Dynamic Determination of Thermal Repository Capacity For Fuel Cycle Analysis

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INTRODUCTION

An algorithm and supporting database for rapid thermal repository capacity calculation implemented in Cyder, a software library for coupled thermal and hydrologic repository performance analysis, is described. Integration of Cyder with the Cyclus fuel cycle simulator is also described. Finally, a proof of principle demonstration is presented in which the rapid calculation method described here is compared with results of a more detailed model.

This algorithm employs a Specific Temperature Change (STC) method [1, 2] and has resulted from combining detailed spent nuclear fuel composition data [3] with a detailed thermal repository performance analysis tool from Lawrence Livermore National Laboratory (LLNL) and the Used Fuel Disposition (UFD) campaign [4]. By abstraction of and benchmarking against these detailed thermal models, Cyder captures the dominant physics of thermal phenomena affecting repository capacity in various geologic media and as a function of spent fuel composition.

Abstraction based on detailed computational thermal repository performance calculations has resulted in implementation of the STC estimation algorithm and a supporting reference dataset. This method is capable of rapid estimation of temperature increase near emplacement tunnels as a function of waste composition, limiting radius, r_{lim}, waste package spacing, S, near field thermal conductivity, K_{th}, and near field thermal diffusivity, α_{th}.

MOTIVATION

The United States is simultaneously considering a number of domestic nuclear fuel cycle and geologic disposal options [5]. These decisions are technologically coupled by repository capacity. That is, the thermal capacity of a geologic repository is a strong function of site geology thermal parameters (see Table 1) as well as spent fuel composition, which varies among alternative fuel cycles.

To inform research and development in this coupled system, a generic geologic disposal performance model capable of dynamic integration with a systems analysis framework is necessary to illuminate capacity constraints and dynamic feedback effects of candidate repository geologies in the context of fuel cycle options. In answer to this need, the algorithm in this work has been implemented in the Cyder software library which integrates with the Cyclus computational fuel cycle systems analysis platform [6, 7].

Thermal Behavior of Various Concepts

	Clay (Bentonite Buffer)	Granite (Concrete Buffer)	Salt (Salt Backfill)	Deep Borehole (Bentonite Buffer)
Buffer Limit $[^\circ C]$	**100**	**100**	**180**	**100**
Reference	[8]	[9]	[9, 10]	[9]
Host Limit $[^\circ C]$	**100**	**200**	**180**	**none**
Reference	[11]	[9]	[8]	[8, 12]
$\alpha_{th}[\frac{10^{-6}m^2}{s}]$	**0.12-0.19**	**0.9-1.8**	**1.3-2.1**	**0.9-1.8**
Reference	[13]	[14, 8, 15]	[8, 16]	[14, 8, 15]
$K_{th}[\frac{W}{m\cdot K}]$	**1-2**	**2-4**	$\sim$ **4**	**2-4**
Reference	[8, 13]	[8, 15, 17, 18]	[8, 16]	[8, 15, 17]
Coalescence	yes	no	yes	no

TABLE 1: Maximum heat load constraints, thermal diffusivity, and thermal conductivities vary among repository concepts and host formations.

A generic repository model appropriate for systems analysis must emphasize modularity and speed while providing modeling options at various levels of detail. Therefore, parameterized simulations and abstraction efforts conducted to develop the method described in this work sought to capture the dominant physics of thermal repository capacity assessment so that the Cyder disposal environment library could meet the simulation speed requirements of the Cyclus fuel cycle simulator.

METHODOLOGY

Cyder Integration With Cyclus

To inform dynamic behavior within the simulator, the repository requires a model capable of quickly arriving at a heat based capacity for an arbitrary waste stream.

More specifically, the Cyder repository model is a type of FacilityModel (see [7]) within Cyclus and interfaces with the simulation by requesting materials from the fuel cycle facilities operating simultaneously with it. It the receives materials according to the capacity that it defines. In the case of Cyder, the heat-limited capacity of the repository is reassessed for each new waste stream composition offered to the repository.

Specific Temperature Change Method

Introduced by Radel, Wilson et al., the STC method uses a linear approximation to arrive at the thermal loading density limit [2, 1]. Since the thermal response in a system with a

long term transient response is strong function of the transient decay power, it is also a strong function of the isotopic composition of the waste. Thus, the time dependent temperature change, ΔT, at the limiting radius, r_{lim}, can be approximated as proportional to the mass loading density. First, ΔT is determined for a limiting loading density of the particular material composition then it is normalized to a single kilogram of that material, Δt, the so called STC.

$$\Delta T(r_{lim}) = m \cdot \Delta t(r_{lim}) \tag{1}$$

where

$$\begin{aligned} \Delta T &= \text{Temperature change due to m } [^\circ K] \\ m &= \text{Mass of heat generating material } [kg] \\ \Delta t &= \text{Temperature change due to 1 kg } [^\circ K] \\ r_{lim} &= \text{Limiting radius } [m]. \end{aligned}$$

For an arbitrary waste stream composition, scaled curves, Δt_i, calculated in this manner for individual isotopes can be superimposed for each isotope to arrive at an approximate total temperature change.

$$\Delta T(r_{lim}) \sim \sum_i m_i \Delta t_i(r_{lim}) \tag{2}$$

where

$$\begin{aligned} i &= \text{An isotope in the material } [-] \\ m_i &= \text{mass of isotope i } [kg] \\ \Delta t_i &= \text{Specifc temperature change due to } i \ [^\circ K]. \end{aligned}$$

Supporting Thermal Response Dataset

To support this calculation in Cyder, a reference data set of temperature change curves was calculated. Repeated runs of a detailed analytic model over the range of values in Table 2 determined STC values over a range of thermal heat limit radii, r_{lim}, thermal diffusivity values, α_{th}, thermal conductivity values, K_{th} and waste package spacings, S. Linear interpolation across the discrete parameter space provides a simple thermal reference dataset for use in Cyder.

The analytic model used to populate the reference dataset was created at LLNL for the UFD campaign. In this tool, heat limited thermal response is calculated analytically for each geology, for many waste package loading densities, and for many fuel cycle options [8, 19, 4]. It employs an analytic model from Carslaw and Jaeger and is implemented in MathCAD [20, 21]. The integral solver in the MathCAD toolset is the primary calculation engine for the analytic MathCAD thermal model, which relies on superposition of point, finite-line, and line source integral solutions.

Thermal Cases

Parameter	Symbol	Units	Value Range
Diffusivity	α_{th}	$[m^2 \cdot s^{-1}]$	$1.0\times10^{-7} - 3.0\times10^{-6}$
Conductivity	K_{th}	$[W \cdot m^{-1} \cdot K^{-1}]$	$0.1 - 4.5$
Spacing	S	$[m]$	2, 5, 10, 15, 20, 25, 50
Radius	r_{lim}	$[m]$	0.1, 0.25, 0.5, 1, 2, 5
Isotope	i	$[-]$	$^{241,243}Am$, $^{242,243,244,245,246}Cm$, $^{238,240,241,242}Pu$ $^{134,135,137}Cs$ ^{90}Sr

TABLE 2: A thermal reference dataset of STC values as a function of each of these parameters was generated by repeated parameterized runs of the LLNL MathCAD model[4, 19].

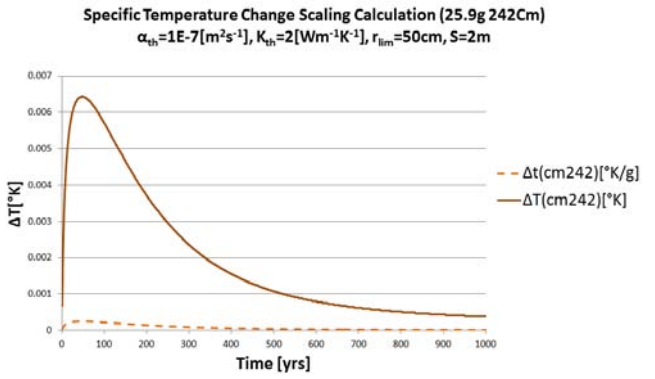

Fig. 1: As a demonstration of the calculation procedure, the temperature change curve for one initial gram of ^{242}Cm and is scaled to represent $25.9g$, approximately the ^{242}Cm inventory per MTHM in 51GWd burnup UOX PWR fuel.

Figure 1 demonstrates the scaling of an STC curve according to equation (1) to represent the heat from $25.9g$ of initial ^{242}Cm using the reference data set.

The supporting database was limited to some primary heat contributing isotopes present in traditional spent nuclear fuel, H, such that the superposition in equation (2) becomes

$$\Delta T(r_{lim}, S, K_{th}, \alpha_{th}) \sim \sum_{i \in H} m_i \Delta t_i(r_{lim}, S, K_{th}, \alpha_{th}) \tag{3}$$

where

$$\begin{aligned} H &= \text{set of high heat isotopes } [-] \\ S &= \text{uniform waste package spacing } [m] \\ K_{th} &= \text{thermal conductivity } [W \cdot m^{-1} \cdot K^{-1}] \\ \alpha_{th} &= \text{thermal diffusivity } [m^2 \cdot s^{-1}] \end{aligned} \tag{4}$$

The use of this superposition is demonstrated in Figure 2.

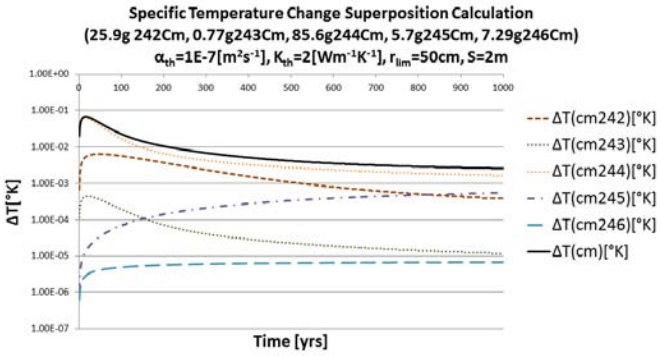

Fig. 2: As a demonstration of the calculation procedure, scaled temperature change curves for five curium isotopes are super imposed to achieve a total temperature change (note log scale).

RESULTS AND ANALYSIS

The primary outcome of this work is a mulitdimensional database of repository temperature change per mass of high heat contributing isotopes supporting the implementation of the STC method in Cyder.

A validation effort concerning this tool was performed to assess the validity of the STC method for the purpose of repository thermal response estimation. Comparison of the results of this method with the LLNL model [4] gave appropriately accurate results and demonstrated the way in which inaccuracies from neglected low heat contributing nuclides are bounded. Figure 3 shows the results of one example validation exercise comparing the combined scaling and superposition calculations demonstrated in Figures 1 and 2 respectively. This particular validation example, containing no neglected nuclides, demonstrates an average error of 1.1% and a maximum error of 4.4%.

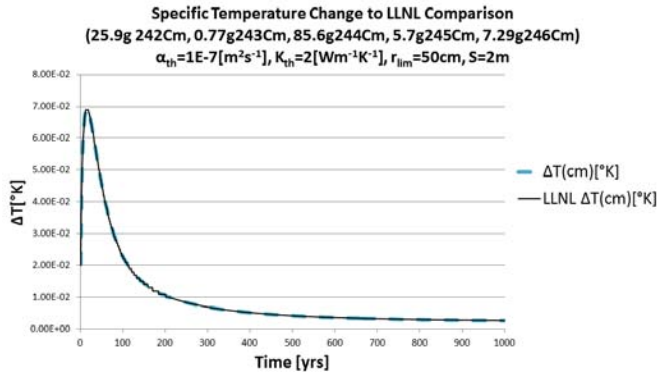

Fig. 3: This comparison of STC calculated thermal response from *Cm* inventory per MTHM in 51GWd burnup UOX PWR fuel compares favorably with results from the analytical model from LLNL.

In addition to this validation effort, continual verification of code behavior is enabled by a suite of unit tests packaged with the tool. These tests may continually be performed to evaluate the implementated behavior of units of functionality within the interpolation and specific temperature change algorithms even as the code is improved in the future.

CONCLUSIONS

The Cyder source code in which these models are implemented as well as associated documentation are freely available for use by model developers in the field of nuclear waste management. The application programming interface to this software library is intentionally general to facilitate the incorporation of the models presented here within software tools in need of a multicomponent repository model.

Furthermore, this work contributes to an expanding ecosystem of computational models available for use with the Cyclus fuel cycle simulator. The Cyder thermal response and hydrologic nuclide transport library, by virtue of its capability to modularly integrate with the Cyclus fuel cycle simulator, has laid the foundation for integrated disposal option analysis in the context of fuel cycle options.

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