions used in the TDT at the package scale. This follows the approach adopted by SKB for the KBS-3V disposal concept. 3D verification included the following tests:

(1) Modelling to test the assumption that the geometry of a container can be represented adequately as a 'line source' (with the analytical end correction factor), for each of the different concepts.

(2) Modelling to consider the effect on the maximum temperature of the buffer material on different choices of the canister materials, e.g. copper and cast iron (high thermal conductivity and moderate thermal conductivity). These calculations were to establish the efficacy of the approximations made and the applicability of analytical approximations (i.e. when it can be made), for each of the different container concepts.

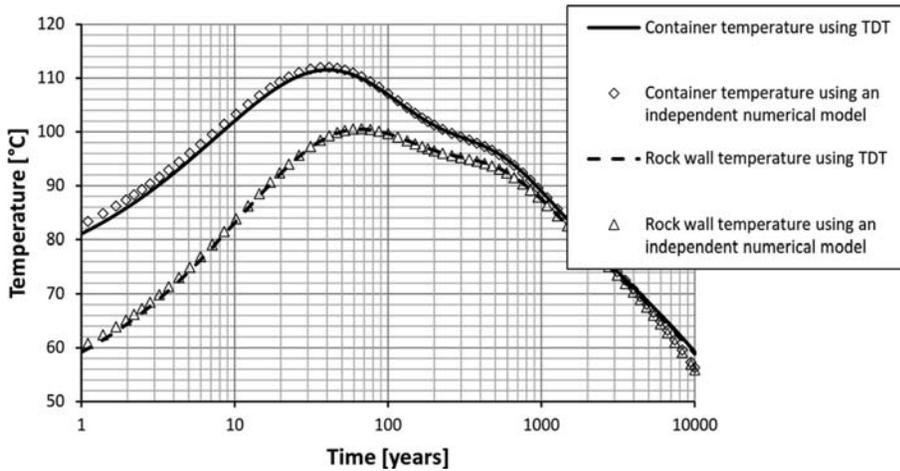


FIG. 6. A comparison between the TDT and a finite element model used to model a single module (an array of vaults) of high-heat-generating waste for disposal Concept A1. It shows the maximum temperature evolution of both the buffer and rock wall. Figure published with permission of the NDA.

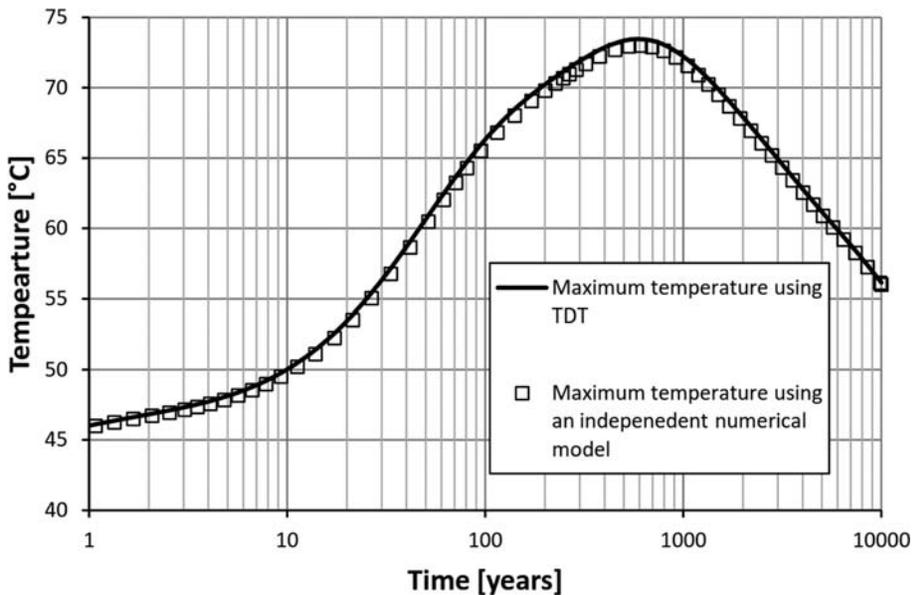


FIG. 7. A comparison between the TDT and a finite element model used to model a single module (consisting of a large array of boreholes) of high-heat-generating waste for disposal Concept A3. It shows the maximum temperature evolution of the rock wall (in contact with the container). Figure published with permission of the NDA.

(3) Modelling to assess the effect of incomplete slots (unfilled capacity in the waste container) or different spent fuel in different slots (radially inhomogeneous) and the profile of heat along the canister if inhomogeneous as a result of either burn-up being higher at the centre of fuel or disposing of shorter fuel elements. This was to assess whether it is

adequate to consider the total heat within the canister to define the power source, for each of the different container concepts.

(4) Initial modelling to scope the effects of other coupled processes, in particular variable saturation.

Extensive verification of the approximations used in TDT has been conducted using detailed

finite-element models. Figures 6 and 7 show two examples of some of the supporting verification of the thermal dimensioning tool (TDT) for disposal Concept A1 and Concept A3, respectively, using an independent numerical model. They demonstrate good agreement between the approaches with temperature differences, for the cases illustrated, typically less than 2% of the maximum.

Summary

The purpose of the TDT model is to explore the parameter space associated with the thermal calculations for each disposal concept and for a variety of high-heat-generating waste types, in order to discover the key parameters that affect the temperature of the buffer material in the GDF and how they affect the temperature evolution of the EBS.

The TDT tool has provided a significant advance in thermal modelling of a range of disposal concepts in the UK. Particular innovations in the tool are that it:

(1) Reads information directly from the project database reducing the possibility of errors being introduced.

(2) Can identify user changes from these 'agreed' values to enable quality assurance checking to be accomplished efficiently.

(3) Allows the flexibility to model a wide range of disposal concepts (five concepts rather than only one allowed for previously).

(4) Speeds up the calculation time by a factor of several hundred times faster than similar semi-

analytical tools and hundreds of thousands times faster than other possible tools.

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References

- Carlsaw, H.S. and Jaeger, J.C. (1959) *Conduction of Heat in Solids*, 2nd Edition. Oxford, Clarendon Press.
- Defra (2007) *DTI and the Devolved Administrations of Scotland, Wales and Northern Ireland, Policy for the Long Term Management of Solid Low Level Radioactive Waste in the United Kingdom*. PB 12522.
- Hökmark, H., Lönnqvist, M. and Kristensson, O. (2009) *Strategy for Thermal Dimensioning of the Final Repository for Spent Nuclear Fuel*. SKB Rapport R-09-04.
- Holton, D., Dickinson, M., Hoch, A., Cowper, M., Thetford, R., Allinson, H., Crockett, G., Cairns, M., Roberts, D., Padovani, C., Johnson, M., Carr, N., Jowett, J., Finch, C., Walsh, C., Southgate, B., Wood, P. and Young, A. (2012) *Project Ankhiale: Disposability and Full Life Cycle Implications of High-heat Generating UK Wastes: Roadmap*. AMEC Report D.006297/001 Issue 1.
- Myers, S., Leung, C. and Holton, D. (2014) *Project Ankhiale, User Guide: the Thermal Dimensioning Tool (TDT) Version 1.01*. AMEC Report 103726-0010-UA00-TLN-0002 Issue 3.
- NDA RWMD (2010) *Geological Disposal: Generic Disposal Facility Designs*. NDA/RWMD/048.