Cyclus Fuel Cycle Simulation Capabilities with the Cyder Disposal System Model

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INTRODUCTION

An algorithm and supporting database for rapid thermal repository loading calculation was implemented in CYDER. 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), Argonne National Laboratory (ANL), 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 with the LLNL semi-analytic model 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}.

CYDER REPOSITORY MODELING PARADIGM

The CYDER disposal system simulator architecture is intended to modularly permit exchange of disposal system Component models (e.g., detailed nuclide transport model vs. less detailed) and data (e.g., exchange clay for granite geologic data) and accept arbitrary waste stream isotopic compositions. Finally, in order to participate in a CYCLUS simulation as a facility model, CYDER must make requests for spent material up to its capacity. Determination of the repository capacity for various types of spent fuel commodities comprises the interfacing functionality of the repository model.

Waste Stream Acceptance

The disposal system simulator must accept arbitrary spent fuel and high level waste streams. A waste stream is a material data object resulting from the CYCLUS simulated fuel cycle. As radionuclides are gained, lost, and transmuted within the spent fuel object, a history of its isotopic composition is recorded. It arrives at the repository and is emplaced if it obeys all repository capacity limits.

For waste streams that vary from each other in composition, the thermal capacity of the repository to receive that waste stream must therefore be recalculated. Since disposable material in most simulations of interest will be of variable composition and therefore heterogeneous in heat production capability, the disposal system simulator will repeatedly need to recalculate its own capacity as new materials are offered.

Waste Stream Conditioning

Waste conditioning is the process of packing a waste stream into an appropriate waste form. As CYCLUS lacks a conditioning facility, the CYDER repository fulfills this need as a part of the repository behavior. As a waste stream is accepted into the repository, it is associated with a waste form according to its commodity name. This pairing is input by the user during simulation setup when a number of waste form Component configurations are specified and associated with allowed waste stream commodities. It is according to these pairings that CYDER loads discrete waste forms with discrete waste stream contaminant vectors as depicted in Figure 1.

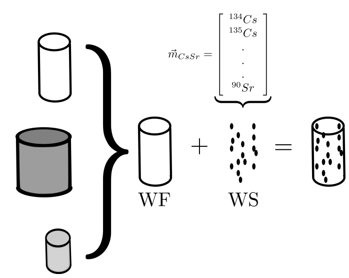

Fig. 1: Waste streams are accepted and conditioned into the appropriate waste form according to user-specified pairings between commodities and waste forms.

Waste Form Packaging

Waste packaging is the process of placing one or many waste forms into a containment package (typcially metallic). Once the waste stream has been conditioned into a waste form, that waste form Component is loaded into a waste package Component, also according to allowed pairs dictated by the user, as depicted in Figure 2.

Package Emplacement

Finally, the waste package is emplaced in a buffer component, which contains many other waste packages, spaced evenly in a grid. The grid is defined by the user input and depends on repository depth, Δz, waste package spacing, Δx,

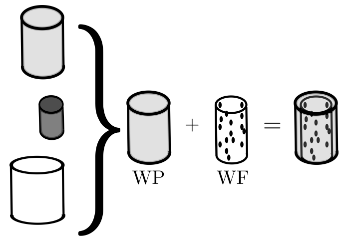

Fig. 2: Waste forms are loaded into the appropriate waste package according to user-specified pairings between forms and packages.

and tunnel spacing, Δy as in Figure 3.

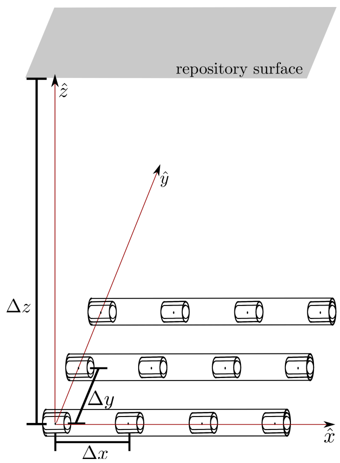

Fig. 3: The CYDER repository emplacement geometry allows generic representation of all semi-regular two dimensional gridded layouts.

Nested Components

The fundamental unit of information in the disposal system simulator is radionuclide contaminant presence at each stage of containment. The disposal system simulator, in this way, is fundamentally a tool to determine thermal and contaminant transport evolution as a result of an arbitrary waste stream. The disposal system simulator in this work conducts this calculation by treating each containment Component as a nested volume in a release chain.

Each Component is defined by a Geometry, some Material Data, a ThermalModel, and a NuclideModel. It is also defined by the Parent Component which contains it and the daughter components which it contains. An emplaced waste package Component, for example, possesses a pointer to the buffer that surrounds it, its Parent Component. It also possesses a list of pointers to the waste form or waste forms within it, its daughter components.

Component Geometry

Each Component of the repository system (i.e. waste form, waste package, buffer, and geologic medium) is modeled as a discrete control volume. Each control volume performs its own mass balance at each time step and assesses its own internal heat transfer and degradation phenomena utilizing boundary condition information provided by adjacent nested Components. This control volume is defined by the Component Geomtry, a class which keeps track of the inner and outer radii, length, and centroid coordinates of the (assumed cylindrical) volume.

Component Material Data

Each Component of the repository system possesses a notion of the material that it is made of. Supporting thermal and hydrologic data for canonical engineered barrier and geologic media is provided with the code in the mat_data.sqlite SQLite database.

Each table in the database holds data related to one of a canonical set of engineered barrier and geologic medium materials (e.g. clay, glass, etc.). The columns of that table hold data required to support all CYDER models. Thermal diffusivity and thermal conductivity comprise the thermal data in the table for each material. The hydrologic and chemical data in the database has one table for each material. Each table contains relative diffusivity coefficients, solubility limits, and sorption parameters for each element.

Component ThermalModel

Each Component possesses a thermal transport model that determines the temperature inside the Component over time. This allows limitations within any barrier at any limiting radius to control the limiting thermal response within the CYDER repository simulator.

Component NuclideModel

Each Component possesses a radionuclide contaminant transport model that determines the contaminant transport inside the Component over time. The choices available for this NuclideModel range in fidelity but emphasize the distinction between dominant transport modes (advective or disperive) in various geologic media as well as dominant retarding geochemistry for specific isotopes (sorption and solubility limitation).

Implicit Timestepping

Each Component passes some information radially outward to the nested Component immediately containing it and some information radially inward to the nested Component it contains.

In the case of radionuclide transport, for example, each Component model requires information about the radionuclides released from the Component it immediately contains. Thus, nuclide release information is passed radially outward from the waste stream sequentially through each containment layer to the geosphere. However, the solutions within each Component often rely on the external boundary conditions of that Component. Thus, the CYDER model uses an implicit timestepping method to arrive at the future state of each Component, radially outward, as a function of both the past state and the current state.

That is, in Component j, some Component in a nested series, the mass flux entering the Component at time t_n is found from the initial state of the cell at time t_n, the inner boundary condition at time t_n and the outer boundary condition at t_{n-1}.

$$\dot{m}_{ij}^n = f(m_j(t_{n-1}), BC_i(t_n), BC_j(t_{n-1})...)$$

where

$$\begin{aligned} m_{ij}(t_n) &= \text{ contaminant mass flux from component i to j } [kg/timestep] \\ BC_i(t_n) &= \text{ inner conditions at } r_i\text{, and time } t_n \\ BC_j(t_{n-1}) &= \text{ outer conditions at } r_j\text{, and time } t_{n-1} \\ f &= \text{ functional form of contaminant transport into j.} \end{aligned}$$

Once the mass flux into the component is found, the mass is removed from the inner cell, updating its state in preparation for the next time step.

$$m_i^{\dagger}(t_n) = m_i(t_n) - m_{ij}(t_n) \tag{1}$$

where

$$m_i^{\dagger}(t_n) = \text{ updated mass in component i } [kg] \tag{2}$$

In this way, the contained mass in the component is described as

$$m_j(t_n) = m_j(t_{n-1}) + \dot{m}_j(t_n).$$

Resulting concentration profiles across the component can then be calculated and one can solve, numerically, for the outer boundary condition at t_n

$$\begin{aligned} BC_j(t_n) &= g\left(m_j(t_n), C_j(t_n)\right) \\ g &= \text{functional form of contaminant transport across j} \end{aligned}$$

This boundary condition can, in turn, be used by the component external to it, k as the t_n inner boundary condition of its own solution and so on.

THERMAL TRANSPORT ANALYSIS

For dynamic thermal capacity analysis in Cyder, a transient model utilizes a linear approximation of heat based capacity quickly for each arbitrary waste stream offered to the repository. This relies on a thermal reference database of repository heat evolution curves covering the thermal coefficient range of the main geologies of interest and over a range of realistic waste package spacings.

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 1 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.

Thermal Cases

Parameter	Symbol	Units	Value Range
Diffusivity	α_{th}	$[m^2 \cdot s^{-1}]$	$1.0 \times 10^{-7} - 3.0 \times 10^{-6}$
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 1: 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, 5].

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 [6, 5, 4]. It employs an analytic model from Carslaw and Jaeger and is implemented in MathCAD [7, 8]. 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.

Figure 4 demonstrates the scaling of an STC curve according to equation (**??**) 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 (**??**) becomes

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

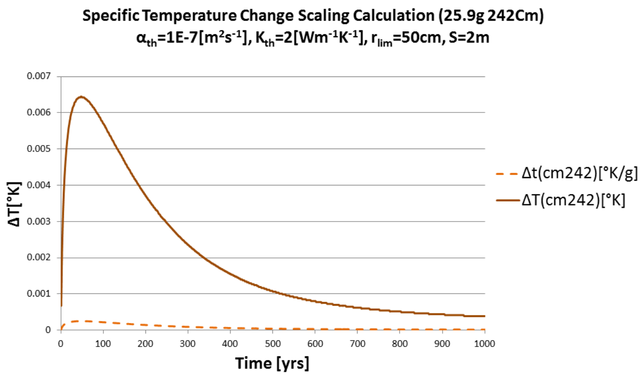

Fig. 4: As a demonstration of the calculation procedure, the temperature change curve for one initial gram of ^{242}Cm and is scaled to represent $25.9g$, approximately the ^{242}Cm inventory per MTHM in 51GWd burnup UOX PWR fuel.

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 5.

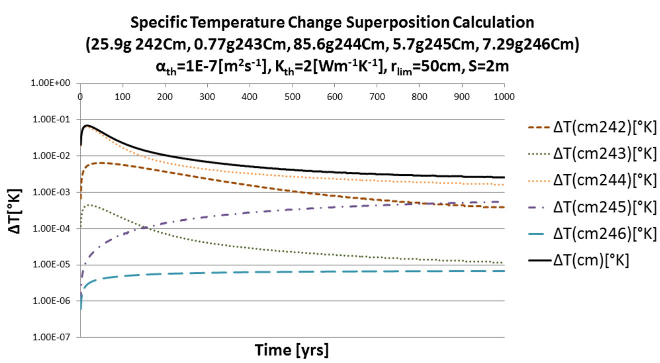

Fig. 5: As a demonstration of the calculation procedure, scaled temperature change curves for five curium isotopes are superimposed to achieve a total temperature change (note log scale).

Thermal Transport Validation

The results here provide an overview of the relative importance of thermal parameters that that affect the repository capacity of simplified generic disposal concept in various geologic media where conduction is the dominant heat transfer mode. The applicability of this sensitivity analysis is thus restricted to enclosed, backfilled concepts.

Parametric Domain

Sensitivity analyses were conducted which span the parametric range of values generated by the reference specific temperature change database and described in Table 1.

These values were selected to provide detail in the near field and at values of α_{th} and K_{th} in the three host media under consideration in this work.

Approach

This analysis utilized the LLNL semi-analytic MathCAD model utilized to derive supporting data and to validate behaviro within the CYDER STC model. It performs detailed calculations of the conductive thermal transport in a generic repository concept with a gridded layout.

It relies on the thermal diffusivity, α_{th} and conductivity K_{th} of the material as well as the waste package spacing, S, and thermally limiting radius, r_{lim}. Finally, it relies on the STC data calculated with the semi-analytic model based on the decay heat profiles of the emplace wastes, Q. The essential decay heat profiles, Q, were retrieved from a UFD database provided by Carter et al. [3].

Thermal Conductivity Sensitivity Validation

The thermal conductivity, K_{th} of geologic repository host media impacts the speed of transport, and therefore the time evolution of thermal energy deposition, in the medium.

LLNL Model Results

In the creation of the STC database, the thermal conductivity was varied across a broad domain for each isotope, i, package spacing, s, limiting radius r_{calc}, and thermal diffusivity α_{th}, considered. By varying the thermal conductivity of the repository model from 0.1 to 4.5 $[W \cdot m^{-1} \cdot K^{-1}]$, this sensitivity analysis succeeds in capturing the domain of thermal conductivities witnessed in high thermal conductivity salt deposits as well as low thermal conductivity clays.

Figure 6 shows the trend in which increased thermal conductivity of a medium decreases thermal energy deposition in the near field. This indicates, then that thermal conductivity is an important parameter for repository geolgic medium selection.

Cyder Results

In a similar analysis, the thermal conductivity was compared both with the spacing between waste packages and the limiting radius.

Figures 7 and 8 validate the trend noted above that increased thermal conductivity of a medium decreases thermal energy deposition in the near field. Additionally, analysis with the CYDER STC database demonstrates the way in which the importance of spacing and the importance of the limiting radius decrease with increasing K_{th}.

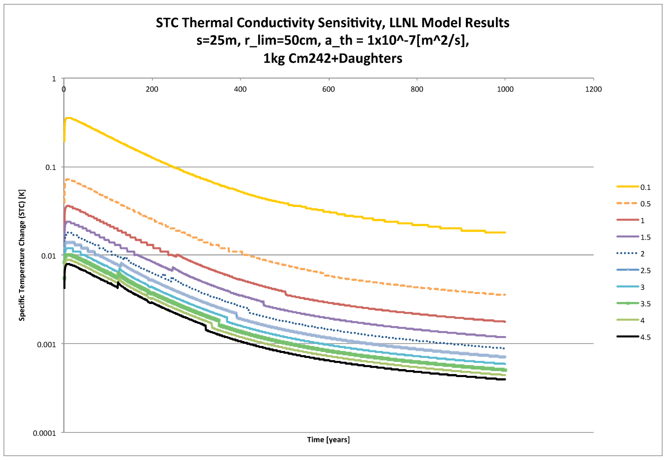

Fig. 6: Increased thermal conductivity decreases thermal energy deposition (here represented by STC) in the near field (here $r_{calc} = 0.5m$).

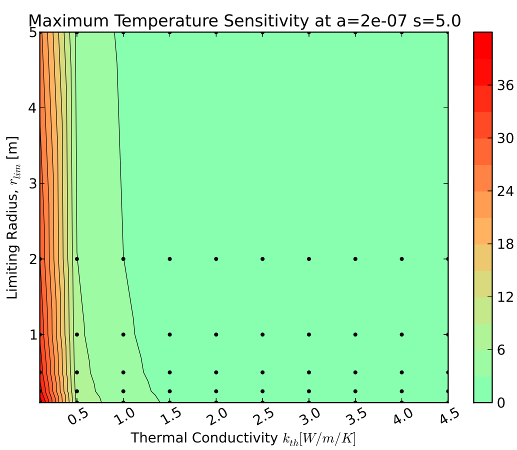

Fig. 7: Cyder results agree with those of the LLNL model. The importance of the limiting radius decreases with increased K_{th}. The above example thermal profile results from 10kg of ^{242}Cm

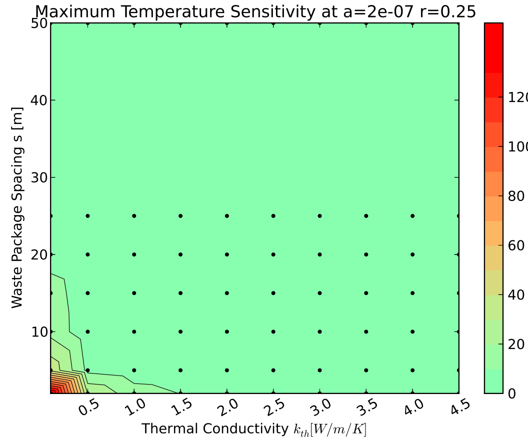

Fig. 8: Cyder results agree with those of the LLNL model. The importance of the limiting radius decreases with increased K_{th}. The above example thermal profile results from 10kg of ^{242}Cm

Thermal Diffusivity Sensitivity Validation

The thermal diffusivity, α_{th} of geologic repository host media describes the tendency of thermal energy to diffuse through, and therefore be deposited, in the medium.

LLNL Model Results

In the creation of the STC database, the thermal diffusivity was varied across a broad domain for each isotope, i, package spacing, s, limiting radius r_{calc}, and thermal conductivity K_{th}, considered. By varying the thermal diffusivity of the disposal system from $0.1 - 3 \times 10^{-6}[m^2 \cdot s^{-1}]$, this sensitivity analysis succeeds in capturing the domain of thermal diffusivities witnessed in high thermal diffusivity salt deposits as well as low thermal diffusivity clays.

Figure 9 shows the trend in which increased thermal diffusivity of a medium decreases thermal energy deposition in the near field. This indicates, then that thermal diffusivity is an important parameter for repository geolgic medium selection. The effect is accentuated by high thermal conductivities, as seen in Figure 10

Cyder Results

In a similar analysis, the thermal diffusivity was compared both with the spacing between waste packages and the limiting radius.

Figures 11 and 12 validate the trend noted above that increased thermal diffusivity of a medium decreases thermal energy deposition in the near field. Additionally, analysis with the CYDER STC database demonstrates the way in which the importance of K_{th} remains constant, but the importance of the limiting radius decreases with increasing α_{th}.

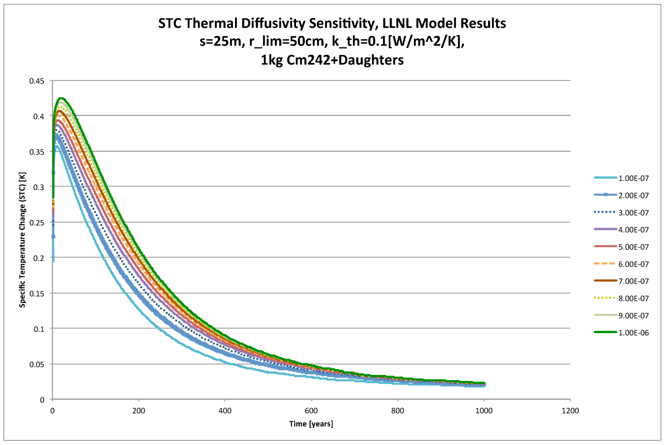

Fig. 9: Increased thermal diffusivity decreases thermal energy deposition (here represented by STC) in the near field (here $r_{calc} = 0.5m$).

Fig. 10: Increased thermal diffusivity decreases thermal energy deposition (here represented by STC) in the near field (here $r_{calc} = 0.5m$).

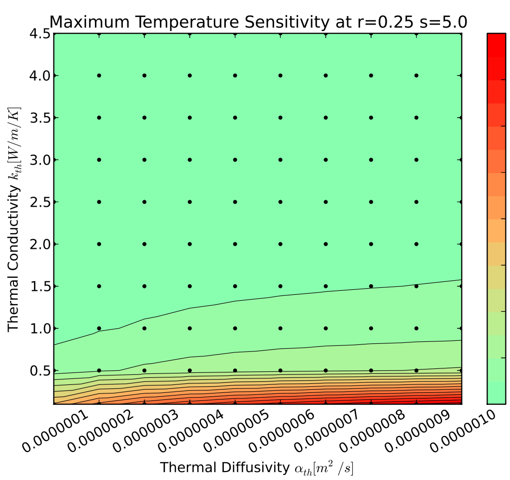

Fig. 11: Cyder trends agree with those of the LLNL model, in which increased thermal diffusivity results in decreased thermal depsoition in the near field. The above example thermal profile results from 10kg of ^{242}Cm.

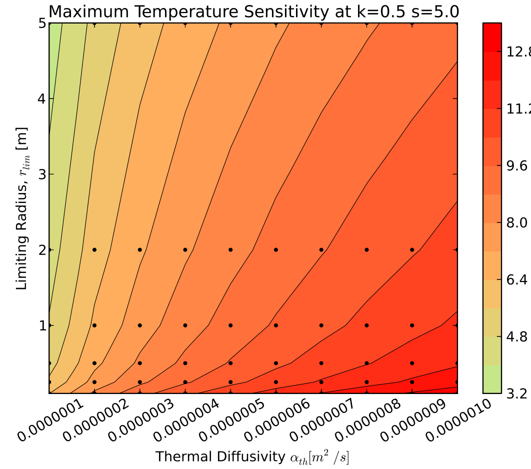

Fig. 12: Cyder trends agree with those of the LLNL model. The importance of the limiting radius decreases with increased K_{th}. The above example thermal profile results from 10kg of ^{242}Cm

Waste Package Spacing Sensitivity Validation

The waste package spacing, s of geologic repository concept effects the areal decay heat burden in the repository and has a strong effect on the thermal energy deposited per unit area in the medium.

LLNL Model Results

In the creation of the STC database, the waste package spacing was varied across a number of values for each isotope, i, limiting radius r_{calc}, thermal diffusivity α_{th}, and thermal conductivity K_{th}, considered. By varying the waste package spacing of the geometric layout from $0.1 - 5[m]$ this sensitivity analysis succeeds in capturing the domain of waste package spacings present in geologic repository concepts under consideration.

Figure 13 shows the trend in which increased waste package spacing of a medium decreases areal thermal energy deposition in the near field. This indicates that waste package spacing is an important parameter for repository concept design.

Similarly, the location of the limiting radius has a strong effect on the waste package loading limit, for a fixed limiting temperature. In Figure 14, the trend is demonstrated in which increased limiting radius decreases the thermal energy contributing to the thermal limit.

Cyder Results

In a similar analysis, the thermal diffusivity was compared both with the spacing between waste packages and the limiting radius.

Figure 15 validates the trend noted above that increased

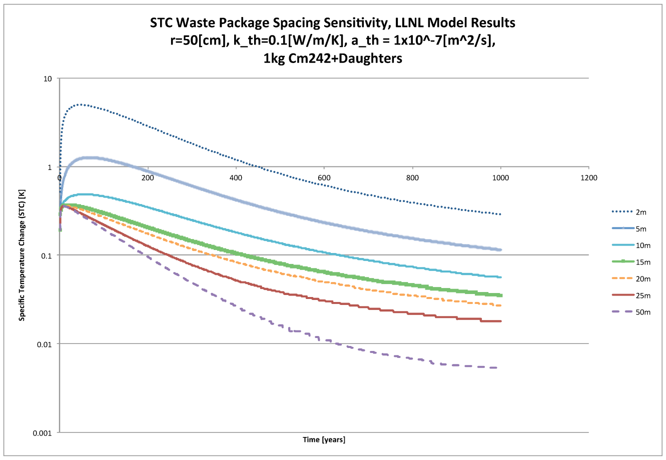

Fig. 13: Increased waste package spacing decreases areal thermal energy deposition (here represented by STC) in the near field (here $r_{calc} = 0.5m$).

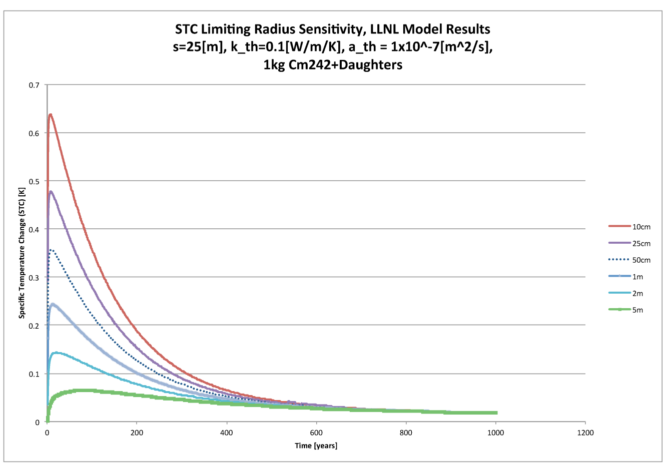

Fig. 14: Increased limiting radius decreases thermal energy deposition contributing to the thermal limit (here represented by STC).

waste package spacing in a repository concept decreases areal thermal energy deposition in the near field. Additionally, analysis with the CYDER STC database demonstrates the way in which the importance of r_{lim}, the limiting radius, impacts the maximum calculated temperature at that radius.

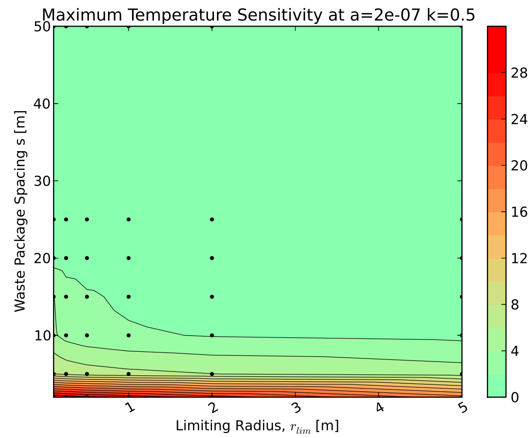

Fig. 15: Cyder results agree with those of the LLNL model. The importance of the limiting radius decreases with increased K_{th}. The above example thermal profile results from 10kg of ^{242}Cm

RESULTS

Computational fuel cycle simulation tools capable of simulating heterogeneous spent fuel isotopics resulting from transition scenarios and alternative fuel cycles have previously lacked equally dynamic repository modeling options. This work demonstrates that the Cyder generic repository model can inform fuel cycle metrics by providing just such a dynamic interface between waste management and fuel cycle technology decisions.

The sensitivity analyses and validation efforts conducted in this work demonstrate the capability of the CYDER tool to provide repository capacity and performance metrics in the context of dynamic fuel cycle feedback effects.

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