Thermal Analysis to Determine Acceptable Package Loading and Spatial Configurations of High-Heat-Generating Wastes - 15411

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ABSTRACT
The inventory of radioactive materials planned for geological disposal in the UK is diverse. This inventory includes a range of high-heat-generating wastes and other radioactive materials not currently declared as waste including some spent nuclear fuel and separated uranium and plutonium. To ensure that safe disposal solutions can be developed, it will be necessary to understand the influence of this heat on engineered barrier systems for the range of generic disposal concepts being considered in the UK. For these reasons, Radioactive Waste Management Limited has established a dedicated project to enhance understanding of the factors affecting geological disposal of high-heat-generating wastes with a view to supporting future decision making and concept selection.

One of the priority areas to be addressed within the High-heat-generating Waste Project (Project Ankhiale) concerns the effect of heat on the engineered barrier systems. The core focus of the work is to identify the thermal constraints on specific outline conceptual designs, building upon the findings of other work activities aimed at understanding the influence of heat on buffer materials. The constraints on the design relate to important features of the engineered barrier system and parameters such as waste package loading, package dimensions and package spacing. Work is underway to identify an acceptable range of designs and parameters for waste package disposal concepts and layout of the GDF.

INTRODUCTION
The Nuclear Decommissioning Authority (NDA) is responsible for planning and implementing geological disposal in the UK and has established the Radioactive Waste Management Limited (RWM) (a wholly owned subsidiary) for this purpose. The RWM work programme is currently at a generic stage as the geological environment for a geological disposal facility (GDF) is not yet known. A range of possible disposal concepts have therefore been identified to enable disposal of the wide range of radioactive wastes in the range of possible geological environments. This is to illustrate the potential range of engineered and natural barriers that could be used for a GDF in the UK, upon which generic safety cases can be developed.

The inventory of radioactive wastes planned for geological disposal in the UK is diverse. This inventory includes a range of high-heat-generating wastes and potentially some other nuclear materials (some spent fuel, uranium and plutonium) that is subject to government policy decisions and therefore may be declared as wastes for geological disposal in the future. The inventory of high-heat-generating UK wastes and materials therefore potentially includes the following [1]:

- Vitrified High Level Waste (HLW) from spent fuel reprocessing;
- Advanced Gas Reactor (AGR) spent fuel (SF) that is not reprocessed;
- LWR SF from Sizewell B (currently the UK's only LWR);
- SF from a potential LWR new build programme;
- "Exotic" fuels (includes a range of fuels from UK research and defence activities);

- Magnox[1] SF (if not reprocessed);
- Mixed-oxide (MOX) SF (from any future re-use of UK plutonium);
- Separated (unirradiated) plutonium.

For the purpose of robust planning, the materials above are assumed to be declared as waste and plans for its disposal in a GDF must therefore be developed.
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 [2] and a paper presented (15339) [3].

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 exploring the spacing out the heat generating waste to ensure these limits are not exceeded is called thermal dimensioning.

DISPOSAL CONCEPTS

The RWM work programme is currently at a generic stage as the geological environment for a GDF is not yet known. A range of possible disposal concepts have therefore been identified to enable disposal of the wide range of radioactive wastes in the range of possible geological environments.

For the purposes of the Project, a range of concept options was selected that is focused on the most likely combinations of waste type, container type and material of construction, buffer material, backfill material, geology and concept geometry. The options have been developed around three basic container types: disposal canisters, multi-purpose containers (MPCs) and supercontainers [4]:

- **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. A higher-strength host rock is assumed.
- **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. It is assumed this is applicable to a lower-strength sedimentary host rock.
- **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 standardised designs, for consistency with international precedents for this concept. A number of disposal containers are emplaced in each deposition hole, separated from each other. The assumed host rock is an evaporite. A backfill of crushed host rock would be used.
- **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.
- **Concept C** (Fig. 2b) – Concept C describes the emplacement of pre-fabricated engineered modules (‘supercontainers’) horizontally along emplacement tunnels. The pre-fabricated engineered modules incorporate a carbon steel disposal container within a cementitious over-

[1] Magnesium-alloy clad metallic uranium fuel used in the UK’s first generation of commercial gas-cooled power reactor.

pack. Any remaining volume in the emplacement tunnels is backfilled with cement. A lower-strength sedimentary host rock is assumed.

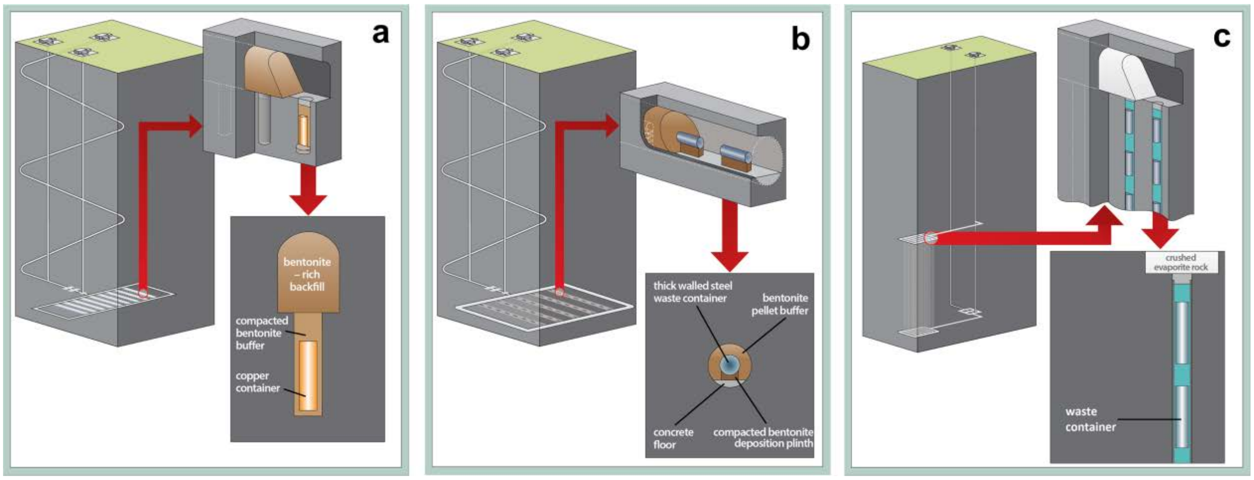

Fig. 1. (a) Concept A1, (b) Concept A2, (c) Concept A3

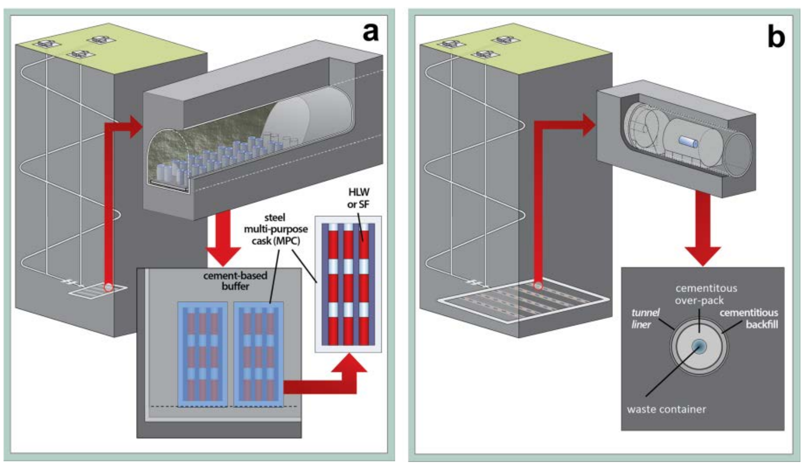

Fig. 2. (a) Concept B, (b) Concept C

THERMAL DIMENSIONING TOOL

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

At this generic stage of development of disposal concepts in the UK the TDT was designed such that:

- It has the ability to efficiently perform thermal dimensioning for a range of disposal concepts for heat generating waste
- 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

- It can model the consequences of parametric uncertainty
- It supports the project principle of quality assurance of data, reinforcing the basic principles of verification and data management
- It has a simple, clear user interface to help the user construct a model

MATHEMATICAL APPROACH

There are broadly two possible approaches to calculating the temperature in the vicinity of a disposal container of high-heat-generating waste. The first is based on analytical or semi-analytical approach, in which closed form solutions can be exploited, or the second is based on purely on a numerical approach where the equations and domain are discretised and solved (e.g. a finite-element model). Both approaches have advantages and disadvantages. The use of a semi-analytical approach is capable of providing more insight into the key parameters influencing the temperature rise and is usually highly 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 phase of work, the semi-analytical approach is most appropriate for thermal modelling, and has been used in the TDT. However, a set of independent detailed numerical calculations have been performed to verify the TDT approximation for a range of disposal concepts.

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 more detailed description of the EBS is required; the rest of the local module; and distant modules. Fig. 3 describes the layout for a typical representation of Concept A1.

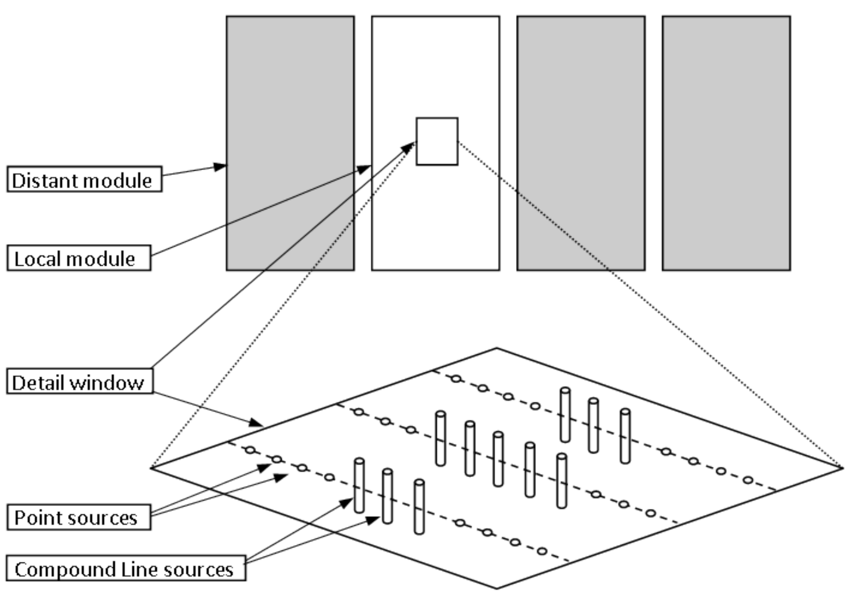

Fig. 3. Concept A1 as modelled by the TDT

This shows how different types of source are arranged. The local module is shown as the larger white rectangle, and the detail window is shown as the smaller rectangle. The distant modules are grey.
The nearest containers to the point of interest are represented as compound line sources (with the main body of the container treated as a line source, and the ends treated as point sources), with the line contribution given by [5, 6]:

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

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 [5, 6]:

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

The rest of the local module, and each distant module, are represented as extended plane sources, whose contribution is described by [5, 6]:

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

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

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

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 a 'negative mirror' source which supplies the 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.

MANAGING TDT DATA

The TDT interfaces with the Project Ankhiale Database, which acts as a quality assured repository for the data (and parametric uncertainty) associated with each disposal concept. This data is 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. Fig. 4 describes the relationship between the Inventory Tool, the Project Ankhiale database and the TDT. Categories of input include:

- Disposal container inventory
- Disposal container design
- Repository design
- EBS thermal properties

- Geosphere thermal properties
- GDF layout

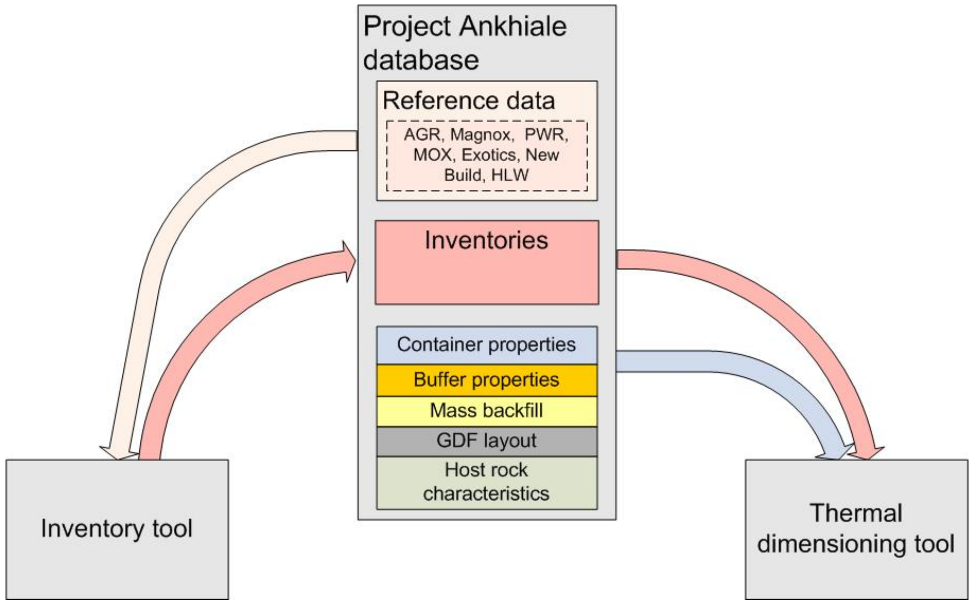

Fig. 4. Relationship between the Inventory Tool, the Thermal Dimensioning Tool and the Project Ankhiale database.

The inventory is input as a list of 229 activities associated with relevant radionuclides. A calculation is then performed to generate a power curve. A series of 15 exponentials is fitted to the power curve to give an efficient evaluation of the power output at a given time.

VERIFICATION AND TESTING

A series of 2D and 3D finite element calculations were completed to both confirm and demonstrate an understanding of the approximations made as part of semi-analytical approach used in the TDT.

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:

- Modelling to test the assumption that the thermal contribution of a container can be represented adequately as a “line source” (with an analytical correction factor to account for heat flux from the ends of the container) for each of the different concepts.
- Modelling to test if distant contributions from the other heat-generating-waste can be adequately approximated by point and plane source terms
- 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. 5 and Fig. 6 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 typically less than 2% of the maximum.

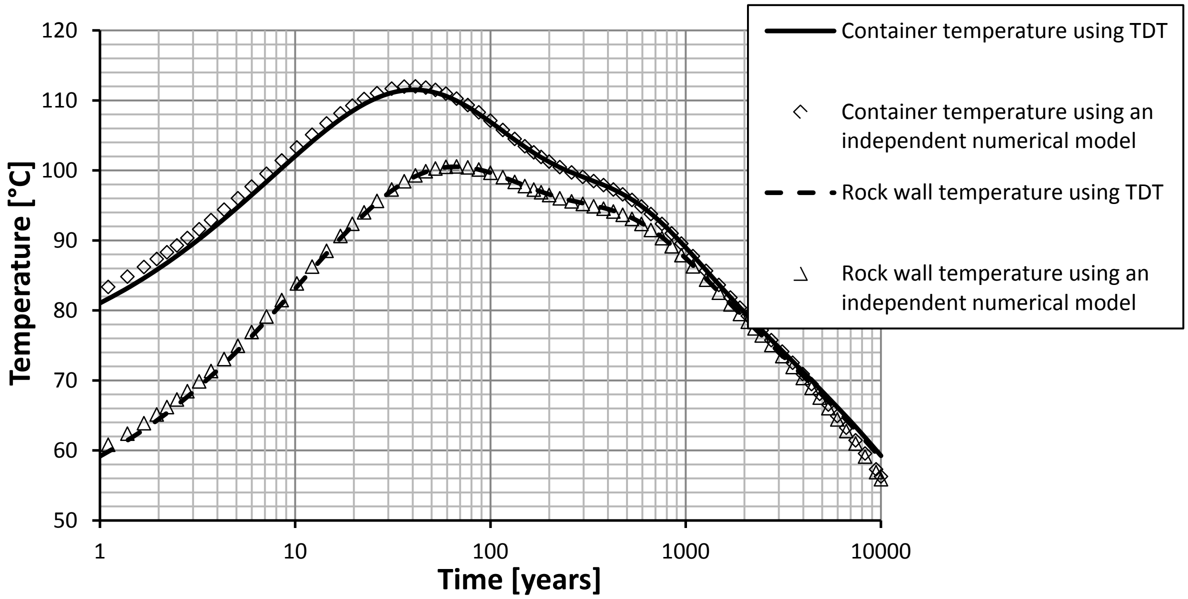

FIG 5. A comparison between TDT and a finite element model used to model a single module of high-heat-generating waste for disposal Concept A-1. It shows the maximum temperature evolution of both the buffer and rock wall.

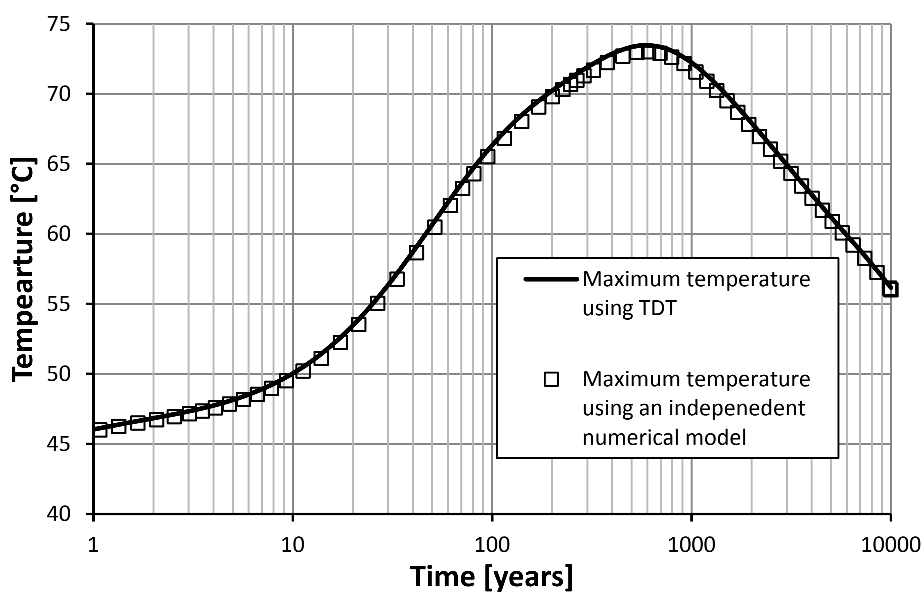

FIG 6. A comparison between the TDT and a finite element model used to model a single module of high-heat-generating waste for disposal Concept A-3. It shows the maximum temperature evolution of the rock wall (in contact with the container).

Extensive verification of the approximations used in TDT has been conducted using detailed finite-element models this has revealed that he analytical approach can be extremely effective at modelling a broad range of geometrical configurations.

AN EXAMPLE OF APPLICATION OF TDT TO A DISPOSAL CONCEPT

The Project Ankhiale Database contains all relevant data for a thermal assessment, for each of the five disposal concepts described above. Data associated with each concept often have a given range of parameters, which represent either physical limits which may exist (such as a minimum tunnel spacing based on geotechnical considerations) or to reflect parametric uncertainty due either to an uncertainty in a measurement, or to the fact that no specific site data are known. Broadly, each parameter has been classified into one of two categories: engineering and layout parameters which may be adjusted as part of the thermal dimensioning (for example, modifying tunnel spacing, package spacing), and material properties (for example, host rock thermal conductivity) which cannot be simply adjusted whose consequences need to be assessed.

As part of the thermal dimensioning analysis of a disposal concept, a range of calculations would be performed. One such may be to identify a nominal 'cautious case' scenario, a circumstance that may be unlikely to occur, however would test the overall limits of the strategy to manage temperature in a GDF. The example presented here is an example of an investigation to determine whether a particular inventory of spent fuel can be emplaced in a GDF using Concept A1 with a set of 'cautious case' parameters, without exceeding a 100°C temperature limit imposed on the bentonite buffer. The 'cautious case' parameters used in this analysis is given in Table 1.

TABLE 1: 'Cautious case' parameters for Concept A1

Property	**Reference value**	**Cautious case value**
Bentonite Thermal conductivity	$1.2\ W{\cdot}m^{-1}{\cdot}K^{-1}$	$0.6\ W{\cdot}m^{-1}{\cdot}K^{-1}$
Bentonite pellets Thermal conductivity	$0.6\ W{\cdot}m^{-1}{\cdot}K^{-1}$	$0.1\ W{\cdot}m^{-1}{\cdot}K^{-1}$
Temperature at ground surface	10.0°C	20.1°C
Higher strength rock density	$2700\ kg{\cdot}m^{-3}$	$2600\ kg{\cdot}m^{-3}$
Higher strength rock specific heat capacity	$820\ J{\cdot}kg^{-1}{\cdot}K^{-1}$	$690\ J{\cdot}kg^{-1}{\cdot}K^{-1}$
Higher strength rock thermal conductivity	$3.0\ W{\cdot}m^{-1}{\cdot}K^{-1}$	$2.2\ W{\cdot}m^{-1}{\cdot}K^{-1}$
Temperature gradient	$2.79E^{-2}\ K{\cdot}m^{-1}$	$3.71E^{-2}\ K{\cdot}m^{-1}$

The inventory investigated for disposal is the anticipated total arisings of spent fuel from spent fuel with a specified future burn-up. The inventory is composed of over 20,000 Spent Fuel (SF) assemblies, housed in approximately 5,000 disposal containers (with four assemblies per container). The inventory is averaged over the assumed operational period of the reactors to represent an average container. This is a reasonable assumption if the contents of each container are a mixture of longer-cooled and shorter-cooled assemblies. The power decay curve associated with the SF is shown in Fig. 7.

The inventory is emplaced in a single module of 54 tunnels of 620m length and spaced 25m apart, each containing 95 containers spaced 6.5m apart. The inventory is assumed to apply at the end of the reactors projected lifetime, to be emplaced 15 years later, so the inventory will decay by 15 years before emplacement, to a power of approximately 2kW.

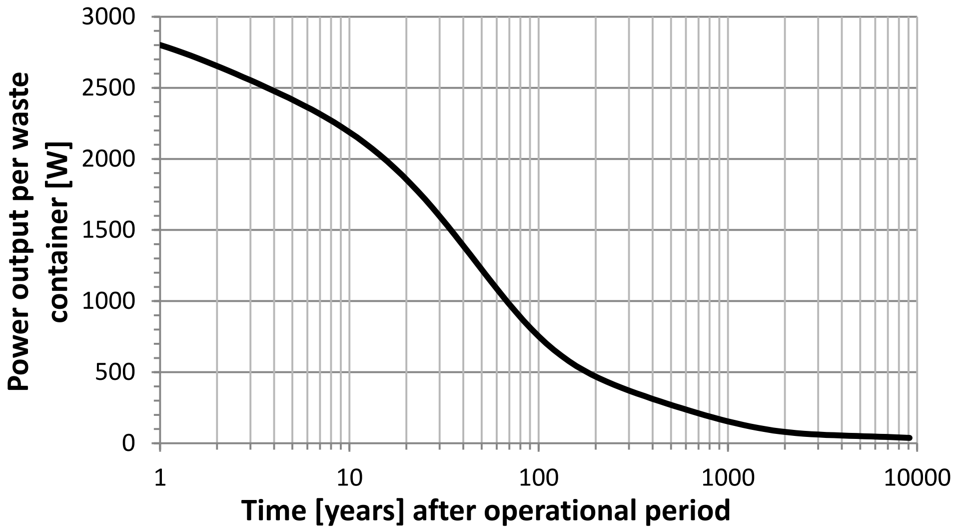

Fig. 7. The power curve for the spent fuel container. The default emplacement year is 15 years following the operational period, so the power at emplacement is around 2kW.

Fig. 8 and Fig. 9 show the evolution of the total rock wall temperature, the maximum buffer temperature, and the temperature at the surface of the local container.

The consequence of this initial power is that the peak buffer temperature is well above the 100°C limit (at 190°C). Therefore, it is clear that potentially significant measures are needed to reduce it. Fig. 8 shows that the contributions to overall temperature from the rock wall from the local container and the ambient temperature alone is almost 80°C. Fig. 9 shows that, at early times, the buffer is over 50°C hotter than the rock wall. The difference between the buffer and the rock wall is driven primarily by the local container, so no amount of increasing spacing (to further separate the containers) will reduce the peak temperature below 100°C. Additional measures that may be taken in conjunction with increasing spacing include increasing the decay storage time in excess of the initial 15 years, or by reducing the number of spent fuel assemblies per container.

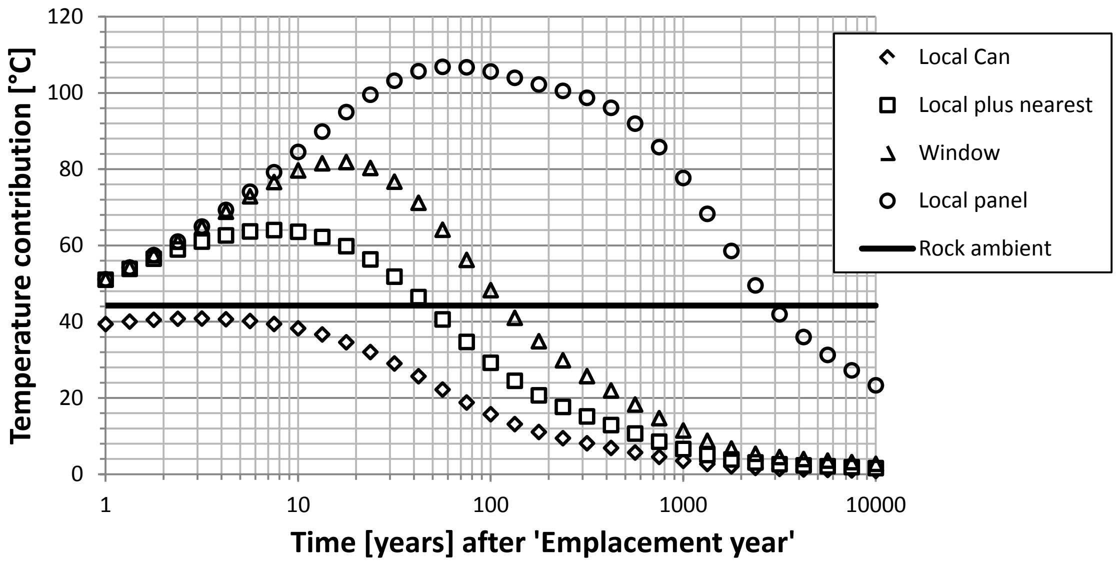

Fig. 8. The contributions to the rock wall temperature from near the local container from a range of portions of the GDF. The diamonds show the evolution of the local container contribution, the squares show the local plus the nearest six containers, the triangles show the detail window contribution, and the circles show the entire local panel contribution. The horizontal line is the ambient rock temperature at the depth of the GDF. The emplacement year is 2100.

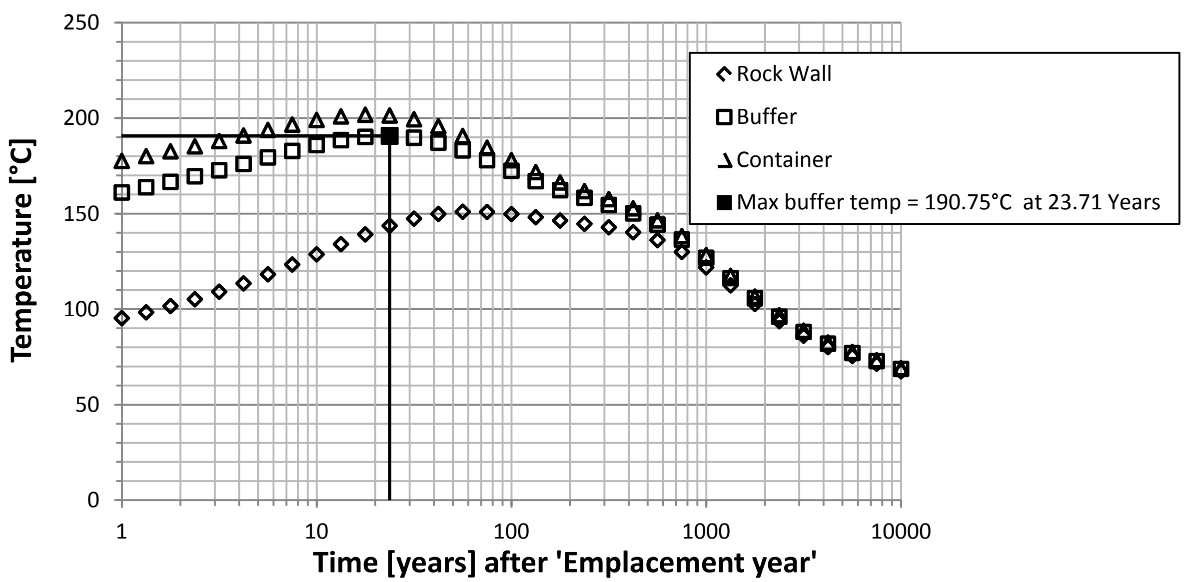

Fig. 9. The contributions to the rock wall temperature from near to the local container. The diamonds show the evolution of the local container contribution, the squares show the local plus the nearest six containers, the triangles show the detail window contribution, and the circles show the entire local panel contribution. The horizontal line is the ambient rock temperature at the depth of the GDF.

The possibility of emplacing this spent fuel (at this fuel loading) for this ‘cautious case’ scenario, without exceeding the temperature constraint, is investigated for the four assemblies per container case, and for a case with three assemblies per container. In both cases the decay storage time and the container spacing parameters are varied. The reduction to three assemblies per container reduces the thermal power of each container, but increases the number of containers by 33%. The result of the analysis is shown in Fig. 10 for the four assembly case; Fig. 11 shows the three assembly case. Both figures show the effect of increasing the container spacing along the tunnel for a range of decay storage times. It can be seen that, in the four assembly case, the spent fuel needs in excess of 50 years decay storage before emplacement is possible. At 85 years decay storage, a container spacing of 11.25m is sufficient to respect the temperature limit. The three assembly case, however, requires only 50 years decay storage, where the required container spacing is again 11.25m. This reduction in the required decay storage period has therefore resulted in a larger disposal module footprint due to the increased spacing of containers.

An illustrative footprint analysis (effective plan area taken up by the disposal system with only this waste) has been carried out, with results shown in Table 2. It is not impossible to emplace the waste with four assemblies per container using only 15 years of decay storage without exceeding the 100°C temperature limit, and this is also true for the three assembly case. Consistent with the previous conclusion, the footprint of the three assemblies per container module at 50 years is larger than the four assembly module at 85 years. It is interesting to note that, comparing both 85 years decay storage cases, the three assembly case has a marginally smaller footprint despite the significantly greater number of containers.

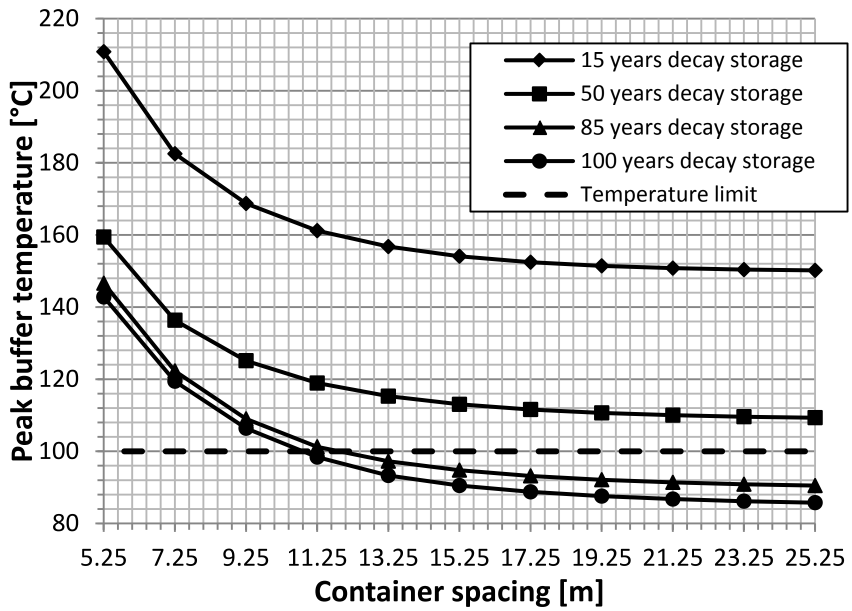

Fig. 10. The example SF inventory packaged at 4 assemblies per container. It shows the dependence of peak buffer temperature on container spacing within a tunnel, for a range of decay storage times. The dashed line shows the temperature limit for bentonite.

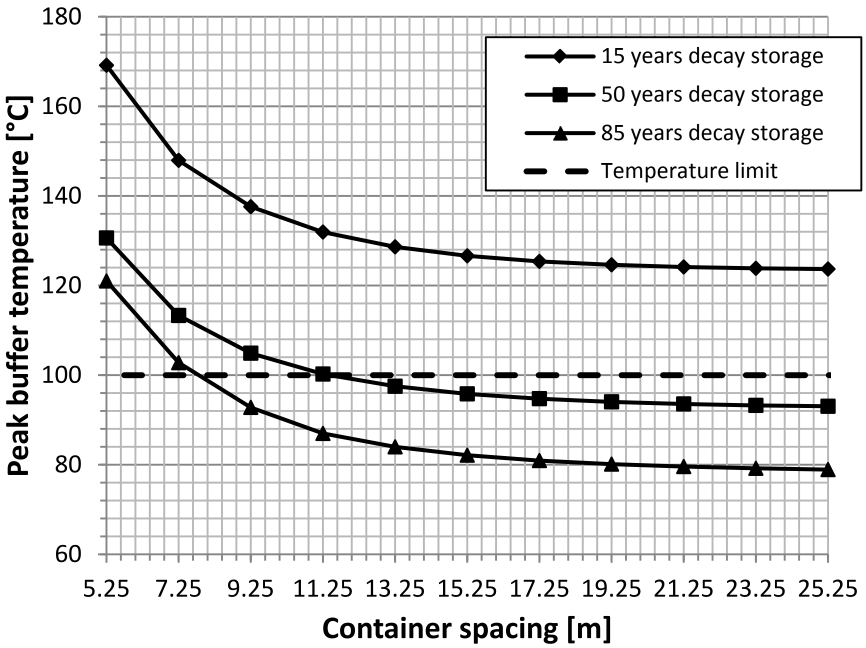

Fig. 11. The example SF inventory packaged at 3 assemblies per container. It shows the dependence of peak buffer temperature on container spacing within a tunnel, for a range of decay storage times. The dashed line shows the temperature limit for bentonite.

TABLE 2: Footprint analysis for the example Spent Fuel module. The footprint of the module is calculated as the area of the smallest rectangle which covers all the containers in the module when the container and tunnel spacings at their minimum values which do not cause the temperature limit to be exceeded. In this model the container and tunnel spacing are equal and the module is square.

Case	Decay storage time	Container spacing for under 100°C	Number of containers	Total footprint
4 assemblies	15	Not possible	5094	-
4 assemblies	50	Not possible	5094	-
4 assemblies	85	17m	5094	$1.4*10^6$ m^2
4 assemblies	100	16.5m	5094	$1.3*10^6$ m^2
3 assemblies	15	Not possible	6786	-
3 assemblies	50	17m	6786	$1.9*10^6$ m^2
3 assemblies	85	14m	6786	$1.3*10^6$ m^2

It should be noted that this theoretical 'cautious case' scenario is unlikely to occur, but the analysis presented here demonstrates that the disposal concept contains enough flexibility to emplace SF at a relatively high power output inventory without exceeding the temperature limit as long as a sufficient period of decay storage is permitted. Naturally, the period of required decay storage can be minimised by adjusting the container spacings and reducing the amount of waste per container. The work presented herein illustrates the utility of the TDT in managing how the temperature in a GDF can be managed within the imposed temperature constraints, and what steps may be taken to emplace waste in more extreme circumstances.

CONCLUSIONS

A thermal dimensioning tool (TDT) has been developed as part of the Project Ankhiale high-heat Integrated Project Team, which:

- has the ability to efficiently perform thermal dimensioning for a range of disposal concepts for heat generating waste
- 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
- can model the consequences of parametric uncertainty
- supports the project principle of quality assurance of data, reinforcing the basic principles of verification and data management
- has a simple, clear user interface to help the user construct a model

The TDT and the mathematical model that it uses have been independently verified against a comprehensive set of detailed finite element simulations for each of the five implemented disposal concepts, and found to compare favourably.

An illustration of the use of the TDT has been presented, which shows how the TDT can inform the design of a GDF intended to emplace a specific waste type. It can also be used to assess different solutions if a scenario is found to exceed the imposed temperature limit for the disposal concept, which can in turn inform the disposal system specification requirements for high-heat-generating wastes.

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