THERMAL MODELLING OF A MARK II CONTAINER

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Abstract

This paper describes the analysis methods, assumptions and results obtained in calculations performed to assess fuel temperatures inside a Mark II used fuel container. The Mark II container is designed to hold 48 used fuel bundles. A variety of cases is considered, including: used fuel container in air, used fuel container in a bentonite buffer box, and used fuel container in the underground repository.

Separate analyses have been performed for repositories hosted in sedimentary and crystalline rock; however, because fuel temperatures are essentially the same in both cases only the sedimentary rock analysis is described.Several sensitivity cases have also been examined to determine the effect of key parameters.

The overall conclusion is that the maximum fuel temperature for fuel with a burnup of 280 MWh/kgU and a 30 year decay time will be less than 60°C during handling of the container, about 75°C during handling of buffer box, and about 114°C after placement in the repository.

Key words: Thermal modelling, heat transfer, nuclear waste

1. Background

The NWMO is designing and assessing the performance of aMark II used fuel container shown in Figure 1. The container consists of an outer copper corrosion-barrier and an inner carbon steel load-bearing shell.Each container is loaded with 48 used CANDU fuel bundles arranged in four storage modules, with each module having 12 horizontal bundle tubes. This Mark II container (12FB-4L) has a diameter of 562 mm and a length of 2,512 mm with hemispherical heads on each end (all dimensions from drawing: APM-ASSY-04302-0001, REV000A, 2014/4/1). The inner steel layer is 46.23-mmthick at the main cylinder and 30-mmthick at the hemispherical ends. The container is coated with a layer of 3-mm-thick copper (Figure 1).

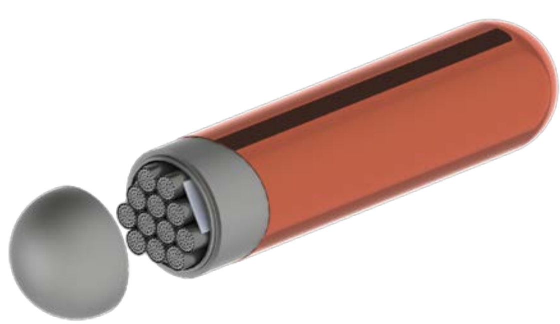
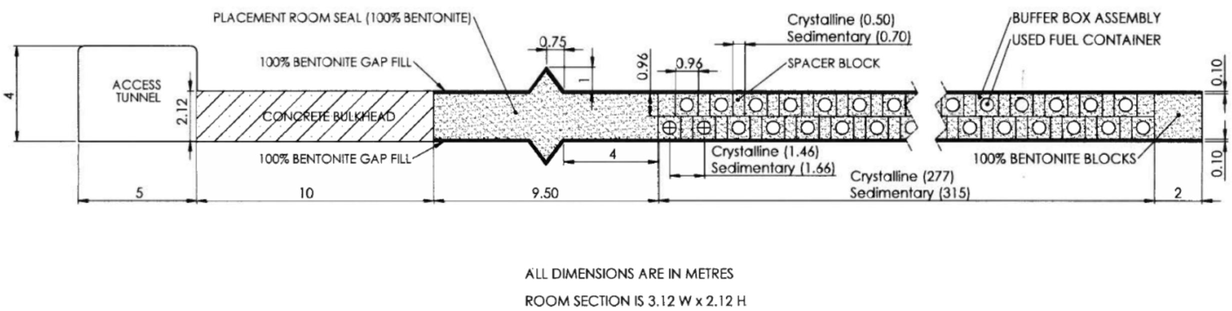


Figure 1: Mark II used fuel container view

In the repository concept assessed, the containers are housed in a highly compacted bentonite buffer box. The buffer boxes are installed in the placement room with the containers perpendicular to the tunnel direction. The deep geological repository (DGR) layout consists of arrays of horizontal, rectangular-shaped placement rooms. The placement rooms are connected by access drifts for the removal of excavated rock, and for the transfer of buffer boxes and backfill materials. The assumed depth of the DGR is 500 m. The placement details are shown in Figure 2. The placement rooms are 2.12 m in height and 3.12 m in width witha layer of 100 mm of gap fill (bentonite pellets) placed around the buffer boxes and the dense backfill blocks in the placement rooms.



From NWMO draft drawing of Mark II design concept for crystalline and sedimentary host rock (APM-PDD-04000-0003)

Figure 2: Mark II 48-bundle Container Placement Room Concept

2. Model Geometry, Boundary and Initial Conditions and Material Parameters

COMSOL version 4.3b was used to perform the simulations. COMSOL is a commercial finite element program[1].

The fuel bundles are assumed to have a decay period of 30 years with a discharge burnup of 220 MWh/kgU. Fuel temperaturesare calculated for three types of boundary conditions: container in air (i.e., in the used fuel packaging plant), container inside a buffer box in air (i.e. during transfer underground), and container placed in a repository.

Separate analyses have been performed for sedimentary and crystalline rock geospheres; however, because fuel temperatures are essentially the same in both environments only the sedimentary rock analysis is described.

For computational efficiency and ease of modelling, a number of submodelsare used, with information passed from one submodel to another via boundary conditions[2]. Specifically:

- For the container in air, a Container Model and a Bundle Model are used. Results from the Container Model are imposed as boundary conditions on the Bundle Model;
- For the container insidea buffer box in air, a Buffer Box Model, a Container Model and a Bundle Model are used. Results from the Buffer Box Model are imposed as boundary

conditions on the Container Model and results from the Container Model are imposed as boundary conditions on the Bundle Model;

- For the container insideabuffer box in abackfilled DGR, a DGR Model, a Container Model and a Bundle Model are used. Results from the DGR model are imposed as boundary conditionson the Container Model and results from the Container Model are imposed as boundary conditions on the Bundle Model.

2.1 Model Geometry

As discussed above, four models are created in the course of this work. These are the DGR Model, the Buffer Box Model, the Container Model and the Bundle Model. Heat conduction is considered in all models while thermal convection is considered only on the outside surfaces of the Buffer Box Model (for the case of the Container inside the Buffer Box in Air) and on the outside surface of the Container Model (for the case of the Container in Air). Thermal radiation heat transfer and thermal convection inside the container and inside the bundle tubes are not considered; however, their effects are examined later via sensitivity studies.

2.1.1 Sedimentary DGR Model

The geometry of the Sedimentary DGR Model, including dimension information, is shown in Figure 3. There are five kinds of materials: rock (sedimentary), buffer box bentonite, spacer blocks (also called backfill blocks), used fuel container and bentonite gap fill (In this modelling exercise, the tunnel spacing was assumed to be 20 m; however, in the reference case for sedimentary rock environment, it is 25 m now).

The horizontal dimensions are 10 m x 0.83 m based on the criterion that the container surface temperature is less than 100°C. The dimensions of the buffer box are 0.962 m x 0.962 m x 2.912 m (there are two one-quarters of the buffer box in each model with dimensions of 0.481 m x 0.962 m x 1.456 m). The vertical dimension of the model unit cell is 1000 m. The bottom of the placement room is 500 m below the top of the model.

The rock should be stratified for the sedimentary repository case; however, for simplification, rock homogeneity is assumed. Because of the requirement that the container surface temperature be lower than 100°C, this assumption will not have a significant effect on the fuel temperature analysis.

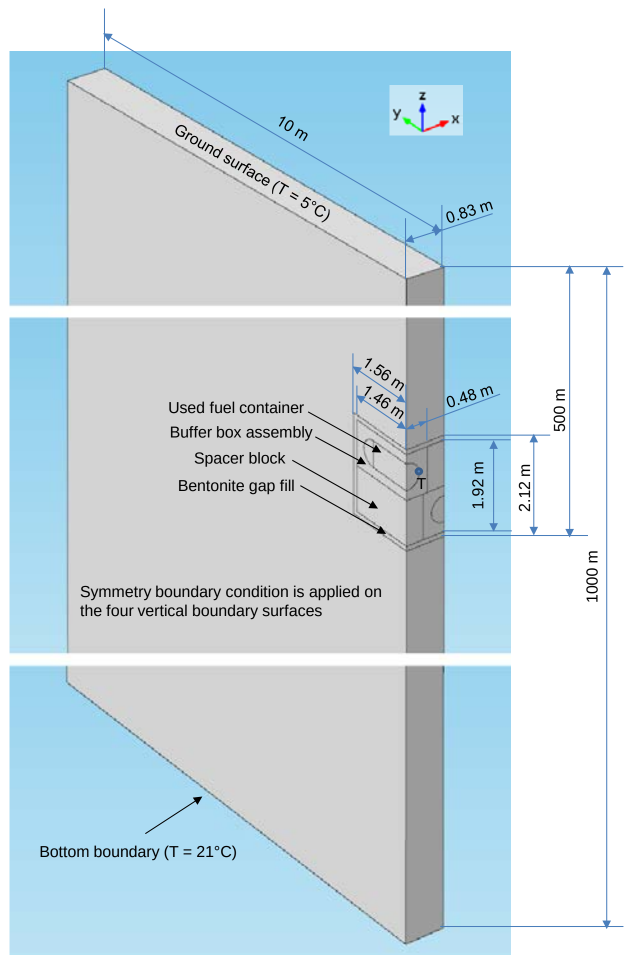


Figure 3: Sedimentary DGR Model Geometry

2.1.2 Buffer Box Model

The Mark II container is placed within a buffer box. The dimensions of the Buffer Box Model are 0.962 m x0.962 m x 1.456 m. Only one-half of the buffer box is modelled because of symmetry (Figure 4). In this Buffer Box Model, there are two kinds of materials. One of the modelled materials is the bentonite of the buffer box while the other modelled material is a 3-mm-thick layer of copper (on the outside of the used fuel container) that is in contact with the inside portion of the buffer box. In this model, full contact is assumed between the copper layer and the buffer box bentonite. The container is not included in the Buffer Box Model and the total heat source from one-half a container is applied on the inside surface of the copper layer.

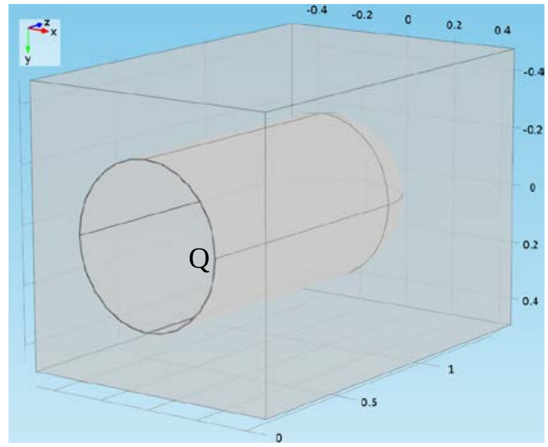


Figure 4: Buffer Box Model Geometry

2.1.3 Container Model

The dimensions of a Mark II container are described in Section 1. Because of symmetry, one-half of the container is represented in the Container Model as shown in Figure 5. The model includes three kinds of materials: copper, steel and air. The outermost layer of the model is the 3-mm-thick copper coating with an outside diameter of 0.562 m. Inside this layer is a steel layer with a 46.23-mm-thick wall and hemispherical end cap with a thickness of 30 mm. Inside the steel layer are twelve 1.03-m-long steel tubes with a wall thickness of 2.5 mm. The space between the tubes and the steel spherical shell is filled with air. The tubes are empty and the heat source from the fuel will be applied on the inside surface of the tubes. It is assumed that there is no physical connection between fuel tubes and the inside surface of the container.

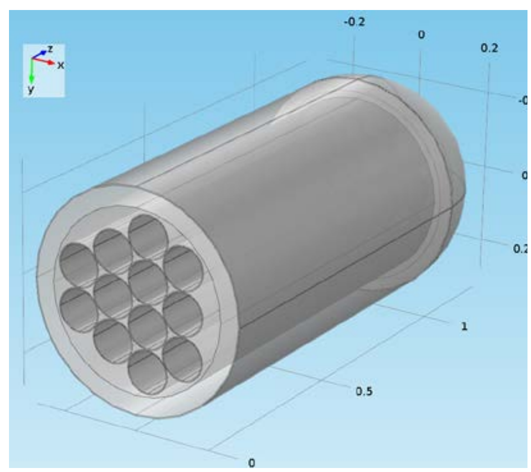


Figure 5: Container Model Geometry

2.1.4 Bundle Model

Inside each container are 48 fuel bundles, with each fuel bundle comprised of 37-element fuel. The geometry of the Bundle Model is shown in Figure 6. Each element consists of UO_2 pellets and cladding.

Due to symmetry, the model represents one-half of a steel tube in a container with the one-half tube segment holding two fuel bundles. The model components are a steel tube, two fuel bundles and air in the void spaces. The outside diameter, inside diameter and length of the steel tube are 0.11 m, 0.105 m and 1.03 m, respectively. Inside the steel tube are two 37 Zircaloy-4 fuel sheaths arranged in the form of a CANDU fuel bundle. The fuel sheaths are 1.03 m long tubes with an outside diameter of 13 mm and wall thickness of 0.4 mm[3]. Each fuel sheath is filled with cylindrical-shaped UO_2 fuel pellets. The space between the fuel sheaths and the steel tube is filled with air. The spacers between fuel pins/sheaths and between fuel pins and bundle tubes are not incorporated in the Bundle Model. This simplification is conservative because it results in higher fuel temperatures.

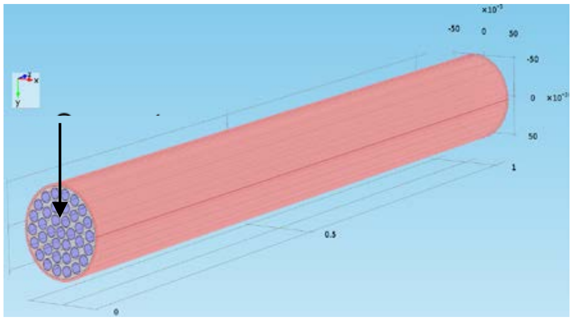


Figure 6: Bundle Model Geometry

2.2 Initial Conditions

The initial temperature for all material types in the Bundle Model, the Container Model and the Buffer Box Model is assumed to be ambient (20°C).

The initial temperature for all material types in the DGR Model is a function of depth and calculated using the following equation[4].

$$T_0 = 5 + 0.016 \cdot z \tag{1}$$

In which T_0 is the initial temperature at depth z, °C; z is the depth from the ground surface, m.

2.3 Boundary Conditions

Figure 7 shows the heat source per 37-element “standard” CANDU bundle,as a function of fuel age, for a bundle with adischarge burnup of 220 MWh/kgU[5].

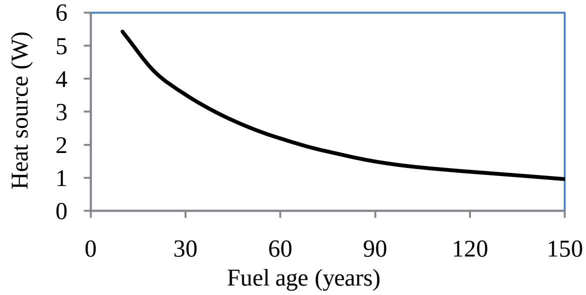


Figure 7: Heat Source Per 37-element Bundle for a Discharge Burnup of 220 MWh/kgU

The boundary conditions for the DGR Model are:

- No heat flow on the four vertical outside surfaces.
- The temperature at the ground surface is 5°C.
- The temperature at the bottom of the model is 21°C.
- Twenty-four times the heat source of a single 37-element bundle is uniformly applied in the (half) volume of the used fuel container.

The boundary conditions for the Buffer Box Model are:

- No heat flow across the symmetrical vertical surface.
- A convective heat flux boundary condition is applied on the outside six surfaces. The outside ambient room temperature is fixed at 20°C.
- One-half (24 bundles) of the total heat source in a used fuel container is uniformly applied as a heat flux on the inside surface of the copper layer.

The boundary conditions for the Container Model are:

- No heat flow across the symmetry surface;
- One-half (24 bundles) of the total heat source is uniformly applied as a heat flux on the inside surfaces of each of the 12 tubes;
- Container surface temperature for three different conditions:
  - For the Container inside the Buffer Box in the DGR Model: The temperature at point T on the outside surface of the container from the DGR Model is applied on the outside surface of the Container Model.
  - For theContainer inside the Buffer Box Model: The temperature at point Qon the inside surface of the copper from the Buffer Box Model is applied on the outside surface of the Container Model.
  - For the Container Model in Air: Convective heat flux is applied on the outside surface of the container with the ambient room temperature fixed at 20°C.

The boundary conditions for the Bundle Model are:

- No heat flow across the symmetry surface at $z = 0$,
- The maximum temperature of the central air determined using the Container Model is applied on the outside surface of the Bundle Model and on the end surface at $z = 1.03$ m,
- The total heat source of two bundles is uniformly applied in the volume of the two 37 UO_2elements (There are two 37-element bundles axially in the Bundle Model).

2.4 Material Parameters

The thermal properties of the materials used are shown in Table 1. Thermal conductivity of $UO_2$is extrapolated from the thermal conductivity of UO_2 at high temperature [6]. The specific heat of Zircaloy-4 cladding is interpolated using the data from IAEA [6].

Table 1: Thermal Properties for the Considered Materials

Materials	Density [kg/m³]	Specific Heat [J/kg·°C]	Thermal Conductivity [W/(m·°C)]	Reference
Limestone	2600	830	2.3	[4]
Bentonite pellets	1410	920	0.4	[7]
HCB	1700	1440	0.5	[7]
Dense backfill	2120	1100	0.8	[7]
Steel*	7800	444	43	
Copper*	8960	385	400	
UO_2 pellets	10637	235	6.955-0.009704*T***	[6]
Zircaloy-4 cladding	6471	255.66+0.1024(*T***+273)	17.5	[6]

*http://www.engineeringtoolbox.com/thermal-conductivity-d_429.html***T* is the temperature, °C.

Convective heat transfer (and hence its coefficient) is difficult to estimate exactly. It depends on the type of media, gas or liquid, the flow properties such as velocity, viscosity and other flow and temperature dependent properties. A convective heat transfer coefficient of 13.1 W/(m^2·°C) is applied on the outside container surface for the Container in Air case. This value is taken from "The Engineering Toolbox".For comparison, Lienhard and Lienhard[8] useda value of 15 W/(m^2·°C) for a copper sphere at a uniform temperature of 40°C suspended in a slow-moving air stream with temperature of 0°C. Compared to the copper sphere case,the value of 13.1 W/(m^2·°C) used here for stationary air with an ambient temperature of 20°C is reasonable.

A convective heat transfer coefficient of 4 W/(m^2·°C) is applied on the buffer box outside surface in air[9]. No data for the convective heat transfer coefficient for bentonite was found and therefore this value corresponds to that for soil.

The emissivity coefficient for the outside surface of the steel bundle tubes, the inside surface of a container, and the inside surfaces of the bundle tubes is 0.7 (this value from "The Engineering Toolbox" online).

For the Zircaloy-4 fuel sheath, the emissivity value for steel bundle tubes is applied.

The thermal parameters used for air are taken from the values for COMSOL built-inmaterials.

3. Modelling Results

3.1 Results from the Three Base Cases

The case of Container in Air: The maximum temperature of the container central air is 69°C.The maximum fuel temperature is 75°C (Figure 8).

The case of Container inside the Buffer Box in Air: The maximum fuel temperature reaches a peak value of 86.5°C at 20 days (Figure 9). The maximum container temperature reaches a peak value of 81.1°C at 20 days. The maximum container outside surface temperature reaches a peak value of 37.2°C at 20 days.

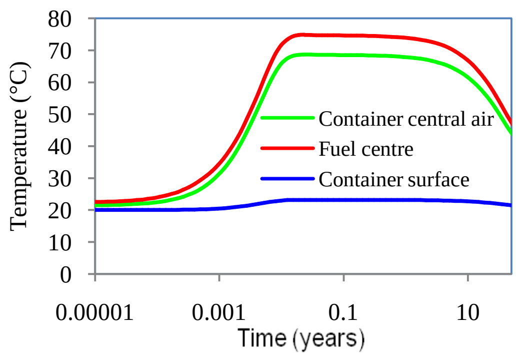


Figure 8: Temperature vs. Time for Container in Air

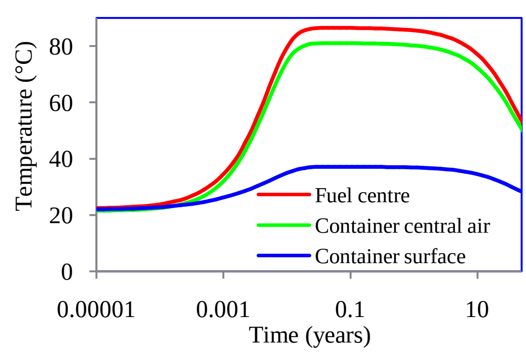


Figure 9: Temperature vs. Time for Container inside a Buffer Box in Air

The case of Container inside a Buffer Box in a Repository: The maximum fuel temperature decreases from a peak value of 126°C at 14.7 years to 116°C at 50 years (Figure 10). The maximum container air temperature decreases from 122°C at 14.7 years to 114°C at 50 years. The maximum container surface temperature decreases from 96°C at 40 years to 95°C at 50 years.

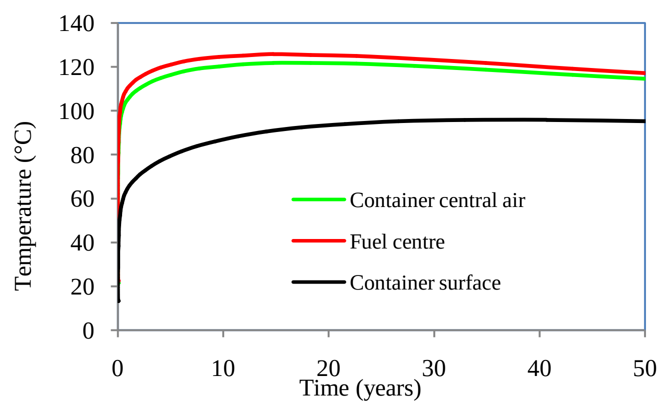


Figure 10: Temperature vs. Time for Container in a Buffer Box in a Sedimentary Repository

3.2 Sensitivity Analyses

This section examines the influence of a gap between a container and a buffer box,the effect of including radiation heat transfer in a container or in a fuel tube, and the influence of higher burnup.

3.2.1 Influence of theGap between the Container and the Buffer Box

In Section 3.1, it is assumed that there is no gap between a container and its surrounding buffer box. In reality, there may be a 3-mm-thick gapalong some upper part of the container surface when the container is first placed in the bufferbox. Over time, the bentonite in the buffer box will saturate and the gap will disappear. The no gap assumption makes the results for the temperature inside the container at early timeslower than it would otherwise be. Modelling results show that ignoring the gap underestimates the container central air temperature by about 3°C and the container surface temperature by about 3.6°C.

3.2.2 Influence of Radiation Heat Transfer on Temperature

Due to the complexity of the container geometry described in Section 2.1, radiation heat transfer has not been included to this point for reasons of computational efficiency. The influence of radiation emitted from the outside surface of the bundle tubes impinging on the inside surface of the container and the influence of radiation emitted in a fuel tube is evaluated based on the Container inside a Buffer Box in a Sedimentary Repository Case.

Modelling results show that ignoring radiationheat transfer overestimates the container central air temperature by17°C at time of maximum air temperature, occurring at 14.7 years.

Based on these results, the maximum temperature of the centre air inside a container filled with 30-year-old fuel in a sedimentary repository when accounting for radiation heat transfer is 105°C. This value is determined by subtracting 17°Cfrom the 122°Cmaximum temperature that arises from the Container Model in a sedimentary repository case. Considering the results from the Bundle Model, the corresponding maximum fuel temperature would be 109°C.

The results also show less than 2°C difference between considering and without considering radiative heat transfer within a fuel bundle.

3.2.3 Influence of Higher Burnup

All of the analysesdescribed above assume a bundle burnup of 220 MWh/kgU. This section evaluates the influence of higher burnup (i.e., 280 MWh/kgU) on the fuel temperature.

The repository layout was based on ensuring that the container surface temperature did not exceed 100°Cif thecontainerswere filled with 30-year-old 220 MWh/kgUburnup bundles. If bundles with higher burnup are emplaced, then to continue meeting the container temperature constraint, fewer high burnup bundles could be emplaced in a given container.

Because the heat source per bundle with a 280 MWh/kgUburnup is about 29% greater than that for a bundle with a 220 MWh/kgU burnup, at most thirty-six 30-year-old 280 MWh/kgUfuel bundles can be placed inside the container. With this number of high burnup bundles, the container outside surface temperature and the container centre temperature will be similar to those (122°C at the container central air and 96°C on the container surface) as described in Section 3.1. However, the fuel temperature difference above the container central air temperature will be 29% higher than that for fuel with 220 MWh/kgUburnup, or about 2°C higher. This means that the fuel temperature would be about 127°C for the higher burnup fuel.

3.3 Summary of the Modelling Results

This paper presents fuel, container central air and container outside surface temperatures for the Container in Air Case, the Container inside the Buffer Box in Air Case, the Container inside the Buffer Box in the Sedimentary Rock Repository Case and the Container inside the Buffer Box in the Crystalline Rock Repository Case. The influences of the small space between the container and the bentonite material in the buffer box, radiation heat transfer between bundle tubes and between bundle tubes and the container inside surface, and radiation heat transfer between fuel elements and between fuel elements and the bundle tube inside surface are also presented.

Table 2summarizes the results of the simulations.The table shows the maximum fuel temperature, the maximum container air temperature, the maximum container surface temperature and the times at which the maximums occur.

Table 2: Summary of Maximum Temperature Results*

Case	Fuel Age (years)	Maximum Fuel Temperature (°C)	Maximum Container Air Temperature (°C)	Maximum Container Surface Temperature (°C)
Container in Air	30	75 (8.6 days)	69 (8.6 days)	
Container inside theBuffer Box in Air	30	87 (20 days)	81 (20 days)	37 (20 days)
Container inside the Buffer Box in a Sedimentary Repository	30	126 (14.7 years)	122 (14.7 years)	96 (40 ears)

*The results are for the cases with fuel having 220 MWh/kgU Burnup, without considering radiation heat transfer effects and without considering the gap between a containers and a buffer box.

Table 3 summarizes the results of the sensitivity analysis simulations. The table shows the influences of different factors.

Table 3: Summary of Sensitivity Analysis Results

Sensitivity Case	Effect
Adding a 3-mm-air gap between Container Surface and the Buffer Box	Increases fuel temperature by about3°C
Accounting for radiation heat transfer between bundle tubes and between bundle tubes and the inside container surface	Reduces fuel temperature by about 17°C
Accounting for radiation heat transfer between fuel elements and between fuel elements and the inside surface of bundle tube	Reduces fuel temperature by about 2°C
Higher bundle burnup (280 MWh/(kgU)instead of 220 MWh/(kgU))	Increases the fuel temperature less than 2°C

Based on the analysis results, the anticipated fuel temperature can be determined using the information presented in Tables 2 and 3as follows:

$$T = T_0 + \Delta T_1 + \Delta T_2 + \Delta T_3 \qquad (1)$$

where: T_0 is the maximum fuel temperature calculated from the Bundle Models in Sections 3.1 and Table 2;

ΔT_1 is the influence of the air gap between the container and the buffer box. For the Container in Air case, ΔT_1 = 0°C, for the Container in Buffer Box case and for the Container in a Repository cases, ΔT_1 = 3°C;

$\Delta T_2$is the influence of radiation heat transfer between the bundle tubes and between bundle tubes and the inside container surface, ΔT_2= -17°C;and

ΔT_3 is the influence of high burnup fuel, , ΔT_3 = 0°C for bundles with a burnup of 220 MWh/(kgU) and ΔT_3 = 2°C for bundles with a burnup of 280 MWh/(kgU).

In the above modification equation, the overestimation caused by ignoring the connections between the bundle tubes and the inside surface of the container is not considereddue to the uncertainty of the width of the connections and is used as a conservative factor.

For different cases, the maximum fuel temperaturecan be modified using Equation 1 and the results shown inTable 4

Table 4: Summary of Modified Maximum Temperature Results

Case	**Fuel Age (years)**	**Maximum Fuel Temperature**(°C)	
		Burnup of 220 MWh/kgU	Burnup of 280 MWh/kgU
Container in Air	30	58	60
Container inside the Buffer Box in Air	30	73	75
Container inside the Buffer Box in a Sedimentary Repository	30	112	114

4. Conclusions

A series of thermal modelling simulations for different conditions has been modelling using COMSOL to determine the maximum internal container temperature and the maximum fuel temperature.

In this modelling activity, there are several assumptions which make the modelling results for the fuel temperature conservative. For example,

- In the container model, the temperature at the mid-container surface from the Buffer Box Model or from the Repository Model, which is the highest temperature on the container surface, is used as the boundary condition for the outside surface temperature and this results in a conservative temperature in theContainer Model,

- Using the centreair temperature in the container as the boundary condition in the Bundle Model, and
- Ignoring the connection between the bundle tubes and the inside surface of the container results in overestimating fuel temperature.

There is only one assumption which may result in lower temperature in the container. This assumption is that there is no air gap between the container and the buffer box and this assumption may give the container central air temperature 3°C lower than if an air gap is included.

The use of higher burnup fuel (280 MWh/kgU) instead of 220 MWh/kgU results in an increase in fuel temperature of about 2°C.

Considering the above two kinds of assumptions, the modelling results show the fuel maximum temperature (for fuel with a burnup of 280 MWh/kgU) is less than 60°C during handling of the container, 75°C during handlingof the buffer box placement, and 114°C after placement in sedimentary rock.

References

[1] COMSOL. Heat Transfer Module User's Guide Version 4.3b,2013.

[2] R. Guo. Thermal modelling of a Mark II container. Nuclear Waste Management Organization Technical Report NWMO-TR-2015-06, 2015.

[3] M.Garamszeghy. Nuclear Waste Projects in Canada – 2015 Update.NWMO TR-2015-19,2015.

[4] R.Guo. Coupled thermal-mechanical modelling of a deep geological repository using the horizontal tunnel placement method in sedimentary rock using CODE_BRIGHT. NWMO TR-2010-22,2010.

[5] J.C.Tait, H. Roman and C.A. Morrison. Characteristics and radionuclide inventories of used fuel from OPG Nuclear Generating Stations. Volume 1 - Main report; and Volume 2 – Radionuclide inventory data. Ontario Power Generation Report 06819-REP-01200-10029-R00, 2000.

[6] IAEA.Thermophysical properties database of materials for light water reactors and heavy water reactors: Final report of a coordinated research project,2006.

[7] P.Baumgartner. Generic thermal- hydraulic - mechanical (THM) data for sealing materials, Volume 1: soil-water relationship. Ontario Power Generation, Nuclear Waste Management Division 06819-REP-01300-10122-R00,2006.

[8] J.H. Lienhard IV and J.H. Lienhard V. A heat transfer textbook (fourth edition). Phlogiston Press. Cambridge Massachusetts,2011,p.38.

[9] A. M.Abdel-Ghany andT. Kozai. On the determination of the overall heat transmission coefficient and soil heat flux for a fog cooled, naturally ventilated greenhouse: Analysis of radiation and convection heat transfer. Energy Conversion and Management. Volume 47, Issues 15-16, 2006, pp. 2612–2628.