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Disposal Systems Evaluation Framework DSEF Version 3.0 User Manual

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DISPOSAL SYSTEMS EVALUATION FRAMEWORK

DSEF VERSION 3.0 USER MANUAL

Used Fuel Disposition Campaign

Level 4 Milestone (M4): M4FT-13LL08060323

Generic Engineered Barrier System Evaluation

(Work Package FT-13LL080603)

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Revision History

LLNL-TR-629812 - March 2013 – Original issue of User Manual for DSEF Version 2.1

LLNL-TR-629812 Rev. 1 - August 2013 – Updated for DSEF Version 3.0

- Extensive revision of disposal system cost model including updated Inputs and Cost Calculation worksheets
- Increased number of cases in the Case Library from 300 to 721, including 4 new Case Catalog sections for easy access to the new cases
- The addition of two new Mathcad thermal-analytical models
  - A model to determine required ventilation time to meet specific temperature acceptance criteria using an iterative convergence model
  - A model allowing temperature-dependent and time-dependent properties of the Engineered Barrier System layers of the thermal analytical model

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List of Acronyms

ANL	Argonne National Laboratory
DOE	Department of Energy
DSEF	Disposal Systems Evaluation Framework
EBS	Engineered Barrier System
EC, E-Chem	Electro-Chemical (with –C or –M indicates ceramic or metal, respectively) HLW waste form
GWd/MT	Gigawatt (thermal) - days per Metric Ton
HLW	High-Level nuclear Waste
LLNL	Lawrence Livermore National Laboratory
MOX	Mixed Oxide Fuel
NBS	Natural Barrier System
PWR	Pressurized Water Reactor
ROM	Rough Order of Magnitude
SNL	Sandia National Laboratories
UFD	Used Fuel Disposition
UOX	Uranium Oxide Fuel
UOX-40	UOX with 40-GWd/MTU burnup
UOX-60	UOX with 60-GWd/MTU burnup
VBA	Visual Basic for Applications
WP	Waste Package

1. Overview

The Disposal Systems Evaluation Framework (DSEF) has been developed at Lawrence Livermore National Laboratory (LLNL) to formalize and facilitate the development and documentation of repository conceptual design options for a range of waste forms, geologic environments, repository design concepts, and repository operating modes. DSEF is one component of the Engineered Barrier System (EBS) family of work packages at several national laboratories led by Sandia National Laboratories (SNL), in support of the DOE Office of Nuclear Energy, specifically of the Used Fuel Disposition (UFD) Campaign within the Office of Used Nuclear Fuel Disposition Research and Development (NE-53).

DSEF is a knowledge management system that allows the user to intelligently access and draw data from a case library of hundreds of completed thermal analyses (currently 721 cases in the library), and draw input from databases of material properties and repository development cost data (currently the data in these databases are drawn from more than 100 references).

The core functionality of DSEF is provided by a Microsoft Office Excel 2010 workbook with macros and form controls that create a structured environment and walk the user through the steps of creating the input data required to perform disposal system evaluations internally and by interfacing with external programs. The user can choose to work with built-in data from the case library of previous analysis cases, from the material property databases, or can define their own input descriptions and data.

DSEF uses the Excel **worksheet protection** (implemented on a sheet by sheet basis) to prevent inadvertent over-writing of formulas with data. When worksheet protection is enabled, the user can see all underlying formulas, and enter data in unprotected cells (the unprotected cells generally correspond to the yellow highlighted cells). Worksheet protection also prevents restructuring the files (adding or deleting rows or columns) and changing the formatting, as well as preventing access to the Visual Basic Editor to prevent modification of the macros. If the user needs to modify the worksheet structure, formulas, or macros, they can contact LLNL to get the password to unprotect the worksheets. However, care should be taken in making any modifications, since the macros and formulas are dependent in some cases on the current structure, range names, and macro subroutines

DSEF is set up to retrieve the results of external thermal analysis program runs, summarize them graphically, and provide a template for adding the new results to the Case Library.   The Case Library worksheet in DSEF is set up to create a Case Library data record for each new analysis case, at the top of the list of prior cases. Therefore, a separate DSEF file (with unique name) should be saved for each run that is to be archived. Users should submit a copy of their DSEF files to LLNL so that their results can be added to the overall Case Library and made available to other laboratories and stakeholders.   LLNL will maintain the DSEF Case Library and make the most current files available on the SNL SharePoint site. The Revision History sheet documents the file evolution.

One of the key objectives of DSEF is to allow the user to compare the results of thermal analyses to the thermal constraints of the design components. These comparisons can then be used to consider design, layout, and operating mode modifications to find combinations that can meet the thermal constraints for a given combination of waste form, geologic medium, surface storage time, and system concept of operation.

DSEF has built-in capabilities to allow a user to graphically compare and contrast material property data, with statistical data summaries for the selected data sets. This is done at the push of a control button, where the user can then select a range or a collection of individual sets of data for comparison, with the freedom to select the placement location of the comparison plot.

As part of the assessment of design concept feasibility, DSEF includes the capability to evaluate the costs of repository design, licensing, construction, maintenance, closure and performance confirmation based on the methodology defined in Carter 2012 and Hardin 2012b. The costs also include waste packages and program integration costs. Similar to the thermal analysis Case Library, DSEF includes five sets of cost data input values from the five generic repository design cases defined in Carter 2012 and Hardin 2012b as example reference cases. The cost data for these five cases can be displayed on the INPUTS worksheet as examples of the cost calculations documented in the subject references, and they can be used directly or over-ridden by user supplied input to analyze different repository design concepts.

Interfaces with various repository analysis codes are possible for further DSEF development. Version 3.0 currently provides input to, and retrieves output data from; several Mathcad Version 15 thermal-analytical models developed at LLNL (see Appendix B).

This User Manual describes the structure and use of the various types of worksheets contained in the DSEF Version 3.0 workbook. Most of the worksheets are fully operational. Some worksheets are placeholders pending potential future development. A Beta test Version 2.0 of the software was delivered previously to the SNL Lead, Carlos Jove-Colon, and the DOE Manager, William Spezialetti; their comments greatly improved the software and this User Manual. The DSEF Version 2.0 Beta Test Excel file and the draft DSEF Version 2.0 User Manual delivered in September and August 2012 respectively met the requirements of Deliverable M4FT-12LL0806043. The DSEF Version 2.1 Excel spreadsheet, Mathcad thermal-analytical model, and the original issue of the DSEF User Manual for Version 2.1 (LLNL-TR-629812 were issued as in March 2013, and posted to the SNL SharePoint server for distribution.

2. Information Flow

As in the DSEF Version 1.0 Progress Report (Sutton 2011), waste forms are examined with respect to three fuel cycles: open (once through), modified open (partial recycle), and closed (full recycle). The six heat-producing waste types from these cycles (one from open, two from modified open, and three from closed) are identified as examples with dimensions, mass, reactor burnup and decay heat properties. Seven disposal environments were initially identified, with the four key mined and saturated repositories (granite, salt, clay/shale and deep borehole) being part of the base case for DSEF evaluations. Together with six fuel types and four pre-emplacement aging times (10, 50, 100, and 200 years), 120 base case models were proposed (including 1 and 4-PWR-assembly options for SNF waste packages in granite, clay, and salt). Additional repository concepts, geological environments, operating modes, waste packages sizes, and spent fuel burnup cases were analyzed and documented in DSEF Version 2.1 (expanding the number of cases in the Case Library to 300) and in Version 3.0 (expanding the number of cases to 721).

Figure 1 is a high-level overview of the structure and approach that is implemented in DSEF to help the user gather the necessary input data, define an analysis case, and compare results to design constraints. It is used in an iterative manner to focus in on feasible repository design concepts for a given combination of heat generating high-level radioactive waste in a given geologic medium using selected repository design and operating concepts.

Figure 1- DSEF Input-Process-Output diagram

INPUTS	PROCESS	OUTPUT
• **GEOLOGIC MEDIA DATA** HOST ROCK TYPE AND MATERIAL PROPERTIES • **WASTE FORM PHYSICAL DATA** WASTE PACKAGE DIMENSIONS AND MATERIALS • **WASTE FORM RADIOLOGICAL DATA** DECAY HEAT DATA BASED ON RADIONUCLIDE INVENTORY • **ENGINEERED BARRIER SYSTEM DATA** EBS LAYERS, MATERIAL TYPES, DIMENSIONS AND MATERIAL PROPERTIES • **REPOSITORY LAYOUT CONCEPTS** PHYSICAL SPACING AND ARRANGEMENT DATA • **STORAGE AND OPERATIONAL DATA** SURFACE STORAGE PRIOR TO EMPLACMENT, AND ASSUMPTIONS FOR OPERATIONS AND CLOSURE • **CASE LIBRARY DATABASE** PREVIOUS ANALYSIS CASE INPUT DATA AND RESULTS • **COST CASE EXAMPLES** PREVIOUS ROM COST REPORT CASE INPUT DATA AND RESULTS	• **DEFINE** THE ANALYSIS CASE PARAMETERS, ASSUMPTIONS, AND DESIGN CONSTRAINTS • **ASSEMBLE** REQUIRED INPUTS FOR EACH CASE • **DOCUMENT** PARAMETER SELECTIONS FOR EACH CASE • **DEVELOP** RANGE OF UNCERTAINTIES FOR PARAMETER UNCERTAINTY ANALYSIS • **VALIDATE** ANALYSIS RESULTS BY COMPARING ANALYTICAL AND FINITE ELEMENT MODEL CALCULATIONS • **COMPARE** THERMAL RESULTS AGAINST DESIGN CONSTRAINTS • **ITERATE** REVISE INPUT ASSUMPTIONS UNTIL CONSTRAINTS CAN BE MET	• **ACCEPTABLE REPOSITORY DESIGN AND OPERATING CONCEPTS** • **TEMPERATURE TRANSIENT RESULTS** • **ROUGH ORDER OF MAGNITUDE COSTS** • **PERFORMANCE ASSESSMENT RESULTS FOR THE REPOSITORY CONCEPT** ** • **OUTPUT DATA TO INTERFACE WITH EXTERNAL PROGRAMS** • **OUTPUT DATA AND RESULTS TO MASTER CASE LIBRARY**

Notes:
**Not currently implemented in DSEF VERSION 3.0.

Figure 2 shows the detailed information flow in DSEF that implements the approach defined in the input-process-output diagram shown in Figure 1. It shows how DSEF can be used to identify feasible repository disposal concepts. TruGrid and DIABLO are used as examples of interfacing external analysis programs. The user could easily substitute CUBIT for the TruGrid as an alternate mesh generation program, and SINDA-G, ARIA, ALBANY, TOUGH2 or TOPAZ for DIABLO as other possible finite element model thermal analyzers.

Figure 2 – Example of the information flow in DSEF
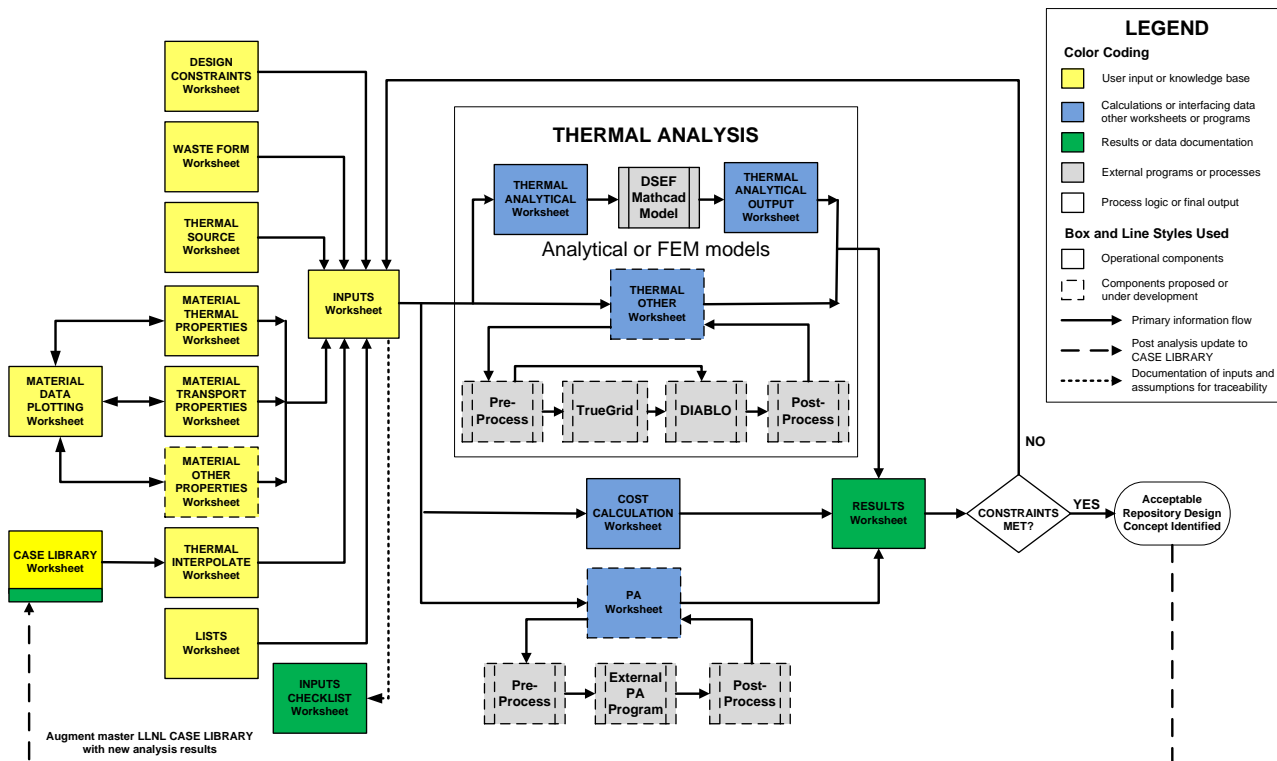
3. Finding Your Way Around – the NAVIGATION, README, LISTS and REV HISTORY Worksheets

Hyperlinks are available throughout the worksheets in the DSEF workbook to help you navigate quickly to related input and data source pages. The NAVIGATION worksheet in DSEF is the first worksheet tab, which allows users to quickly move to any worksheet and can be found by clicking on the Excel control for scrolling through the worksheet tabs. It is shown in Figure 3, with the arrow pointing to the "go to the first tab" button. Clicking on that will always take you to the NAVIGATION worksheet.

Figure 3 – Using the Excel tab navigation bar
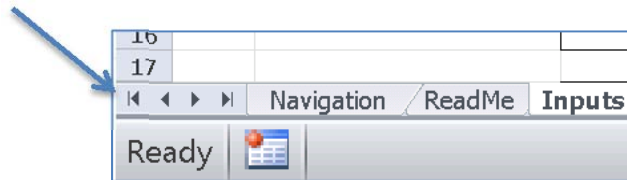
On the NAVIGATION worksheet, there are two lists as shown in Figure 4. The list on the left shows the names of the worksheets in the sequence that they appear in the DSEF workbook. The list on the right consists of the same names but sorted alphabetically and hyperlinked to the worksheets themselves. Using the control shown in Figure 3 and the hyperlinks shown in Figure 4 enables quick navigation to any worksheet with two simple mouse clicks.

The README worksheet gives a brief overview of DSEF. At the bottom, there is an "Information Flow" description that explains the relationships between many of the worksheets. That part of the README worksheet serves the same purpose as this User Manual, but can be updated more easily when minor modifications and improvements are made to DSEF.

The LISTS worksheet is a tool primarily used by the DSEF Development Team. It is a central location for all drop-down lists and look-up tables used by other worksheets. Some advanced users may choose to view this worksheet to globally see the range of choices in these lists and to recommend additional choices to the DSEF Development Team.

The REV HISTORY worksheet documents the development history of DSEF. Advanced users may choose to view this worksheet to determine comparability of runs with earlier DSEF versions with current runs.

Figure 4 – The two lists of worksheets in the NAVIGATION worksheet

Worksheets in order of appearance		Hyperlinks to Worksheets in alphabetical order
Navigation (this sheet)		Case Library
Readme		Cost Calculations
Inputs		Cost References
Inputs Checklist		Design Constraints
Case Library		Environment
Thermal-Interpolate		Inputs
Results		Inputs Checklist
Interface Parameters		Interface Parameters
Design Constraints		Lists
Waste Form		Material Data Plotting
Environment		Materials
Thermal		Materials-Other Properties
Thermal-Source		Materials-References
Thermal-Analytical		Materials-Thermal Properties
Thermal-Analytical Output		Materials-Transport Properties
Thermal-FEM		Navigation (this sheet)
Performance Assessment		Performance Assessment
Cost Calculations		Readme
Cost References		Results
Materials		Rev History
Material Data Plotting		Thermal
Materials-Thermal Properties		Thermal-Analytical
Materials-Transport Properties		Thermal-Analytical Output
Materials-Other Properties		Thermal-FEM
Materials-References		Thermal-Interpolate
Rev History		Thermal-Source
Lists		Waste Form

4. Getting Started – Working with the DSEF Workbook

Opening DSEF for the First Time – Enabling the Macros

DSEF is a Microsoft Excel workbook with macros, and therefore has a file extension of ".xlsm" is used instead of the typical ".xlsx" for a workbook without macros. The macros developed in the built-in Visual Basic for Applications (VBA) programming language allow DSEF to automate a number of process steps coupled with the use of Form controls (such as command buttons and drop-down lists).

The first time that you open the DSEF workbook, you may get a prompt at the top of the workbook (below the Ribbon) notifying you that macros have been disabled for your protection and asking you if you want to enable macros. **In order for the Form controls to work, you must *enable macros*.** If you do not see this prompt, and the drop-down lists and other controls do not respond, you must change some settings in Excel. A detailed step-by-step procedure is outlined in Appendix A, complete with screen shots that point out exactly which options to select.

The Color Coding Conventions for Types of Cells and Information in DSEF

The DSEF file includes a significant amount of error checking and messages, and uses color codes for hyperlinks, errors, and inputs. Color coding conventions to help you recognize where input is needed, and where input is being used from other worksheets are the following:

- **Yellow highlighted cells**: Input cells or controls that help you select or input data
- **White highlighted cells**: Normal cells that contain data or formulas
- **Cells with a gray background and blue lettering** contain hyperlinks to other worksheets
- **Light gray highlighting of cells with black text** is used to distinguish different subsets of analysis cases for some of the CASE CATALOGs and some of the cases in the CASE LIBRARY. It is also used to distinguish the five cost case example data sets available on the INPUTS worksheet
- Light blue highlighted cells: Cells that retrieve data from other worksheets
- Cross-check / Caution cells:
  - **White background with black text** - Cross-check cells that provide confirmation of valid input
  - **Light red background with red text** – Cross-check cells that caution the user of a potential inconsistency when the cross-check confirmation fails
- **Green arrows and text**: Point to cells that have special range names used in formulas elsewhere

Working with the Form Controls

There are several kinds of Form controls used in DSEF, and for the most part, their use is straightforward (such as command buttons and check boxes). Figure 5 and Figure 6 show two examples.

The Form controls can serve three purposes

- They allow you to select from a pre-defined set of options, or allow you to enter a "user defined" option
- They can automatically run a macro program based on the selection you made. For example the control shown in Figure 5 runs a macro that copies the decay heat data for the selected waste form **from** a library of decay heat data on the THERMAL-SOURCE worksheet **to** the named range that defines the decay heat that will be used in the current analysis.
- They can limit the range of values you can use. For example the spinner control shown in Figure 6 only allows values between 5 years and 300 years of surface storage.

Figure 5 – A drop-down list to select the waste form
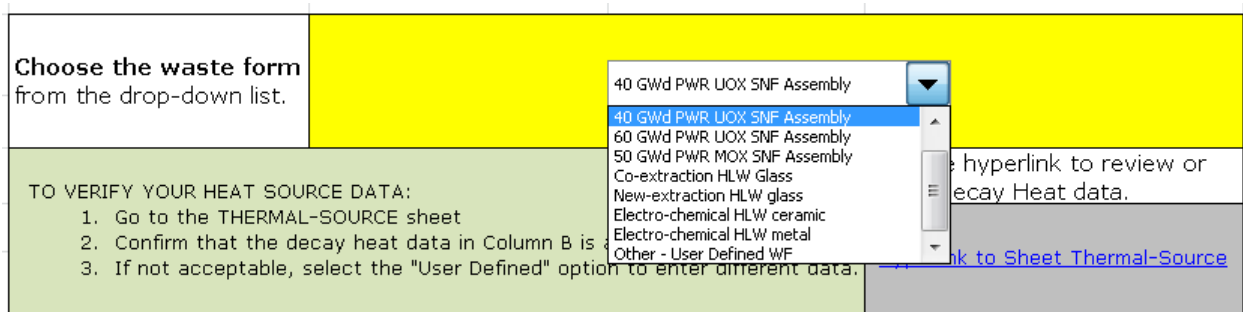
Figure 6 – A spinner control to select the number of assemblies in a waste package

In a number of cases, the data entry sections of the DSEF worksheet will look different depending on the selections you make using these controls. This is done by using conditional formatting to hide unused data entry cells and to display others, and by running macros that can hide some of the other controls.

Naming and Saving Files

DSEF is a template and is provided as a read-only, macro-enabled (xlsm), Excel spreadsheet. You must use the SAVE-AS menu command to save a DSEF workbook with your own data in it. The INPUTS worksheet helps you construct a file name with a standard set of information that will be common to all users and has a macro button to save the file (to the current directory) using the file name DSEF itself constructs. It is highly recommended you use this capability, rather than manually using the SAVE-AS Excel command. The name will include the DSEF version, date, your initials, and some information about waste form and medium from other selections you make on the INPUTS worksheet. The name will also include text that you specify after picking from the initial menus, and also a case number if you do multiple runs based on a similar configuration.

Suggested file name =

DSEF [Version]-[date]-[user's initials]-[waste form & geologic medium]-[a 4 to 30 character case description]-[case number of up to 6 alpha numeric characters].xlsm

After new design cases have been analyzed using DSEF and an external thermal analyzer like Mathcad, the DSEF file will include the results of your analysis on the RESULTS and THERMAL-ANALYTICAL OUTPUT worksheets, and will have a new data record for the analyzed design case on the CASE LIBRARY worksheet (just below the Case Catalog and the list of references).

As described in Section 11 of the User Manual, you can use a macro button on the THERMAL-ANALYTICAL OUTPUT worksheet to format the results written by Mathcad, and after doing that, you need to manually save this file using the FILE SAVE command in Excel. A copy of the completed DSEF file should be sent to LLNL to allow consolidation and augmenting of the master Case Library, thereby allowing updating and sharing of the new information between laboratories via the SNL SharePoint website.

5. The Starting Point to Define an Analysis Case - the INPUTS Worksheet

The central data entry worksheet in DSEF is the INPUTS worksheet. This worksheet builds the analysis case in steps (which are numbered and shown on the left edge). The user can proceed linearly through the worksheet, from top to bottom following the instructions on the worksheet, and completely define the analysis case. DSEF also provides two types of assistance in addition to the linear process:

- Hyperlinks to other worksheets are provided to allow the user to inspect libraries of properties (see Section 12). Some of these worksheets include tools to organize and/or visualize information being considered. The user can then return to the INPUTS worksheet (via another hyperlink, or by manual navigation) and input the parameter.
- Numbered cases in the CASE LIBRARY (see Section 7). The user can select a prior case number in several places on the INPUTS worksheet, resulting in pre-population of some input cells. The user can then overwrite parameters that are different than the "reference" case being used for that set of parameters in the INPUTS worksheet. The user can also use a hyperlink to jump to the THERMAL INTERPOLATE worksheet, which has tools to organize and visualize selected parameters for a selected set of cases (see Figure 22 - Side-by-side case comparison table).

For experienced users, the cells in the linear process that require decisions or inputs are colored, allowing fast input without reading all the instructions for each use of DSEF.

Automatic Entry of Inputs

The power of DSEF can be used to automatically fill in many of the inputs by simply selecting a CASE LIBRARY case number. Different reference cases can be used for the natural and engineered barrier properties and configurations. Ideally, users can select a common reference case number to set the starting inputs for both NBS and EBS (DSEF won't stop you from using different cases, but it will alert you if you have). An example is shown in Figure 7.

Figure 7 - An example of some of the cross-checks and cautions displayed in the INPUTS worksheet

Designation of Case from Sheet "Case Library" for Initial EBS parameter data values					
Table1: Summary of EBS Component Selection Using CASE:		23	<-- EBS_case_select		CAUTION – The NBS and EBS case selections don't match!
CAUTION – The waste form for selected case does not match the waste form selected above!			CROSS-CHECK – The waste package spacing for selected case matches the spacing entered above.		
CROSS-CHECK – The waste package capacity for selected case matches the waste package capacity selected above.			CROSS-CHECK – The drift/borehole spacing for the selected case matches the spacing entered above.		
Case Number	DSEF Case Descripton	Waste Form	WP Capacity	EBS Components	Design Mode (Enclosed/Open)
23	Salt 4-UOX-40, Storage time=10 y, WP spacing=20 m, Drift/borehole spacing=20 m, EBS based on 200°C properties	UOX-40	4	WP, crushed Salt (to 3.048 m, calc rad = 4 m)	Enclosed

DSEF has several different constructs to use existing data. Some situations provide drop-down lists of data selections, and others have single data entry value displays and over-ride options. An example of the second approach is shown in Figure 8, in which the yellow override cells change the reference-case-

populated values to the left. The resulting set of values (some from the pre-population and others from the overrides) are shown to the right of the yellow cells.

Figure 8 - An example of one of the ways DSEF lets you use data from the case library, or override the data with user input

Default EBS Component Names	User Input Names for EBS Components	EBS Component Names	Component Radial Thickness, m for Case 229	User Input Component Radial Thickness	Component Radial Thickness	Inner Radius m	Outer Radius m
Waste Form		Waste Form	0.89		0.89	N/A	0.89
Canister		Canister	0		0	0.89	0.89
Waste Package		Waste Package	0.11		0.11	0.89	1
Buffer		Buffer	0	0.1	0.1	1	1.1
Envelope	Buffer Layer 2	Buffer Layer 2	0	0.2	0.2	1.1	1.3
Backfill		Backfill	1.225	0.925	0.925	1.3	2.225
Liner		Liner	0.025		0.025	2.225	2.25
					Host Rock Inner Radius, m ---->	2.25	

Steps in the INPUTS Worksheet Process

The INPUTS worksheet is designed to guide the user in developing an analysis case in a structured manner. To assist new or infrequent users, instructions are provided near the entry fields. Color conventions are used to enable frequent users to move through the steps quickly, skipping those instructional fields. For all users, DSEF checks many of the inputs for consistency and provides feedback in cells labeled "Cross-Check".

The user should follow these steps sequentially in the DSEF INPUTS worksheet:

- Step 1 provides the user with the DSEF version number. No action is required, but the user should be aware that DSEF evolution from version to version could compromise comparability of results with earlier runs. The REV HISTORY worksheet documents the changes.

- Step 2 builds the case name and includes a macro for the initial saving of the file using the case name. The user inputs the date, their initials, some descriptive text, and a case number. Because the case name includes the geologic medium and the waste form, the user also selects (from pull-down lists) those parameters in Step 2. Step 2 also includes a macro button that allows the user to "Clear Previous Thermal Output Results" if the same Excel file is being used as a starting point to prepare multiple analysis cases.

- Step 3 selects the waste package capacity, in terms of the number of spent nuclear fuel assemblies or high-level waste canisters. A spinner control enables selection of integer numbers. A check box enables input of a non-integer number (for the situations of rod consolidation or non-standard canister sizes).

- Step 4 selects the storage time, which is the time between removal from the reactor flux to the emplacement in the repository.

- Step 5 selects the repository depth. Three inputs are required: depth, surface temperature, and geothermal gradient. DSEF uses these three inputs to calculate the initial temperature at the

repository horizon (which is the initial temperature of the infinite medium in the THERMAL-ANALYTICAL worksheet approach). DSEF also uses the depth in the COST CALCULATIONS worksheet.

- Step 6 develops the repository layout. The THERMAL-ANALYTICAL worksheet uses a two-dimensional model that calculates thermal response from a central waste package, its axial neighbors, and its lateral neighbors. Thus, axial spacing and lateral spacing are the two inputs. Spacing values are center-to-center. The THERMAL-ANALYTICAL worksheet approach calculates the temperature near a central waste package with four axial (point source) neighbors on each end, and four line-source lateral neighbors on each side. For in-drift emplacement, axial spacing is between waste packages, and lateral spacing is between drifts. For horizontal borehole emplacement, axial spacing is between waste packages, and lateral spacing is between boreholes. For vertical boreholes with one waste package per borehole, the two-dimensional approximation turns each WP to be horizontal, with the axis aligned with the axis of the turned WPs in each neighboring borehole; thus, the axial spacing is the borehole spacing, and the lateral spacing is the drift spacing (the boreholes are drilled in the drift floor). For deep borehole emplacement, the axial spacing is between waste packages, and the lateral spacing is between boreholes (this only calculates one plane of the repository, but lateral spacing is wide enough that the adjacent planes can be ignored).

- Step 7 specifies the natural system material name and properties (thermal conductivity and thermal diffusivity). The user is invited to enter a case number for display of values from that reference case, directly to the left of the yellow input cells. The user may override any or all of these values in the input cells. Directly to the right of the input cells are the values DSEF will use (which are the displayed reference case values if no values are directly input). Hyperlinks to the CASE LIBRARY and the MATERIALS worksheets are provided to enable the user to view available cases and material properties, prior to making their input choices.

- Step 8 specifies the EBS material names, radial thicknesses, thermal conductivities, and thermal diffusivities. EBS layers include the waste form, canister, waste package, buffer, envelope, backfill, and liner. The drift or borehole radius is the outer radius of the liner. The inner three layers are provided for dimensional purposes only; the THERMAL-ANALYTICAL worksheet treats everything inside of the waste package outer radius to be a thermal source with a thermal flux imposed at that location. The outer four layers can be renamed to accommodate a variety of designs. If a layer thickness is zero, it is as if that layer does not exist in the THERMAL-ANALYTICAL worksheet approach. As in Step 7, the user is invited to enter a case number for display of values from that reference case, which may be a different reference case than used in the Step 7. Table 8.B in DSEF, part of which is shown in Figure 8, allows the user to keep the reference case values or override them with user input (where the yellow cells are provided for user input). Table 8.C. displays a summary of the data that will be used, and that is passed to the THERMAL-ANALYTICAL worksheet, which is the interface with the Mathcad component of DSEF. Hyperlinks to the CASE LIBRARY worksheet and the MATERIALS worksheet are provided to enable the user to view prior runs and the assembled set of reference properties, prior to making their input choices.   Finally, in Table 8.D, the user specifies a second in-rock

compliance point. The Mathcad component of DSEF will calculate temperature history (and the value and time of peak temperature) at this location in addition to the outer radius of the waste package, all of the EBS component interfaces, and the drift/borehole radius.   The Mathcad component returns the results of the transient temperature calculations to the THERMAL-ANALYTICAL OUTPUT worksheet.

- Step 9 specifies the parameters required to calculate the thermal behavior of an "open mode" repository design concept that includes pre-closure ventilation. These parameters include the ventilation duration and the subsequent unventilated duration during which backfill is emplaced, the ventilation efficiency, the rock wall emissivity, and the waste package emissivity.   As in the preceding steps, the user is provided with the reference values from the EBS reference case (from Step 8), and can make their own direct inputs or overrides. The resulting values are shown to the right of the yellow input cells. The step ends with a hyperlink to the THERMAL worksheet which manages the calculation and documentation of the thermal performance. The user should return to this point in the INPUTS worksheet afterward, to address the COST calculation, should it be desired.

- Step 10 specifies the input parameters necessary to generate an approximate cost for the design choices made above. For costing, the entire repository must be specified, rather than the central waste package and neighbors specified above for the thermal performance calculations. Figure 9 shows an example of the repository-level cost input data, where the user enters the repository capacity (MTU) and annual receipt rate (MTU/yr) as well as other variables. The user can also choose one of five example cost calculation cases from the Carter/Hardin model for comparison purposes (see Section 9 on the COST worksheets). Figure 10 shows an example of user data entry for high and low range contingency percentages.

- Step 11 allows the user to input and output constraint data. The user supplies a constraint value for minimum lateral spacing of drifts for drift structural stability that is used to cross-check the repository design concept input data.   The other constraint inputs are all related to temperature criteria for maximum waste package surface temperature, and maximum EBS and NBS material thermal constraints. The calculated results are checked against these constraint values, and the RESULTS worksheet displays a color-coded set of temperature compliance results as well as displaying quantitative margins (see Figure 11).

- Step 12 allows the user to document and check the single analysis reference case that was defined in steps 1 to 11. Step 12 sends the user to the INPUTS CHECKLIST worksheet, which allows the user to track the status of the input data entry, and provides a place to document decisions and data-selection choices, identify references used, and add notes with respect to the data entries. To perform a "one-off" parameter sensitivity study, proceed to Step 13.

- Step 13 allows the user to either select a "single" calculation mode that uses all of the input data for the reference case defined in Steps 1 through 12, or to select a "parametric" study calculation mode. Figure 12 shows the options available for parametric studies, where the basic inputs have been set, but the user can then define up to 10 data values for one of six possible parameters –

waste package spacing, drift spacing, storage time, ventilation duration, rock thermal conductivity, and backfill thermal conductivity. Caution should be taken because the single value already input will be overwritten for the thermal, but not in the cost calculation. Therefore, the user is encouraged to choose to make one of the parametric values match the "single" value input defined in Steps 1 through12 for easier comparison with the other parametric input results.

- Step 14 sends the user to the RESULTS worksheet, which displays the inputs and results in a reviewable and printable format.

Figure 9 – Example of repository level cost input data with Carter/Hardin example case data

Note: The light blue cells below are input elsewhere. The user should consider the options and consider overriding if appropriate. Consultation of the 5 cases documented in FCRD-UFD-2012-000211, Rev. 1 can be informative. The yellow cells need to be input directly. One can consult the data directly on the LISTS worksheet as shown in the data tables named "Table_Shafts_5_Case", "Table_Surface_Facility_Costs_5_Case", "Table_Assumptions_5_Case", "Table_Ramps_Drifts_5_Case", "Table_O_and_M_Unit_Cost_Assumptions_5_Case" or for any single case by selecting one of the standard cases and looking at Column D in the table immediately below.

FCRD-UFD-2012-000211, Rev 1
Case description

The cell one row down and one column to the left is where one selects "User Defined" or one of the Carter cases - simply click on it to show the menu

Repository operations related inputs	Thermal Calculation Related Inputs	ROM Cost Case 4 – Clay/Shale (open)	User Defined Over-ride Inputs			
MTU per Repository	140,000	140,	**Select Cost Case or User Defined** Select one of the 5 repository concept cost cases defined in FCRD-UFD-2012-000211, Rev 1 [Generic Repository ROM Cost Study; Joe T. Carter, Phillip O. Rodwell, and Mark Dupont (SRNL), Sept. 5, 2012], or select "User Defined" to input your own data.	140000	<-- Repository_MTU
Repository Annual Waste Throughput (MTU/yr)	3,000	3,0		3000	<-- Repository_MTU_per_year
Waste Package Capacity	21	2		21	<-- WP_capacity_for_cost
Ventilation Duration (yr)	250	25		250	<-- Ventilation_Duration
Ventilation Surface Facility Annual Costs (MM$/yr)		1		1	<-- Vent_Surface_Facility_Annual_Cost
Ventilation Operations Unit Cost per Emplacement Drift Length ($/m-yr)		50		50	<-- Vent_Operations_per_Drift_Length_Unit_Cost
Closure Duration (yr)	10	10		10	<-- Closure_Duration
Closure Facility Annual Cost (MM$/yr)		10		10	<-- Closure_Surface_Facility_Annual_Cost

Figure 10 – Example of cost contingency input data

For User-Defined Cases, the DSEF team recommends the User consult the contingencies for the 5 Carter cases. These can be seen in "Table_Contingencies_Carter_5_Case" or for any single case by selecting one of the standard cases and looking at Column D in the table immediately below. Those values can be "pasted-special" in Column C immediately below.	Case Related Description				
Contingency Factors	User Defined Inputs	ROM Cost Case 4 - Clay/Shale (open)	User Defined Over-ride Inputs		
Facility Design & Startup - Low	5%	5%		5%	<-- Contingency_Facility_Design_and_Startup_Low
Facility Design & Startup - High	53%	53%		53%	<-- Contingency_Facility_Design_and_Startup_High
Surface Facility Construction - Low	5%	5%		5%	<-- Contingency_Surface_Facility_Construction_Low
Surface Facility Construction - High	53%	53%		53%	<-- Contingency_Surface_Facility_Construction_High
Subsurface Facility Construction - Low	5%	5%		5%	<-- Contingency_Subsurface_Facility_Construction_Low
Subsurface Facility Construction - High	53%	53%		53%	<-- Contingency_Subsurface_Facility_Construction_High
Ventilation Construction & Startup - Low	5%	5%		5%	<-- Contingency_Ventilation_Construction_and_Startup_Low
Ventilation Construction & Startup - High	53%	53%		53%	<-- Contingency_Ventilation_Construction_and_Startup_High
Operations & Maintenance - Low	5%	5%		5%	<-- Contingency_Operations_and_Maintenance_Low
Operations & Maintenance - High	34%	34%		34%	<-- Contingency_Operations_and_Maintenance_High
Closure Costs - Low	10%	10%		10%	<-- Contingency_Closure_Costs_Low
Closure Costs - High	50%	70%		70%	<-- Contingency_Closure_Costs_High
Waste Packages - Low	5%	5%		5%	<-- Contingency_Waste_Packages_Low
Waste Packages - High	30%	30%		30%	<-- Contingency_Waste_Packages_High
Regulatory & Licensing - Low	5%	5%		5%	<-- Contingency_Regulatory_and_Licensing_Low
Regulatory & Licensing - High	9%	9%		9%	<-- Contingency_Regulatory_and_Licensing_High
Monitoring - Low	10%	10%		10%	<-- Contingency_Monitoring_Low
Monitoring - High	50%	50%		50%	<-- Contingency_Monitoring_High
Performance Confirmation - Low	5%	5%		5%	<-- Contingency_Performance_Confirmation_Low
Performance Confirmation - High	43%	43%		43%	<-- Contingency_Performance_Confirmation_High
Program Integration - Low	10%	10%		10%	<-- Contingency_Program_Integration_Low
Program Integration - High	50%	50%		50%	<-- Contingency_Program_Integration_High

Figure 11 – Example of comparison of thermal results against thermal constraints from the RESULTS worksheet

Number of parametric sensitivity study cases = 3							
Summary of Peak Temperatures and Times		Ventilation Duration 200, yr		Ventilation Duration 250, yr		Ventilation Duration 300, yr	
Location	Radius, m	Peak Temp, C	TooR, yr	Peak Temp, C	TooR, yr	Peak Temp, C	TooR, yr
Second Compliance Point	5.25	183.58	600.00	175.39	680.00	167.86	705.00
Peak Rock	2.25	200.19	525.00	190.62	600.00	182.25	665.00
Liner inner surface	2.23	200.20	525.00	190.63	600.00	182.26	665.00
Backfill inner surface	1.00	237.70	455.00	225.19	515.00	214.34	580.00
Envelope inner surface	1.00	237.70	455.00	225.19	515.00	214.34	580.00
WP surface	1.00	237.70	455.00	225.19	515.00	214.34	580.00
Comparison against Thermal Constraints							
Location / medium	Thermal Constraint, °C	Margin (Constraint - Peak Temp)		Margin (Constraint - Peak Temp)		Margin (Constraint - Peak Temp)	
Host rock / Clay	100	-100.2		-90.6		-82.3	
Liner	None	N/A		N/A		N/A	
Backfill	120	-117.7		-105.2		-94.3	
Envelope	None	N/A		N/A		N/A	
Buffer	None	N/A		N/A		N/A	
WP surface	300	62.3		74.8		85.7	

Figure 12 – Example of parametric study input data from Step 13 on the INPUTS worksheet

6. The INPUTS CHECKLIST Worksheet

The INPUTS CHECKLIST worksheet provides a checklist to follow the user's progress in developing an analysis case, and provides documentation for the combination of built-in options chosen versus new user-defined inputs. It also provides a convenient location to document the references and to make explanatory notes to supplement the DSEF data options chosen. Figure 13 shows an example of the checklist style documentation structure of the INPUTS CHECKLIST worksheet. The INPUTS CHECKLIST worksheet also includes a section at the bottom that echoes all of the cross-check and caution warnings that are utilized on the INPUTS worksheet.

If sufficient display monitor space is available, the user can open both the INPUTS and INPUTS CHECKLIST worksheets side-by-side. As decisions are made on the INPUTS worksheet, the cells in the INPUTS CHECKLIST worksheet are automatically populated. The two columns to the right are places the user can document references used and to place notes on the thought process or rationale for the decisions made. The INPUTS CHECKLIST worksheet is narrow enough to be printed for hard-copy retention of case definition.

Figure 13 - Example from a section of the inputs checklist

Category of input	Subcategory	Subcategory	Data from the INPUTS sheet	References for User defined inputs	Notes
Natural Barriers System - Geologic media		Media type	Clay		
		Thermal conductivity	1.75		
		Thermal diffusivity	6.45E-07		
		Transport properties			
		Constraint temp, °C	100		
Waste form properties		Mechanical properties			
		SNF type	40 GWd PWR UOX SNF Assembly		
		SNF burnup	See SNF type		
		Number of assemblies	32		
		Waste package description	Assembly waste package		
Waste form / waste package geometry		Decay heat source data			
		Waste form outer radius, m	0.89		
		Waste package outer radius, m	1.000		
		Waste package length, m	5		
		Waste package material	Carbon Steel		
		Waste package wall thickness	0.11		
Engineered Barriers System - Layer data	EBS layer 4 - closest to waste package	Layer descriptive name	Buffer		
		Layer material	None		
		Layer thermal kth	N/A		
		Layer thickness, m	0		
		Layer outer radius, m	1		
		Constraint temp, °C	None		
	EBS layer 3 - inner mid-layer	Layer descriptive name	Envelope		
		Layer material	None		
		Layer thermal kth	N/A		
		Layer thickness, m	0		
		Layer outer radius, m	1		
		Constraint temp, °C	None		
	EBS layer 2 - inner mid-layer	Layer descriptive name	Backfill		
		Layer material	70% Bentonite 30% Sand		
		Layer thermal kth	1.2		
		Layer thickness, m	1.225		
		Layer outer radius, m	2.225		
		Constraint temp, °C	120		
	EBS layer 1 - closest to host rock	Layer descriptive name	Liner		
		Layer material	Steel		
		Layer thermal kth	46		
		Layer thickness, m	0.025		

7. Reviewing Previous Analyses – the CASE LIBRARY and the THERMAL-INTERPOLATE Worksheets

DSEF provides user-friendly ways to rapidly access and compare a large number of completed thermal analysis cases through the combination of the CASE LIBRARY and the THERMAL-INTERPOLATE worksheets. The CASE LIBRARY is a flat-file database contained in a named range called the *Interp_Data_Table*. THERMAL INTERPOLATE directly predicts new results by using linear interpolation to get a first-order prediction of the effects of potential changes in a selected set of independent variables.

The database table currently has 721 records (rows) with 56 fields (columns) of data. Figure 14 shows the data fields. DSEF Version 2.1 included 300 analysis cases in the database. DSEF Version 3.0 added cases 301 to 401 from Greenberg 2013a, and cases 402 to 721 from Greenberg 2013b.

The CASE LIBRARY also includes an easy-to-use CASE CATALOG that categorizes the cases in the library and allows the user to quickly jump to a relevant record. Figure 15 through Figure 21 show the CASE CATALOG tables for enclosed mode cases, open mode cases, open mode sensitivity cases, required ventilation calculations, and dual-purpose canister calculations respectively. Each table includes a macro button to jump to the selected case in the CASE LIBRARY.

The "enclosed" mode referred to for Figure 15 means that the space between the waste package and drift or borehole wall is filled with engineered barrier components such as a buffer or backfill. In Figure 15, "Salt 200" is an abbreviation for cases with the thermal properties of salt within the EBS region being evaluated at 200°C, as opposed to the properties in the host rock which were evaluated at 100°C. For "Salt 100" cases, all properties were evaluated at 100°C.

Follow these steps to use the Case Catalog tables to examine specific case records in the library:

- Examine the Case Catalog tables to select a case of interest
- Click on the catalog case number of interest
- Click on the "*Jump to Selected Case*" macro button. This utilizes the Excel "freeze panes" feature to place the data field names at the top of the screen, with the first record being the selected case.
- Just above the field names (after the jump), there is another macro button that says "*Click Here to Go Back to the Case Library*". Clicking on that macro button will put you back at the particular case catalog table you were looking at when you selected the case to review.
- Also above the field names, there is a counter for the "Number of Filtered Rows". When looking at the Case Library the user can click on the Excel menu choice DATA – FILTER to set the auto-filter mode on. In this mode, the Case Library data can be filtered to identify specific sets of cases that meet the filter criteria. The number of filtered cases is displayed in the cell with the counter. Note that the DATA – FILTER operation will not work while the normal DSEF worksheet protection is enabled. A password must be used to first "unprotect" the worksheet before filtering. Contact LLNL if you need the password.

Figure 14 - The data fields used in the CASE LIBRARY

	Columns in Interp_Data_Table			Columns in Interp_Data_Table (continued)
1	Case Number		29	Envelope Wall kth, W/m-K
2	Case Description		30	Backfill kth, W/m-K
3	Design Mode		31	Liner kth, W/m-K
4	Date of Calc		32	Rock k_th, W/m-K
5	Reference Document		33	Rock alpha, m2/s
6	Author / Org		34	Time Out of Reactor (Storage Time, yr)
7	Geologic Medium		35	Depth of Repository Horizon, m
8	Waste Form		36	Ambient T, °C
9	WP Capacity (# SNFAs or Canisters)		37	Center to Center Axial Spacing, m
10	WP Length, m		38	Center to Center Lateral Spacing, m
11	EBS Components		39	Time of Peak T at Rock Wall, yr
12	Waste Form Outer/ Canister Inner Radius, m		40	Peak Rock Wall T, °C
13	Canister Wall Thickness m		41	% Contribution to Peak Rock Wall T from Central WP
14	WP Wall Thickness m		42	% Contribution to Peak from Axial Neighbor WPs
15	Buffer Thickness m		43	% Contribution to Peak from Lateral Neighbor WP Lines
16	Envelope Thickness m		44	Time of Peak WP T, yr
17	Backfill Thickness m		45	Peak WP T, °C
18	Liner Thickness m		46	Third T Location
19	Calculated Rock Wall Radius, m		47	Time of T at Third Location (Note 1)
20	Canister Wall Material		48	Third Location T, °C (Note 1)
21	WP Wall Material		49	Ventilation thermal efficiency %
22	Buffer Material		50	Ventilation Period (yr)
23	Envelope Material		51	Backfill Duration
24	Backfill Material		52	Time of Operation
25	Liner Material		53	Rock Wall Emissivity
26	Canister Wall kth, W/m-K		54	Waste Package Emissivity
27	WP Wall kth, W/m-K		55	Single Case or Parameter Studied
28	Buffer kth, W/m-K		56	Number of Parameter Values in Study

Figure 15 - The enclosed mode analysis case catalog

Case Number Catalog for Enclosed Mode Analysis Cases						
Disposal Scenarios			Click Here to Jump to Selected Case			
Geology	Waste Form	Assemblies / WP	10 Year Storage	50 Year Storage	100 Year Storage	200 Year Storage
Granite	4-UOX-60-SNFA	4	1	55	109	163
	4-UOX-40-SNFA	4	2	56	110	164
	1-UOX-60-SNFA	1	3	57	111	165
	1-UOX-40-SNFA	1	4	58	112	166
	4-MOX-50-SNFA	4	5	59	113	167
	1-MOX-50-SNFA	1	6	60	114	168
	Co-Extraction	1	7	61	115	169
	New Extraction Glass	1	8	62	116	170
	EC-Ceramic	1	9	63	117	171
	EC-Metal	1	10	64	118	172
Clay	4-UOX-60-SNFA	4	11	65	119	173
	4-UOX-40-SNFA	4	12	66	120	174
	1-UOX-60-SNFA	1	13	67	121	175
	1-UOX-40-SNFA	1	14	68	122	176
	4-MOX-50-SNFA	4	15	69	123	177
	1-MOX-50-SNFA	1	16	70	124	178
	Co-Extraction	1	17	71	125	179
	New Extraction Glass	1	18	72	126	180
	EC-Ceramic	1	19	73	127	181
	EC-Metal	1	20	74	128	182
Salt 100	4-UOX-60-SNFA	4	21	75	129	183
	1-UOX-60-SNFA	1	24	78	132	186
	4-MOX-50-SNFA	4	33	87	141	195
	1-MOX-50-SNFA	1	35	89	143	197
	Co-Extraction	1	40	94	148	202
	New Extraction Glass	1	41	95	149	203
	EC-Ceramic	1	42	96	150	204
	EC-Metal	1	43	97	151	205
Salt 200	1-UOX-60-SNFA	1	25	79	133	187
	1-UOX-40-SNFA	1	26	80	134	188
	2-UOX-60-SNFA	2	27	81	135	189
	2-UOX-40-SNFA	2	28	82	136	190
	3-UOX-60-SNFA	3	29	83	137	191
	3-UOX-40-SNFA	3	30	84	138	192
	4-UOX-60-SNFA	4	22	76	130	184
	4-UOX-40-SNFA	4	23	77	131	185
	12-UOX-60-SNFA	12	31	85	139	193
	12-UOX-40-SNFA	12	32	86	140	194
	1-MOX-50-SNFA	1	36	90	144	198
	2-MOX-50-SNFA	2	37	91	145	199
	3-MOX-50-SNFA	3	38	92	146	200
	4-MOX-50-SNFA	4	34	88	142	196
	12-MOX-50-SNFA	12	39	93	147	201
	Co-Extraction	1	44	98	152	206
	New Extraction Glass	1	45	99	153	207
	EC-Ceramic	1	46	100	154	208
	EC-Metal	1	47	101	155	209
Deep Borehole	1-UOX-60-SNFA	1	48	102	156	210
	1-UOX-40-SNFA	1	49	103	157	211
	1-MOX-50-SNFA	1	50	104	158	212
	Co-Extraction	0.291	51	105	159	213
	New Extraction Glass	0.291	52	106	160	214
	EC-Ceramic	0.291	53	107	161	215
	EC-Metal	0.291	54	108	162	216

Figure 16 - The open mode analysis base case catalog

Case Number Catalog for Open Mode Analysis Cases					
Catalog of Base Cases		Click Here to Jump to Selected Case			
Disposal Scenarios		50 Year Storage		100 Year Storage	
Geology	Waste Form	LLNL-TR-572252 Case #	CASE LIBRARY Case Number	LLNL-TR-572252 Case #	CASE LIBRARY Case Number
Clay	4-UOX 40	#13	217	#14	218
	4-UOX 60	#15	219	#16	220
	12-U0X 40	#17	221	#18	222
	12-UOX 60	#19	223	#20	224
	21-UOX 40	#21	225	#22	226
	21-UOX 60	#23	227	#24	228
	32-UOX 40	#25	229	#26	230
	32-UOX 60	#27	231	#28	232
Alluvium	4-UOX 40	#41	233	#42	234
	4-UOX 60	#43	235	#44	236
	12-U0X 40	#45	237	#46	238
	12-UOX 60	#47	239	#48	240
	21-UOX 40	#49	241	#50	242
	21-UOX 60	#51	243	#52	244
	32-UOX 40	#53	245	#54	246
	32-UOX 60	#55	247	#56	248

Figure 17 - The open mode sensitivity studies case catalog

Case Number Catalog for Open Mode Analysis Cases

Catalog of Open Mode Sensitivity Study Cases		Click Here to Jump to Selected Case

Media	Parameter Studied												
Clay	Ventilation Thermal Efficiency. All cases assume - 21-UOX, 40 GWd/MTHM, 50 yr Storage, 300 yr total Operation, 310 yr backfill	Ventilation Efficiency	50%	60%	70%	75%	80%	90%				
		LLNL-TR-572252 Case #	#21a	#21b	#21c	#21	#21d	#21e				
		CASE LIBRARY Case #	249	250	251	225	252	253				
Clay	Ventilation Duration. All cases assume - 21-UOX, 40 GWd/MTHM, 50 yr Storage, Ventilation Eff. 90%	Ventilation Duration	250 y, DS=30	200 y, DS=30	150 y, DS=30	100 y, DS=30	50 y, DS=30	50 y, DS=40	50 y, DS=50			
		LLNL-TR-572252 Case #	#21e	#21f	#21g	#21h	#21i	#21j	#21k			
		CASE LIBRARY Case #	253	254	255	256	257	258	259			
Clay	Drift / Borehole Spacing. All cases assume - 21-UOX or 32-UOX, 40 GWd/MTHM, 50 yr Storage, 300 yr close	Variable Value	30 m, WP=21	40 m WP=21	50 m WP=21	60 m WP=21	70 m WP=21	30 m WP=32	40 m WP=32	50 m WP=32	60 m WP=32	70 m WP=32
		LLNL-TR-572252 Case #	#21	#21w	#21x	#21y	#21z	#25	#25a	#25b	#25c	#25d
		CASE LIBRARY Case #	225	260	261	262	263	229	264	265	266	267
Generic	Host Rock Thermal Conductivity (W/m-K). All cases assume - 21-UOX, 40 and 60 GWd/MTHM, 50 yr Storage	Variable Value	kth=1 BU=40	kth=2 BU=40	kth=3 BU=40	kth=4 BU=40	kth=5 BU=40	kth=1 BU=60	kth=2 BU=60	kth=3 BU=60	kth=4 BU=60	kth=5 BU=60
		LLNL-TR-572252 Case #	#57	#58	#59	#60	#61	#62	#63	#64	#65	#66
		CASE LIBRARY Case #	277	278	279	280	281	282	283	284	285	286
Clay	Backfill Thermal Conductivity. All cases assume - 21-UOX, 40 GWd/MTHM, 50 yr Storage, 300 yr close, 10 yr backfill	Variable Value	kth=1 BU=40	kth=2 BU=40	kth=3 BU=40	kth=4 BU=40	kth=5 BU=40					
		LLNL-TR-572252 Case #	#67	#68	#69	#70	#71					
		CASE LIBRARY Case #	268	269	270	271	272					
Clay #21's Alluvium #49's	Uncertainty in Rock Properties. All cases assume - 21-UOX, 40 GWd/MTHM, 50 yr Storage, 300 yr close, 10 yr backfill	Variable Value	-2 std. dev.	-1 std. dev.	Mean	+1 std. dev.	+2 std. dev.	-2 std. dev.	-1 std. dev.	Mean	+1 std. dev.	+2 std. dev.
		LLNL-TR-572252 Case #	21m	21r	21	21s	21n	49a	49c	49	49d	49b
		CASE LIBRARY Case #	273	287	225	288	274	275	289	241	290	276
Clay	Design Test Cases. All cases assume - 21-UOX, 40 GWd/MTHM, cases 72-74, 50 yr storage, cases 75-77, 100 yr storage	Variable Value	No backfill	backfill kth=2	backfill kth=1.2	backfill kth=0.6	rDW = 5.25 m	No backfill	backfill kth=2	backfill kth=1.2	backfill kth=0.6	rDW = 5.25 m
		LLNL-TR-572252 Case #	72	73	73b	73a	74	75	76	76b	76a	77
		CASE LIBRARY Case #	291	292	293	294	295	296	297	298	299	300

Case Number Catalog for Repository Layout and Required Ventilation Trade Studies in Clay / Shale

			12-PWR waste package DSEF cases 221 (t-store 50) and 222 (t-store 100)		21-PWR waste package DSEF cases 225 (t-store 50) and 226 (t-store 100)						32-PWR waste package DSEF cases 229 (t-store 50) and 230 (t-store 100)					
			WP Spacing, m		Waste Package Spacing, m						Waste Package Spacing, m					
			10		10		15		20		10		15		20	
TC	Dr Sp, m	t-store, yr	LLNL-TR-638880 Case #	CASE LIBRARY Case #	LLNL-TR-638880 Case #	CASE LIBRARY Case #	LLNL-TR-638880 Case #	CASE LIBRARY Case #	LLNL-TR-638880 Case #	CASE LIBRARY Case #	LLNL-TR-638880 Case #	CASE LIBRARY Case #	LLNL-TR-638880 Case #	CASE LIBRARY Case #	LLNL-TR-638880 Case #	CASE LIBRARY Case #
100	30	50	221-1	301	225-1	315	225-10	333	225-19	342	229-1	351	229-10	369	229-19	378
100	30	100	222-1	302	226-1	316					230-1	352				
100	45	50	221-2	303	225-2	317	225-11	334	225-20	343	229-2	353	229-11	370	229-20	379
100	45	100	222-2	304	226-2	318					230-2	354				
100	60	50	221-3	305	225-3	319	225-12	335	225-21	344	229-3	355	229-12	371	229-21	380
100	60	100	222-3	306	226-3	320					230-3	356				
120	30	50	221-4	307	225-4	321	225-13	336	225-22	345	229-4	357	229-13	372	229-22	381
120	30	100	222-4	308	226-4	322					230-4	358				
120	45	50	221-5	309	225-5	323	225-14	337	225-23	346	229-5	359	229-14	373	229-23	382
120	45	100	222-5	310	226-5	324					230-5	360				
120	60	50	221-6	311	225-6	325	225-15	338	225-24	347	229-6	361	229-15	374	229-24	383
120	60	100	222-6	312	226-6	326					230-6	362				
140	30	50	221-7	313	225-7	327	225-16	339	225-25	348	229-7	363	229-16	375	229-25	384
140	30	100	222-7	314	226-7	328					230-7	364				
140	45	50			225-8	329	225-17	340	225-26	349	229-8	365	229-17	376	229-26	385
140	45	100			226-8	330					230-8	366				
140	60	50			225-9	331	225-18	341	225-27	350	229-9	367	229-18	377	229-27	386
140	60	100			226-9	332					230-9	368				

Catalog of Open Mode Sensitivity Study Cases

Click Here to Jump to Selected Case

LLNL-TR-638880 - Required Ventilation Time Trade Study in clay/shale, as a function of Temperature Criteria (TC), Drift spacing, Storage time, and Waste package spacing. Cases analyzed for 2013 IHLRWM conference paper LLNL-CONF-614294

Figure 19 - Case number catalog for repository layout and required ventilation trade studies in clay/shale (2 of 2)

Case Number Catalog for Repository Layout and Required Ventilation Trade Studies in Clay / Shale							
Catalog of Open Mode Sensitivity Study Cases		Click Here to Jump to Selected Case					
LLNL-TR-638880 - Required Ventilation Time Trade Study in clay/shale, as a function of Temperature Criteria (TC), Drift spacing, Storage time, and Waste package spacing Additional base cases to extend WP spacing to 30 m and Drift spacing to 90 m		32-PWR waste package, 40 GWd/MT burnup DSEF base case 229					
		Waste Package Spacing					
		10		20		30	
TC	Dr Sp	LLNL-TR-638880 Case #	CASE LIBRARY Case #	LLNL-TR-638880 Case #	CASE LIBRARY Case #	LLNL-TR-638880 Case #	CASE LIBRARY Case #
100	30	229-1	351	229-19	378	229-67	393
100	60	229-3	355	229-21	380	229-64	394
100	90	229-37	387	229-49	390	229-61	395
120	30	229-4	357	229-22	381	229-68	396
120	60	229-6	361	229-24	383	229-65	397
120	90	229-38	388	229-50	391	229-62	398
140	30	229-7	363	229-25	384	229-69	399
140	60	229-9	367	229-27	386	229-66	400
140	90	229-39	389	229-51	392	229-63	401

(Clay/shale row label spans the left of the data rows)

Figure 20 - Case number catalog for scoping thermal analysis of alternative DPC disposal concepts in clay/shale (subset 1)

Case Number Catalog for Scoping Thermal Analysis of Alternative DPC Disposal Concepts in Clay / Shale (subset 1)									
Catalog of Open Mode Sensitivity Study Cases		Click Here to Jump to Selected Case							
Case # Definition Table (Each parametric study case in LLNL-TR-639869 includes ten DSEF transient calculations)		LLNL-TR-639869 - Repository Layout and Thermal Gradient Trade Study for Large Waste Packages in Clay-Shale 32-PWR WP, 40 GWd/MT, Storage time = 50 years, Drift spacing = 70 m DSEF base case 229							
		Ventilation Duration (yr)							
		100		75		50		25	
Waste Package Spacing (m)	CP2* (m)	LLNL-TR-639869 Case #	CASE LIBRARY Case #	LLNL-TR-639869 Case #	CASE LIBRARY Case #	LLNL-TR-639869 Case #	CASE LIBRARY Case #	LLNL-TR-639869 Case #	CASE LIBRARY Case #
15	1	500-1	402	500-6	452	500-11	502	500-16	552
	2	500-2	403	500-7	453	500-12	503	500-17	553
	3	500-3	404	500-8	454	500-13	504	500-18	554
	4	500-4	405	500-9	455	500-14	505	500-19	555
	5	500-5	406	500-10	456	500-15	506	500-20	556
16	1	500-1	407	500-6	457	500-11	507	500-16	557
	2	500-2	408	500-7	458	500-12	508	500-17	558
	3	500-3	409	500-8	459	500-13	509	500-18	559
	4	500-4	410	500-9	460	500-14	510	500-19	560
	5	500-5	411	500-10	461	500-15	511	500-20	561
17	1	500-1	412	500-6	462	500-11	512	500-16	562
	2	500-2	413	500-7	463	500-12	513	500-17	563
	3	500-3	414	500-8	464	500-13	514	500-18	564
	4	500-4	415	500-9	465	500-14	515	500-19	565
	5	500-5	416	500-10	466	500-15	516	500-20	566
18	1	500-1	417	500-6	467	500-11	517	500-16	567
	2	500-2	418	500-7	468	500-12	518	500-17	568
	3	500-3	419	500-8	469	500-13	519	500-18	569
	4	500-4	420	500-9	470	500-14	520	500-19	570
	5	500-5	421	500-10	471	500-15	521	500-20	571
19	1	500-1	422	500-6	472	500-11	522	500-16	572
	2	500-2	423	500-7	473	500-12	523	500-17	573
	3	500-3	424	500-8	474	500-13	524	500-18	574
	4	500-4	425	500-9	475	500-14	525	500-19	575
	5	500-5	426	500-10	476	500-15	526	500-20	576
20	1	500-1	427	500-6	477	500-11	527	500-16	577
	2	500-2	428	500-7	478	500-12	528	500-17	578
	3	500-3	429	500-8	479	500-13	529	500-18	579
	4	500-4	430	500-9	480	500-14	530	500-19	580
	5	500-5	431	500-10	481	500-15	531	500-20	581
21	1	500-1	432	500-6	482	500-11	532	500-16	582
	2	500-2	433	500-7	483	500-12	533	500-17	583
	3	500-3	434	500-8	484	500-13	534	500-18	584
	4	500-4	435	500-9	485	500-14	535	500-19	585
	5	500-5	436	500-10	486	500-15	536	500-20	586
22	1	500-1	437	500-6	487	500-11	537	500-16	587
	2	500-2	438	500-7	488	500-12	538	500-17	588
	3	500-3	439	500-8	489	500-13	539	500-18	589
	4	500-4	440	500-9	490	500-14	540	500-19	590
	5	500-5	441	500-10	491	500-15	541	500-20	591
23	1	500-1	442	500-6	492	500-11	542	500-16	592
	2	500-2	443	500-7	493	500-12	543	500-17	593
	3	500-3	444	500-8	494	500-13	544	500-18	594
	4	500-4	445	500-9	495	500-14	545	500-19	595
	5	500-5	446	500-10	496	500-15	546	500-20	596
24	1	500-1	447	500-6	497	500-11	547	500-16	597
	2	500-2	448	500-7	498	500-12	548	500-17	598
	3	500-3	449	500-8	499	500-13	549	500-18	599
	4	500-4	450	500-9	500	500-14	550	500-19	600
	5	500-5	451	500-10	501	500-15	551	500-20	601

Figure 21 - Case number catalog for scoping thermal analysis of alternative DPC disposal concepts in clay/shale (subset 2)

Case Number Catalog for Scoping Thermal Analysis of Alternative DPC Disposal Concepts in Clay / Shale (subset 2)

Catalog of Open Mode Sensitivity Study Cases

Click Here to Jump to Selected Case

Case # Definition Table (Each parametric study case in LLNL-TR-639869 includes ten DSEF transient calculations)

LLNL-TR-639869 - Repository Layout and Thermal Gradient Trade Study for Large Waste Packages in Clay-Shale
32-PWR WP, 60 GWd/MT, Storage time = 50 years, Drift spacing = 70 m or 90 m, Ventilation = 150 years
DSEF base case 231

| WP Spacing (m) | CP2 (m) | WP spacing ranges from 16 to 34 m | | | | WP spacing ranges from 32 to 50 m | | | |
| | | Drift spacing = 90 m | | Drift spacing = 70 m | | Drift spacing = 90 m | | Drift spacing = 70 m | |
		LLNL-TR-639869 Case #	CASE LIBRARY Case #	LLNL-TR-639869 Case #	CASE LIBRARY Case #	LLNL-TR-639869 Case #	CASE LIBRARY Case #	LLNL-TR-639869 Case #	CASE LIBRARY Case #
16	1	500-21	602	500-26	652				
	2	500-22	603						
	3	500-23	604						
	4	500-24	605						
	5	500-25	606						
18	1	500-21	607	500-26	653				
	2	500-22	608						
	3	500-23	609						
	4	500-24	610						
	5	500-25	611						
20	1	500-21	612	500-26	654				
	2	500-22	613						
	3	500-23	614						
	4	500-24	615						
	5	500-25	616						
22	1	500-21	617	500-26	655				
	2	500-22	618						
	3	500-23	619						
	4	500-24	620						
	5	500-25	621						
24	1	500-21	622	500-26	656				
	2	500-22	623						
	3	500-23	624						
	4	500-24	625						
	5	500-25	626						
26	1	500-21	627	500-26	657				
	2	500-22	628						
	3	500-23	629						
	4	500-24	630						
	5	500-25	631						
28	1	500-21	632	500-26	658				
	2	500-22	633						
	3	500-23	634						
	4	500-24	635						
	5	500-25	636						
30	1	500-21	637	500-26	659				
	2	500-22	638						
	3	500-23	639						
	4	500-24	640						
	5	500-25	641						
32	1	500-21	642	500-26	660	500-32	662	500-27	672
	2	500-22	643					500-28	673
	3	500-23	644					500-29	674
	4	500-24	645					500-30	675
	5	500-25	646					500-31	676
34	1	500-21	647	500-26	661	500-32	663	500-27	677
	2	500-22	648					500-28	678
	3	500-23	649					500-29	679
	4	500-24	650					500-30	680
	5	500-25	651					500-31	681
36	1					500-32	664	500-27	682
	2							500-28	683
	3							500-29	684
	4							500-30	685
	5							500-31	686
38	1					500-32	665	500-27	687
	2							500-28	688
	3							500-29	689
	4							500-30	690
	5							500-31	691
40	1					500-32	666	500-27	692
	2							500-28	693
	3							500-29	694
	4							500-30	695
	5							500-31	696
42	1					500-32	667	500-27	697
	2							500-28	698
	3							500-29	699
	4							500-30	700
	5							500-31	701
44	1					500-32	668	500-27	702
	2							500-28	703
	3							500-29	704
	4							500-30	705
	5							500-31	706
46	1					500-32	669	500-27	707
	2							500-28	708
	3							500-29	709
	4							500-30	710
	5							500-31	711
48	1					500-32	670	500-27	712
	2							500-28	713
	3							500-29	714
	4							500-30	715
	5							500-31	716
50	1					500-32	671	500-27	717
	2							500-28	718
	3							500-29	719
	4							500-30	720
	5							500-31	721

Once the user finds a case of interest that may be used as a starting point for a new variation or analysis, the INPUTS worksheet can automatically populate some of the key data inputs from the selected case, so that the user can either accept it as is, or input their own values. This is discussed in Section 5.

The THERMAL-INTERPOLATE worksheet includes two tools that can be used to develop a new analysis case from the ensemble of existing runs. The first tool allows the user to compare and contrast combinations of cases and data fields from a set of comparison cases, using the worksheet template shown in Figure 22. Following the color conventions introduced in Section 4, the yellow highlighted cells along the left column and in the top row of Figure 22 allow the user to enter case numbers on the left, and selected data fields (from Figure 14) on the top row.

Once the case numbers and selected data fields have been reviewed in the first tool, the user can select two appropriate case numbers for the interpolation. For example, in Figure 23, the Case 225 and 260 rows show results for open mode drift spacing (i.e., lateral spacing) of 30 m and 40 m. The user is responsible to select cases in which other potential independent variables are identical or at least very similar. In these two cases, the geologic medium, the waste package capacity, the burnup, the waste package spacing (i.e., axial spacing), the surface storage time, and the ventilation duration are identical, as shown in the case description. The user can verify these parameters by inputting their parameter numbers (from the list in Figure 14) on the top row of Figure 22 (the first tool). Other parameters should also be checked using Figure 23 (including thermal conductivities, thermal diffusivities, and EBS dimensions).

Once the two cases are chosen, the user proceeds to the second tool on the THERMAL-INTERPOLATE worksheet, which requires two case numbers, an independent variable, and a dependent variable. Based on the discussion above, lateral spacing could be the independent variable for interpolating between cases 225 and 260. Consider the case where the waste package peak temperature is the dependent variable, with a desired value of 150°C, as an example of using the tool. Figure 23, panel (a), displays that example, with a linearly-predicted peak waste package temperature of 154.72°C at a lateral spacing of 35 m, obtained from the peak temperatures previously calculated for lateral spacing of 30 and 40 m. The user can simply iterate on the lateral spacing until the interpolated result is as close as desired to the target value. It should be noted that the tool also will extrapolate, but the user should be wary of extrapolating a significant distance.

Figure 23, panel (b), shows the error message if the user inadvertently specifies the same point for each end of the interpolation. Figure 23, panel (c), shows an example of one of the drop-down lists and some of the choices for independent variables.

Figure 22 - Side-by-side case comparison table

Side by side Case Comparison Section - see the CASE LIBRARY for additional description of the categories of cases in the library

Column # -->	2	40	39	45	44	21	38	37	50	
Case Number	Case Description	Peak Rock Wall T, °C	Time of Peak T at Rock Wall, yr	Peak WP T, °C	Time of Peak WP T, yr	WP Wall Material	Center to Center Lateral Spacing, m	Center to Center Axial Spacing, m	Ventilation Period [yr]	
225	Open Mode Case 21 , Clay 21-UOX-40, Storage time=50 y, WP spacing=10 m, Drift/borehole spacing=30 m, Base case for sensitivity studies in clay, WP=21, 40 GWd/MT UOX TS=50	134.592	593	164.099	488	Carbon Steel	30	10	250	
260	Open Mode Case 21w, Clay 21-UOX-40, Storage time=50 y, WP spacing=10 m, Drift/borehole spacing=40 m, Sensitivity to Drift Spacing = 40 m	116.053	641	145.345	470	Carbon Steel	40	10	250	
55	Granite 4-UOX-60, Storage time=50 y, WP spacing=10 m, Drift/borehole spacing=20 m	100.7	87	141.2	65	Steel	20	10	NA	

Figure 23 - The template for variable interpolation between relevant cases

(a) – Good selection with no error messages.

Independent variable (Select column name)				Dependent variable (Select column name)			
Lateral Spacing, m ▼				Peak Waste Package T, °C ▼			
Interpolation Table Column #	38			Interpolation Table Column #	45		

WARNING!!! CHOOSE CASES IN WHICH ALL OTHER INDEPENDENT VARIABLES ARE ROUGHLY EQUAL.	Case Number	Independent Variable		Dependent Variable	
	225	X_1	30	Y_1	164.099
	OK	X	35	Y	154.722
	260	X_2	40	Y_2	145.345

(b) – An example of an error message that helps guide the user

Independent variable (Select column name)				Dependent variable (Select column name)			
Lateral Spacing, m ▼				Peak Waste Package T, °C ▼			
Interpolation Table Column #	38			Interpolation Table Column #	45		

WARNING!!! CHOOSE CASES IN WHICH ALL OTHER INDEPENDENT VARIABLES ARE ROUGHLY EQUAL.	Case Number	Independent Variable		Dependent Variable		
	225	X_1	30	Y_1	164.099	**Select Cases with Different Independent Variable Values**
	Reselect	X	35	Y	#DIV/0!	
	225	X_2	30	Y_2	164.099	

(c) – An example of what the drop down lists contain (they scroll to other selections besides the ones shown here)

Independent variable (Select column name)				Dependent variable (Select column name)			
Lateral Spacing, m ▼				Peak Waste Package T, °C ▼			
Interpolation T	Lateral Spacing, m			Interpolation Table Column #	45		
	Peak Rock Wall T, °C						
	Peak Waste Package T, °C						
	T at Third Location, °C						
	Ventillation thermal efficiency %			Independent Variable		Dependent Variable	
	Ventilation Period (yr)						
CHOOSE	Backfill Duration		5	X_1	30	Y_1	164.099
OTHER INDEPENDENT VARIABLES	Time of Operation	OK		X	35	Y	154.722
ARE ROUGHLY EQUAL.			260	X_2	40	Y_2	145.345

8. Getting a Quick Overview of the Latest Analysis – the RESULTS and the THERMAL-ANALYTICAL OUTPUT Worksheets

The RESULTS worksheet contains a concise summary of the input data from both the INPUTS worksheet; the THERMAL-SOURCE worksheets (providing both tabular and graphical summaries of the decay heat data; and results of the COST CALCULATIONS worksheet used in the current analysis case. The output data also includes results from the THERMAL-ANALYTICAL OUTPUT worksheet, including the plots shown later in Section 11 (Figure 36 and Figure 37).

Section 1 of the RESULTS worksheet summarizes the input data as follows:

- 1.A. Case Name and User Information.
- 1.B. Waste Characteristics and Waste Package Capacity.
- 1.C. Repository Design - including layout and ventilation system data.
- 1.D. Host Rock – including geometry, properties, and temperature.
- 1.E. EBS Components – including geometry, material names, and material properties.
- 1.F. Decay Heat – including both tabular and graphical representations.

Section 2 of the RESULTS worksheet summarizes the analysis results as follows:

- 2.A. Peak and Transient Temperature Results – these include peak temperatures and the times of the peaks for the host rock wall, the various EBS component interface locations, and the waste package surface. Figure 11 shows an example of the peak temperature results summary and the results compared to the thermal constraints. When a parametric study is performed in DSEF (as described in Step 12 on the INPUTS sheet), and shown in Figure 12, the full set of peak temperature values and times of the peaks for the parametric study are shown on the RESULTS worksheet, but the graphical results are only shown for the first case of the parametric study, or the single analysis case if no parametric study is performed. The RESULTS worksheet provides a hyperlink to the THERMAL-ANALYTICAL OUTPUT worksheet to allow the user to examine the full set of transient tabular and graphical results when a parametric study is analyzed.
- 2.B. Potential New Case Library Data Entry – this section provides a hyperlink to the CASE LIBRARY, just below the Case Catalog where the current analysis results are displayed in the form of a Case Library record.
- 2.C. Cost Results – this section shows the overall summary of raw, low contingency, and high contingency cost data from the COST CALCULATIONS worksheet (see Figure 28 from Section 9 of this user manual), as well as a short summary of the emplacement drift length calculation based on the thermal analysis model, that is used in the cost calculations.

Note that when the Mathcad component of DSEF returns a table of peak temperatures and times, and one or more sets of transient temperatures (one set for each parametric sensitivity study case) to the THERMAL-ANALYTICAL OUTPUT worksheet, the Excel formatting is lost. There is a macro button on the top of the worksheet which needs to be pressed once to restore the formatting, which makes the results easier to read. There is another macro button which is used to clear all of the transient results in the event the user wishes to use the same Excel file with a few modifications to evaluate another case.

There is a similar macro button to clear previous transient results provided on the INPUTS worksheet in Step 2.G.

9. The COST Worksheets

As part of the assessment of design concept feasibility, DSEF includes the capability to evaluate the costs of constructing and operating a repository concept that uses the design values from the DSEF INPUTS worksheet. In DSEF Version 2.1, the cost calculations were limited to mining and backfill costs of the repository subsurface only. Version 3.0 extends the cost model to include the total system cost.

Rough order-of-magnitude (ROM) cost data were developed in Carter 2012, and presented in Hardin 2012b, and referred to here as the Carter/Hardin cost model. DSEF Version 3.0 has been revised to address all of the cost categories covered in the Carter/Hardin model. The cost categories have been slightly regrouped to take advantage of repository design details available in DSEF, but are generally comparable to the Carter/Hardin results.

Specifically, the Carter/Hardin model includes two high-level cost categories of "Facility Design, Construction, and Startup", and "Operations & Maintenance". The DSEF calculations use five cost categories whose total is comparable to the total of the two Carter/Hardin categories; the DSEF categories are "Facility Design and Startup", "Surface Facility Construction", "Subsurface Facility Construction", "Ventilation", and "Operations and Maintenance". It should be noted that DSEF construction categories include all such construction, while Carter/Hardin include the first phase of construction in their first category, and subsequent modular construction as part of O&M. Also, DSEF includes both construction and O&M for ventilation in the "Ventilation" category. The remaining Carter/Hardin categories are directly comparable to DSEF categories. These are "Closure", "Waste Package costs", "Regulatory & Licensing", "Monitoring", "Performance Confirmation", and "Program Integration".

The DSEF approach was to match the Carter/Hardin costs for their five base cases, for the sum of the first two Carter/Hardin cost categories, for each of the other six Carter/Hardin cost categories, and for the overall total. This was accomplished by calculating costs as the product of a unit cost times the number of units (meters of excavation, number of waste packages, years of operation, etc.), or as the sum of several of these products. The unit costs were specified to produce agreement with the Carter/Hardin costs and to maintain as much consistency and logic as possible across the five disparate base cases.

The DSEF INPUTS worksheet now includes over 80 new input categories to address these calculations, and includes a set of five example cases that were analyzed in by Hardin and Carter using a drop-down menu to select the example case, and then providing the sample case data for each input so that it can either be used or over-ridden by providing user input for the current analysis case.

Note that the DSEF geologic material selection of "granite" corresponds to the crystalline rock type, and the geologic material selection of "alluvium" corresponds to the sedimentary rock type in the cost cases below.

The five example cost cases are defined in the Carter/Hardin model as follows:

1. Crystalline (enclosed) - Vertical borehole emplacement is used with a copper waste package (e.g., Swedish KBS-3 concept) with a clay buffer installed at emplacement. Access drifts are backfilled with low-permeability clay-based backfill at closure (Hardin 2012b, Section 1.4.5.1).

2. Generic Salt Repository (enclosed) – A repository in bedded salt in which carbon steel waste packages are placed on the floor in drifts or alcoves, and immediately covered (backfilled) with run-of-mine salt (Hardin 2012b, Section 1.4.5.2).

3. Clay/Shale (enclosed) – SNF or HLW is emplaced in blind, steel-lined horizontal borings constructed from access drifts. SNF is emplaced in carbon steel packages with a clay buffer. HLW glass is emplaced in stainless steel pour canisters, within a steel liner (Hardin 2012b, Section 1.4.5.3).

4. Shale Unbackfilled (open) – A repository in a thick shale formation constructed so that ventilation is maintained for at least 50 to 100 years after waste emplacement. Emplacement drifts are not backfilled at closure, but all other openings are backfilled to provide waste isolation (Hardin 2012b, Section 1.5.1).

5. Sedimentary Backfilled (open) – Constructed in sedimentary rock so that ventilation is maintained for at least 50 to 100 years after waste emplacement. All waste emplacement and other openings are backfilled with low-permeability clay-based backfill prior to repository closure (Hardin 2012b, Section 1.5.2).

The specific data for these cases is captured in a set of Excel lookup tables on the DSEF LISTS worksheet, and then used as described above on the INPUTS worksheet. DSEF provides a hyperlink to the relevant section of the LISTS worksheet that allows the user to examine the cost data summary tables if desired. The user can also see all the inputs for a single Carter/Hardin base case by simply selecting it. Then, the user can copy the values desired for a user design case, row by row, as appropriate, and then change to User-Defined in the case selection menu. The unit cost data were extracted from both Carter 2012 and Hardin 2012b, or were back calculated to match the Carter results in each category listed above. A number of the key reference tables from Hardin 2012b are included on the COST REFERENCES worksheet.

Error! Reference source not found.Error! Reference source not found. Figure 24, Figure 25, and Figure 26summarize the five example cases from the Carter/Hardin model, and Figure 27 is an example of the detailed cost data for one of the examples (where the details for all of them are shown on the COST REFERENCES worksheet).

Figure 24 - Summary of waste package numbers for the 5 example cost cases

(From Hardin 2012b Tables 2.1-1 and 4-1)

Table 2.1-1 -Numbers of Different Size Waste Packages for a 140,000 MT SNF Repository

	4-PWR/9-BWR	12-PWR/24-BWR	21-PWR/44-BWR
PWR	52,250	17,417	9,952
BWR	30,333	11,375	6,205
Total	82,583	28,792	16,157

Table 4-1 - Summary of Waste Package Numbers for 5 Disposal Concepts

	Package Capacity (PWR/BWR)	**140,000 MT Repository**		**Disposal Overpack**
		Total Waste Packages	**Annual Waste Packages**	**Material**
Crystalline (enclosed)	4/9	82,583	1,757	Copper
Generic Salt Repository (enclosed)	12/24	28,792	616	Carbon Steel
Clay/Shale (enclosed)	4/9	82,583	1,757	Carbon Steel
Shale Unbackfilled (open)	21/44	16,157	344	Carbon Steel
Sedimentary Backfilled (open)	21/44	16,157	344	Carbon Steel

Figure 25 - Summary of mined opening length and volume for the 5 example cost cases

(From Hardin 2012b Table 4-2)

Table 4-2 - Summary of Mined Opening Length and Volume for 5 Disposal Concepts

	Access Drift		Disposal Drifts/ Borings		Service Drift		Repository Total	
	Length (m)	Volume (m³)	Length (m)	Volume (m³)	Length (m)	Volume (m³)	Length (m)	Volume (m³)
Crystalline (enclosed)	8.3E5	2.7E7	8.3E5	1.8E6	2.3E5	7.7E6	1.9E6	3.7E7
Generic Salt Repository (enclosed)	3.1E5	1.7E7	3.5E5	4.4E6	1.3E5	7.2E6	7.9E5	2.9E7
Clay/Shale (enclosed)	3.9E5	9.2E6	8.3E5	4.6E6	3.7E5	8.7E6	1.6E6	2.3E7
Shale Unbackfilled (open)	7.7E4	2.2E6	1.4E5	2.3E6	9.3E4	2.2E6	3.1E5	6.7E6
Sedimentary Backfilled (open)	8.5E4	2.0E6	2.2E5	3.5E6	5.8E4	1.4E6	3.6E5	6.9E6

Figure 26 - Summary of shaft and ramp quantities for the 5 example cost cases

(From Hardin 2012b Table 4-3)

Table 4-3 - Summary of Shaft and Ramp Quantities for a 140,000 MT SNF Repository

	Air Intake	Rock Waste	Ventilation Exhaust	Waste Emplacement	
				Shafts	Ramps
Crystalline (enclosed)	1	1	2	1	0
Generic Salt Repository (enclosed)	1	1	2	1	0
Clay/Shale (enclosed)	1	1	2	0	1
Shale Unbackfilled (open)	8	1	4	0	1
Sedimentary Backfilled (open)	10	1	5	0	1

Figure 27 – Cost example case 1 - crystalline (enclosed) repository drift panel detail summary

(From Hardin 2012b Table 4.1-1 and 4.1-2)

Table 4.1-1 - Crystalline (enclosed) Repository Drift Panel Detail Summary

Drift/Boring Function	Diameter (m)	Length (m)	Number (per panel)	Total Length (m)	Spacing (m)	Closure
Waste Emplacement	1.66	10	1,200	12,000	10	Bentonite clay backfilled at emplacement and shield plug installed
Access Drifts	6.5	1000	12	12,000	20	Backfilled with 30% bentonite clay and 70% crushed rock
Service Drifts	5.5	326 1100	4 2	3,352	N/A	Backfilled with 30% bentonite clay and 70% crushed rock
Panel Total				27,352		

Table 4.1-2 - Crystalline (enclosed) Concept Repository Waste Emplacement Details

Emplacement Mode	PWR/BWR Package Size	Waste Package Spacing (m)	Waste Packages per Emplacement Drift	Waste Packages Per Panel	Waste Package Description
Vertical Borehole	4/9	10	100 WP per 1,000 m segment	1200	Stainless steel SNF canister with 5 cm thick copper overpack

As shown on the NAVIGATION worksheet in Figure 4, there are two cost-related worksheets

- COST CALCULATIONS
- COST REFERENCES

The COST CALCULATIONS worksheet (below the summary information described in the next two paragraphs) follows the Carter/Hardin model cost categories with the changes described above. Depending on the availability of source data, the calculations can be done at three increasing levels of detail. In some cases, there are detailed data on unit costs, and a specific measure of the number of units is available, such as cost per unit volume to excavate emplacement drifts, and emplacement drift lengths. In this case, the calculation could start at level 3 (the most detailed) and build up the costs of subsurface construction to be added together at level 2 or level 1. In other cases, the detailed information may not be available, so the user can put data in at level 2 for several cost components to be summed up at level 1. If there isn't enough detail to break the calculation down further, such as for regulatory & licensing, then the user may enter the data at level 1. As on the INPUTS worksheet, data transferred from other worksheets or data areas in DSEF is shown in light blue, and cells that allow the user to override or directly input data are highlighted in yellow. It is recommended that the user do the overrides in the INPUTS worksheet. Overrides in the COST CALCULATIONS worksheet persist even if the user makes changes in INPUTS, so the user should scan the COST CALCULATIONS override columns to avoid inadvertent overrides for subsequent cases.

The top-left section of the COST CALCULATION worksheet summarizes the raw costs in each category as well as the low and high contingency values. Figure 28 shows an example of the top-left section. The low contingency values are copied from the three-level detailed table below it (as described in the preceding paragraph), and the raw and high contingency values are calculated in the summary table, using the contingencies selected in the INPUTS worksheet. As detailed in the Carter/Hardin model documentation, the values applied for low and high contingency adjustment vary by the cost calculation category. The lookup tables in the LISTS worksheet (which supply contingency values to the INPUTS sheet for the five Carter/Hardin examples) assume the low contingency value is 5% in most cases (except where it is given explicitly by Carter). These lookup tables also include high contingency values that were derived from the summary low and high contingency cost results in Carter/Hardin. This approach yielded good agreement with the five example cases, as shown below. Since the DSEF modeling was based on matching the low contingency values, the raw cost values were obtained by dividing the low contingency calculated values by 1 plus the low contingency, and the high contingency values were then calculated by multiplying the raw cost values by 1 plus the high contingency.. A table showing the general rules for applying contingency factors that were used in the Carter/Hardin model is included in the COST REFERENCES worksheet. The user can override the recommended contingency values in INPUTS.

Figure 28 – Cost summary table example as shown on the RESULTS worksheet

Cost in MM$	Current Case		
	Case evaluation below is ROM cost study case: ROM Cost Case 4 - Clay/Shale (open)		
Cost Category	Raw	Low Contingency	High Contingency
Facility Design & Startup	$705	$740	$1,080
Surface Facility Construction	$1,303	$1,368	$1,997
Subsurface Facility Construction	$1,744	$1,831	$2,674
Ventilation	$1,938	$2,035	$2,971
O&M (not including ventilation)	$6,714	$7,050	$9,024
Upper Half Subtotal	**$12,404**	**$13,024**	**$17,746**
Closure	$1,296	$1,425	$2,203
Waste Package costs	$2,616	$2,747	$3,406
Regulatory & Licensing	$397	$417	$434
Monitoring	$3,019	$3,320	$4,528
Performance Confirmation	$400	$420	$571
Program Integration	$3,393	$3,732	$5,089
Lower Half Subtotal	**$11,120**	**$12,061**	**$16,230**
Total	**$23,524**	**$25,085**	**$33,977**

The five Carter/Hardin cost cases (that had detailed costing in unreleased documentation) were used to construct the DSEF cost model, using cost results summarized by Carter and Hardin at the category level. That comparison is documented on the top-right section of the COST CALCULATIONS worksheet, where the DSEF calculated numbers are compared to the "Low and High Contingency" numbers from Carter/Hardin. The comparisons are shown in Figure 29 through Figure 33, and are generally within 5% of the total costs. In a number of cases, the DSEF modeling was based on estimating some scaling factors, such as scaling backfill costs for emplacement drifts per unit volume or length while accounting for a volume reduction fraction due to drift inverts. The Carter/Hardin unit costs were shifted slightly to allow for this kind of user input, while still calculating a reasonable total backfill cost.

Figure 29 – Cost summary table comparing Carter/Hardin Case 1 (Crystalline Enclosed) results with DSEF results

Costs in MM$	DSEF	Carter	DSEF/ Carter	DSEF	Carter	DSEF/ Carter
Cost Category	Low	Low	Low %	High	High	High %
Facility DC&S		$3,754			$5,495	
Facility D&S	$1,026			$1,498		
Surface	$1,368			$1,997		
Subsurface	$12,484			$18,227		
Ventilation	$0			$0		
O&M (incl some constr)		$17,545			$22,475	
O&M (n/i ventilation)	$7,050			$9,024		
Upper Half Subtotal	$21,928	$21,299	103%	$30,746	$27,970	110%
Closure	$9,698	$9,563	101%	$13,224	$13,704	96%
WPs	$16,682	$17,489	95%	$20,685	$21,647	96%
Regulatory & Licensing	$424	$424	100%	$441	$441	100%
Monitoring	$10,436	$10,685	98%	$14,231	$14,571	98%
PC	$420	$411	102%	$571	$561	102%
Integration	$1,575	$1,575	100%	$2,148	$2,142	100%
Lower Half Subtotal	$39,235	$40,147	98%	$51,300	$53,066	97%
Total	$61,163	$61,446	100%	$82,046	$81,036	101%

Figure 30 – Cost summary table comparing Carter/Hardin Case 2 (Salt Enclosed) results with DSEF results

Costs in MM$	DSEF	Carter	DSEF/ Carter	DSEF	Carter	DSEF/ Carter
Cost Category	Low	Low	Low %	High	High	High %
Facility DC&S		$3,896			$5,595	
Facility D&S	$1,015			$1,482		
Surface	$1,368			$1,997		
Subsurface	$2,893			$4,224		
Ventilation	$0			$0		
O&M (incl some constr)		$7,947			$10,259	
O&M (n/i ventilation)	$7,050			$9,024		
Upper Half Subtotal	$12,326	$11,843	104%	$16,727	$15,854	106%
Closure	$855	$832	103%	$1,322	$1,363	97%
WPs	$3,801	$3,998	95%	$4,713	$4,950	95%
Regulatory & Licensing	$368	$368	100%	$383	$379	101%
Monitoring	$4,646	$4,580	101%	$6,336	$6,246	101%
PC	$560	$567	99%	$762	$773	99%
Integration	$2,136	$2,136	100%	$2,913	$2,907	100%
Lower Half Subtotal	$12,366	$12,481	99%	$16,428	$16,618	99%
Total	$24,692	$24,324	102%	$33,155	$32,472	102%

Figure 31 – Cost summary table comparing Carter/Hardin Case 3 (Clay/Shale Enclosed) results with DSEF results

Costs in MM$	DSEF	Carter	DSEF/ Carter	DSEF	Carter	DSEF/ Carter
Cost Category	Low	Low	Low %	High	High	High %
Facility DC&S		6,872			10,064	
Facility D&S	1,547			2,259		
Surface	1,368			1,997		
Subsurface	22,949			33,506		
Ventilation	0			0		
O&M (incl some constr)		26,884			34,525	
O&M (n/i ventilation)	7,050			9,024		
Upper Half Subtotal	$32,914	$33,756	98%	$46,786	$44,589	105%
Closure	5,199	5,556	94%	8,035	8,334	96%
WPs	7,185	7,542	95%	8,909	9,337	95%
Regulatory & Licensing	414	414	100%	431	429	100%
Monitoring	9,028	9,021	100%	12,311	12,302	100%
PC	756	758	100%	1,028	1,034	99%
Integration	2914	2,914	100%	3,974	3,965	100%
Lower Half Subtotal	$25,496	$26,205	97%	$34,688	$35,401	98%
Total	$58,410	$59,961	97%	$81,474	$79,990	102%

Figure 32 – Cost summary table comparing Carter/Hardin Case 4 (Clay/Shale Open) results with DSEF results

Costs in MM$	DSEF	Carter	DSEF/ Carter	DSEF	Carter	DSEF/ Carter
Cost Category	Low	Low	Low %	High	High	High %
Facility DC&S		3,303			4,711	
Facility D&S	740			1,080		
Surface	1,368			1,997		
Subsurface	1,831			2,674		
Ventilation	2,035			2,971		
O&M (incl some constr)		9,702			12,408	
O&M (n/i ventilation)	7,050			9,024		
Upper Half Subtotal	$13,024	$13,005	100%	$17,746	$17,119	104%
Closure	1,425	1,622	88%	2,203	2,515	88%
WPs	2,747	2,882	95%	3,406	3,569	95%
Regulatory & Licensing	417	417	100%	434	421	103%
Monitoring	3,320	3,395	98%	4,528	4,629	98%
PC	420	423	99%	571	576	99%
Integration	3732	3,732	100%	5,089	5,084	100%
Lower Half Subtotal	$12,061	$12,471	97%	$16,231	$16,794	97%
Total	$25,085	$25,476	98%	$33,977	$33,913	100%

Figure 33 – Cost summary table comparing Carter/Hardin Case 5 (Sedimentary Open) results with DSEF results

Costs in MM$	DSEF	Carter	DSEF/ Carter	DSEF	Carter	DSEF/ Carter
Cost Category	Low	Low	Low %	High	High	High %
Facility DC&S		5,410			7,599	
Facility D&S	1,282			1,872		
Surface	1,368			1,997		
Subsurface	1,923			2,807		
Ventilation	3,010			4,395		
O&M (incl some constr)		9,614			12,264	
O&M (n/i ventilation)	7,050			9,024		
Upper Half Subtotal	$14,633	$15,024	97%	$20,095	$19,863	101%
Closure	2,075	2,263	92%	3,207	3,558	90%
WPs	2,747	2,882	95%	3,406	3,569	95%
Regulatory & Licensing	668	668	100%	695	679	102%
Monitoring	3,780	3,775	100%	5,155	5,148	100%
PC	798	798	100%	1,085	1,088	100%
Integration	6878	6,878	100%	9,379	9,370	100%
Lower Half Subtotal	$16,946	$17,264	98%	$22,927	$23,412	98%
Total	$31,579	$32,288	98%	$43,022	$43,275	99%

The bottom section of the COST CALCULATION worksheet retains some of the emplacement drift mining calculations that were performed in DSEF Version 2.1, summarizing required drift length based on waste package capacity, drift dimensions, and waste package spacing information. In the future, this section could be expanded to calculate lengths of access drifts and service drifts for various layouts, as well as shaft and ramp counts and lengths.

The top section of the COST-REFERENCES worksheet includes tables extracted from Hardin 2012b summarizing the data and assumptions for the five example cases that DSEF displays on the cost section of the INPUTS worksheet. The bottom section of the COST-REFERENCES worksheet provides a number of web pages for current data related to backfill material properties and costs. However, this is neither an endorsement nor a recommendation for using these particular web pages, which were chosen as examples for a ballpark estimate as a starting point for the user.

10. The WASTE FORM Worksheet

The WASTE FORM worksheet summarizes the waste form and waste package dimensions assumed for all of the enclosed mode and open mode cases.   Currently there is a limited set of sizes that have been considered. Figure 34 shows the tables of data from the enclosed mode and open mode repository design cases analyzed in FY11 and FY12 included on the WASTE FORM worksheet. The enclosed mode waste package dimensions were based on the reference international repository design concepts (see Hardin 2011).

Figure 35 shows is a lookup table for PWR waste form outer radius (waste package inner radius), and the geometric figures that form the basis for the development of the lookup table.   The WASTE FORM worksheet also includes data on PWR and BWR fuel basket designs from storage cask vendor designs. This data was used to define the unit cell dimensions used in the PWR waste form radius lookup table. As shown on the WASTE FORM worksheet, a cross-check of the calculation methodology used to construct the table for the 21-PWR waste package inner radius agrees closely with the value assumed in the open mode thermal analysis for that waste package size.

Although not currently planned, other potential developments of this worksheet might be used to define an equivalent internal thermal conductivity for waste packages for the purpose of determining peak cladding or HLW glass temperatures during thermal transients. This has not been investigated until now since the waste package surface temperature results have been low enough that this does not appear to be an issue.

Figure 34 – Tables from the WASTE FORM worksheet

Enclosed Mode Cases		
Waste Form	Geologic Medium	Waste Package Wall thickness (m)
SNF (UOX and MOX)	Granite	0.1
	Clay	0.11
	Salt	0.03
	Deep borehole	0.011
HLW (Co-X, New-X, EC-C, and EC-M)	Granite	0.01
	Clay	0.01
	Salt	0.01
	Deep borehole	0.011

Open Mode Cases		
Waste Form	Geologic Medium	Waste Package Wall thickness (m)
SNF (UOX)	Clay	0.11
	Alluvium	0.11

Open Mode Cases	
Waste Form	Waste Package Length (m)
SNF (UOX)	5

Enclosed Mode Cases	
Waste Form	Waste Package Length (m)
SNF (UOX and MOX)	5
HLW (Co-X, New-X, and EC-C)	4.572 (15 ft)
HWL (EC-M)	3.048 (10 ft)

Open Mode Cases		
Number of SNF Assemblies	Waste Package Inner Radius (m)	Waste Package Outer Radius (m)
4	0.3	0.41
12	0.535	0.645
21	0.69	0.8
32	0.89	1

Enclosed Mode Cases						
Number of Assemblies or Canisters	Geologic Medium	Waste Package Inner Radius (m)	Waste Package Outer Radius Granite (m)	Waste Package Outer Radius Clay (m)	Waste Package Outer Radius Salt (m)	Waste Package Outer Radius Deep Borehole (m)
1 SNF assembly	All Except Deep Borehole	0.19	0.29	0.3	0.22	
2 SNF assemblies		0.38	0.48	0.49	0.41	
3 SNF assemblies		0.38	0.48	0.49	0.41	
4 SNF assemblies		0.38	0.48	0.49	0.41	
12 SNF assemblies		0.555	0.655	0.665	0.585	
1 HLW canister		0.295	0.305	0.305	0.305	
1 assembly (with rod consolidation)	Deep Borehole	0.159				0.17
0.291 canisters (modified smaller radius HLW canister)		0.159				0.17

Figure 35 - WASTE FORM worksheet – calculated waste form outer radius lookup table

Number of Assemblies	PWR Waste Form Outer Radius (m)
1	0.168
2	0.335
3	0.335
4	0.335
5	0.375
6	0.427
7	0.427
8	0.503
9	0.503
10	0.503
11	0.530
12	0.530
13	0.593
14	0.593
15	0.691
16	0.691
17	0.691
18	0.691
19	0.691
20	0.691
21	0.691
22	0.749
23	0.749
24	0.749
25	0.855
26	0.855
27	0.855
28	0.855
29	0.855
30	0.855
31	0.855
32	0.855

5 Assemblies
r = (sqrt(10) / 2)*Unit_side

7 Assemblies
r = (sqrt(13) / 2)*Unit_side

9 Assemblies
r = (3*sqrt(2))/2)*Unit_side

10 Assemblies
r = (3*sqrt(2))/2)*Unit_side

12 Assemblies
r = sqrt(5)*Unit_side

14 Assemblies
r = 2.5*Unit_side

21 Assemblies
r = (sqrt(34))/2)*Unit_side

32 Assemblies
r = sqrt(13)*Unit_side
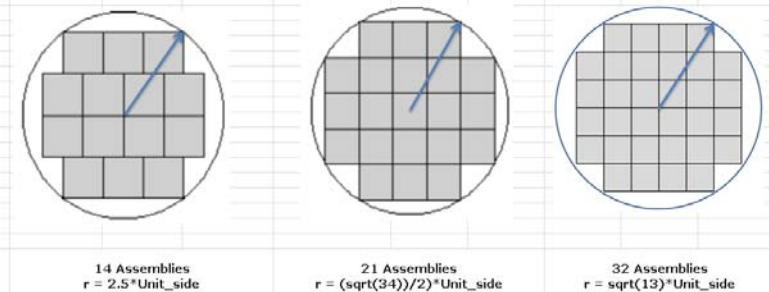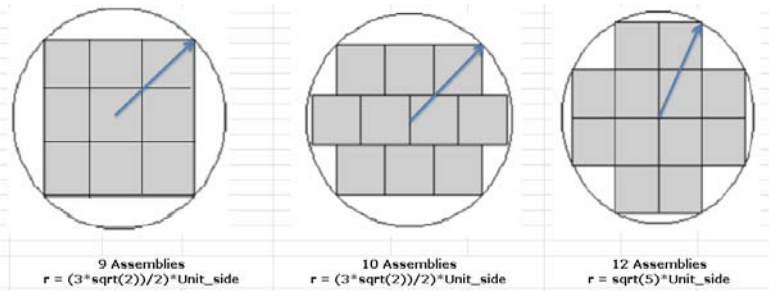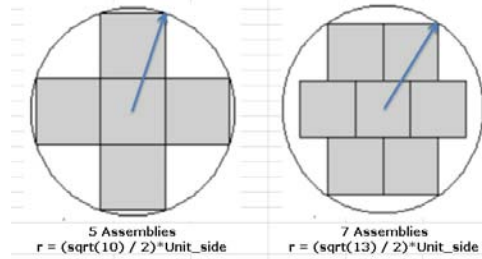
11. Defining Thermal Data Inputs and Outputs -the THERMAL Worksheets

As shown on the NAVIGATION worksheet in Figure 4, there are a series of thermal worksheets

- THERMAL
- THERMAL-ANALYTICAL
- THERMAL-ANALYTICAL OUTPUT
- THERMAL-FEM (see Section 13)
- THERMAL-INTERPOLATE (discussed in Section 7 with the CASE LIBRARY)
- THERMAL-SOURCE

These worksheets are all linked together by the main THERMAL worksheet. Besides including hyperlinks to the other worksheets, the THERMAL worksheet also displays plots of the decay heat chosen for the current analysis case on the THERMAL-SOURCE worksheet. The following describes the use of these other worksheets.

The THERMAL-ANALYTICAL Worksheet - Passing Input Data to Mathcad

The THERMAL-ANALYTICAL worksheet is the interface for passing data to the Mathcad thermal analytical component of DSEF. No numerical calculations are performed in this worksheet, but the formulas in the worksheet cells pull data from the INPUTS and THERMAL-SOURCE worksheets to a standard location cited in the Mathcad file.

The Mathcad file and the DSEF Excel file need to be in the same directory to facilitate the data transfer. As described in Appendix B, the Excel file name is entered in the Mathcad variable "file". Before Mathcad can read the Excel file, the Excel file must be closed. By default the Mathcad DSEF file has the calculation mode set to manual, and the variable "Write_OK" is set to "No". This allows the user to make adjustments and look at results prior to writing them back to the DSEF Excel file. To calculate a screen at a time as the user pages through the Mathcad file, press F9 or use the Mathcad TOOLS – CALCULATE menu to select CALCULATE NOW, alternatively the user can calculate the entire document by pressing CTRL-F9 or selecting the menu option TOOLS – CALCULATE - CALCULATE WORKSHEET. After reviewing the results in MathCad, set the variable "Write_OK" to "Yes" and recalculate the Mathcad document to write the results back to the Excel file in the THERMAL-ANALYTICAL OUTPUT worksheet. To preserve a record of the full Mathcad calculation, the user should print the file to a PDF file for future reference.

The THERMAL-ANALYTICAL OUTPUT Worksheet – Getting Results Back from Mathcad

After running an analysis case in Mathcad the summary of peak temperatures and times, and the full transient outputs are passed back to the THERMAL-ANALYTICAL OUTPUT worksheet, which in turn passes this data to the RESULTS worksheet of DSEF.

The THERMAL-ANALYTICAL OUTPUT worksheet also creates several kinds of plots. There are two plots that are specifically related to parametric studies, as shown in Figure 36. In addition to those plots, for each case in the parametric study two additional plots are provided. One showing the temperature

transients at various locations within the EBS and at a second compliance point within the host rock, and another showing the contributions to the rock wall surface temperature are shown in Figure 37.

Figure 36- Example of parametric study plots on the THERMAL-ANALYTICAL OUTPUT worksheet
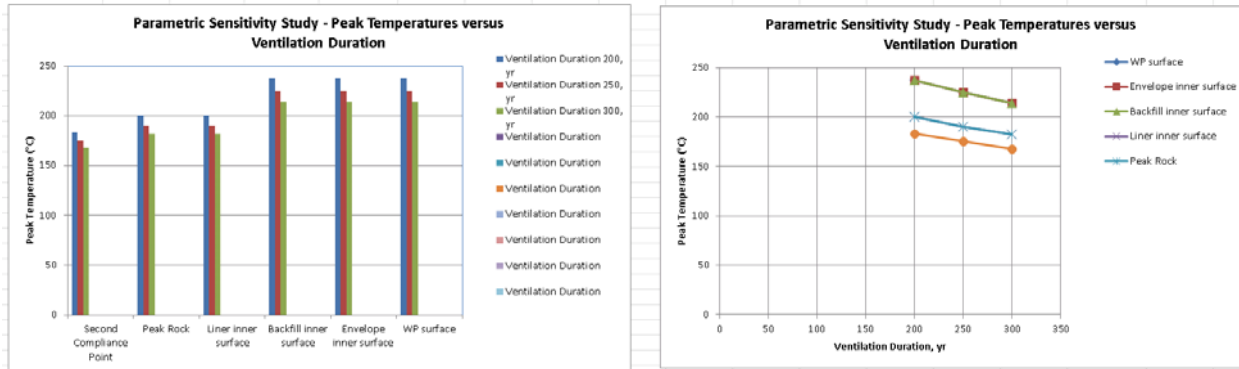
Figure 37 - Example transient output data plotted in the THERMAL-ANALYTICAL OUTPUT worksheet
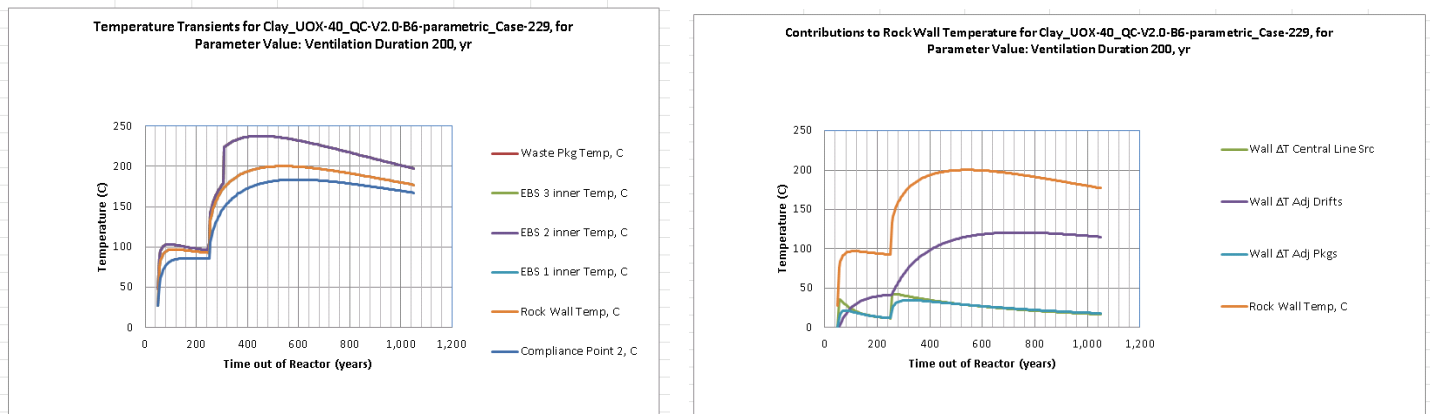
The THERMAL SOURCE Worksheet – Defining the Waste Form Decay Heat

The THERMAL SOURCE worksheet includes a fully documented set of decay heat curves for a set of seven waste forms previously analyzed from three potential fuel cycles

- A once-through LWR fuel cycle with UOX SNF of either 40 GWd/MTU or 60 GWd/MTU burnup
- A partial recycle fuel cycle with MOX SNF of 50 GWd/MTU burnup, and co-extraction glass HLW waste forms (COEX)
- A full recycle based on an Advanced Burner Reactor (ABR) with three HLW waste forms – new-extraction glass (NUEX), Electro-chemical ceramic (E-Chem Ceramic), and Electro-chemical metal (E-Chem Metal).

In addition to these options there is a user-defined option for input from another fuel cycle or modifications to any of the pre-defined cases. Figure 38 shows a plot of the pre-defined waste form decay heat data available for selection on the THERMAL-SOURCE worksheet (Greenberg 2012a).

Figure 38 – Decay heat data built-in to the THERMAL-SOURCE worksheet
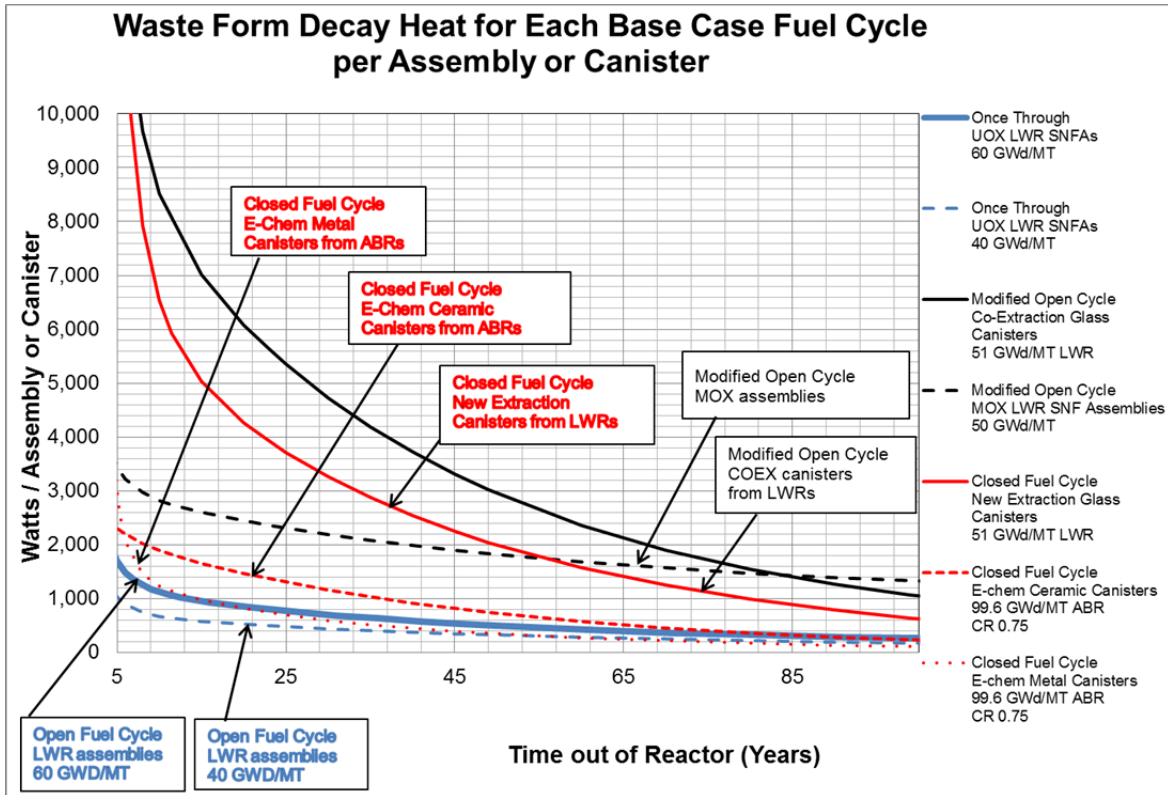
A drop-down list on the INPUTS worksheet allows the user to select one of these data sets, or choose to enter their own data. A prompt and a hyperlink are provided to go the THERMAL-SOURCE worksheet to examine the data, and to click on a macro button to update the decay heat input curve if necessary. Figure 39 shows an example of the "*Update Decay Heat*" macro button and the two types of prompts.

Figure 39 - Examples of decay heat update caution and confirmation prompts

The caution prompt:

The confirmation prompt:

12. Finding and Comparing Material Properties - the MATERIALS Worksheets

As shown on the NAVIGATION worksheet in Figure 4, there are a series of material worksheets

- MATERIAL DATA PLOTTING
- MATERIALS
- MATERIALS-OTHER PROPERTIES (discussed in Section 13)
- MATERIALS-REFERENCES
- MATERIALS-THERMAL PROPERTIES
- MATERIALS-TRANSPORT PROPERTIES

These worksheets are all linked together by the main MATERIALS worksheet, which includes hyperlinks to the other materials worksheets, and then back to the INPUTS worksheet where the derived material properties will be used.

The MATERIAL DATA PLOTTING Worksheet

The MATERIAL DATA PLOTTING worksheet only contains a short list of instructions and a *Click here to plot data distribution* macro button. After clicking on that macro button a Select a Range user input box appears, as shown in Figure 40. At this point the user is free to navigate between material data worksheets by clicking on their tabs at the bottom of the screen, and then scrolling with the mouse to any set of data on those worksheets. The only restriction is that the range of data must be restricted to two yellow-highlighted columns, representing the high and low values of a single data parameter.

The range of data selected can be a continuous block of data values or a separate collection of different data sets (use the CTRL key with the mouse to select non-contiguous sets of data). Any blank rows in the middle of a range of data will be ignored. After clicking OK on the range selection box the user is returned to the MATERIAL DATA PLOTTING worksheet where they pick a location to place the statistical data and the plot, as shown in Figure 41 and Figure 41. However, the user is not restricted to placing the output data and plot on this worksheet. It can be placed on any other worksheet by navigating to the new location before clicking OK to insert the plot.

Figure 40 - The first step – selecting the materials data to plot

TH-N-9	Clay	Opalinus clay			0	
TH-N-10	Clay	Opalinus clay		1.38	1.24	1.31	Ref. C-27, citing Ref. C-31, assumed to be isotropic
TH-N-11	Clay	Opalinus clay			0.81	Ref. C-27, (by inverse modeling, two boreholes) - perpendicular to bedding
TH-N-12	Clay	Opalinus clay			1.87	Ref. C-27, (by inverse modeling, two boreholes) - parallel to bedding
TH-N-13	Clay	Opalinus clay		1.49	1.20	1.345	Ref. C-27, (by inverse modeling, two boreholes) - mean (assuming isotropic)
TH-N-14	Clay	Opalinus clay		1.136	0.916	1.026	Ref. C-27, citing C-32, for perpendicular to bedding
TH-N-15	Clay	Opalinus clay		2.27	1.81	2.04	Ref. C-27, citing C-32 for parallel to bedding
TH-N-16	Clay	Opalinus clay		2.5		2.5	Ref. C-18
TH-N-17	Clay	Opalinus clay		2.2		2.2	Ref. C-18, citing Ref. C-12
TH-N-18	Clay	Opalinus clay		2.5		2.5	Ref. C-18, citing Ref. C-33

Figure 41 - Example output of the materials data plotting macro
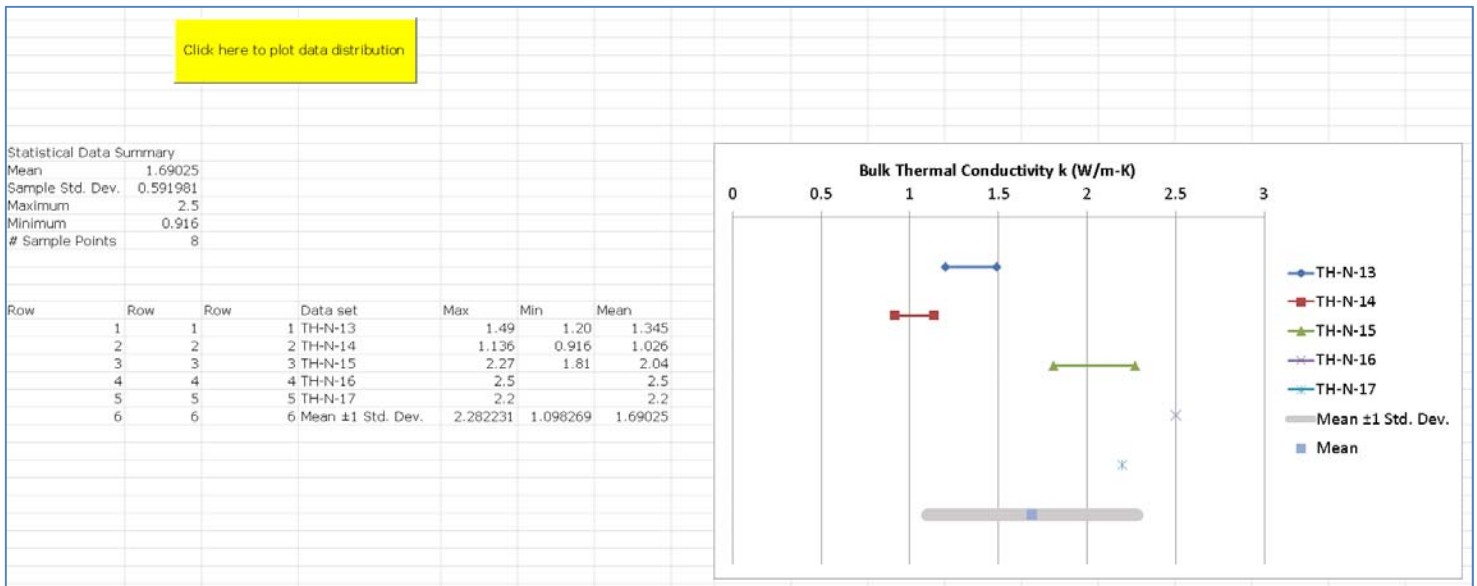
The MATERIALS-THERMAL PROPERTIES Worksheet

The data records on the MATERIALS-THERMAL PROPERTIES worksheet are identified with a sequential data set number starting with TH-N (for natural material properties) or TH-E for engineered material properties. The natural property data is grouped into major categories of rock, and then subcategories, as shown in Figure 42.

Figure 42 - Example of data structure in the MATERIALS-THERMAL PROPERTIES worksheet

Data Set Number	Host Rock General Material Category	Specific Material Data Source	Source Organization / Reference	Range High Bulk Thermal Conductivity k (W/m-K)	Low Bulk Thermal Conductivity k (W/m-K)	Mean Bulk Thermal Conductivity k (W/m-K)	Bulk Thermal Conductivity Comments
TH-N-1	Clay	Boom Clay	NIRAS/ONDRAF, Belgium Ref. C-01	1.69		1.69	Ref. C-01
TH-N-2	Clay	Clay - non-specific	Handbook of Heat Transfer, R-03	1.3		1.3	Ref. R-03, Table 2.35 - Thermophysical Properties of Miscellaneous Materials

The MATERIALS-TRANSPORT PROPERTIES Worksheet

The data records on the MATERIALS-TRANSPORT PROPERTIES worksheet are identified with a sequential data set number starting with TP-N (for natural material properties) or TP-E for engineered material properties. The natural property data is grouped into major categories of rock, and then subcategories, as shown in Figure 43.

Figure 43 - Example of data structure in the MATERIALS-TRANSPORT PROPERTIES worksheet

| Data Set Number | Host Rock | | Source Organization / Reference | Range | | Mean | |
	General Material Category	Specific Material Subcategory		High Permeability (m²)	Low Permeability (m²)	Permeability (m²)	Permeability Comments
TP-N-1	Granite	Canadian Shield granite, measured values		1.00E-17	1.00E-19	5.05E-18	Ref. G-06
TP-N-2	Granite	Äspö diorite		1.00E-19	1.00E-20	5.5E-20	Ref. G-08 - for undisturbed rock

The MATERIALS-REFERENCES Worksheet

The MATERIALS-REFERENCES worksheet contains around 100 references that include both primary and secondary reference citations. These references are listed in groups with category letters as follows:

- A – alluvium
- C – clay
- EBS – engineered barrier materials
- G – granite
- R – general reference documents like handbooks or textbooks
- S – salt
- T – tuff

At LLNL a large number of these references are hyperlinked to the source documents on the network drive, but the distribution copy of DSEF Version 3.0 has all of these hyperlinks removed.

13. Placeholder worksheets for future development

No work is currently planned to develop these placeholder worksheets; however, their potential use is described below:

The INTERFACE PARAMETERS Worksheet

This worksheet has limited current operability, with the capability to read and write "comma delimited files", which are universally accepted by most computer codes.

The DESIGN CONSTRAINTS Worksheet

This worksheet currently documents existing calculations and other references that formed the basis for assumed design constraints in previous calculations, and provides background information for the users. Design constraint data are currently entered in Step 11 of the INPUTS worksheet. However, the DESIGN CONSTRAINTS worksheet could also allow documentation of experimental results and other information currently being developed that might form the basis for design constraints.

The ENVIRONMENT Worksheet

This worksheet is only a placeholder with no detailed description. This worksheet could be used to interface repository design an analysis to NEPA type of environmental impact statement related data such as passing the data on the volume of excavated muck, required concrete, and electricity / diesel fuel requirements – derived from the COST worksheets (for example).

The PERFORMANCE ASSESSMENT Worksheet

This worksheet is a placeholder intended to pass repository design data – repository layout and dimensions, material quantities and properties, and thermal transient data input to performance assessment external programs.

The MATERIALS-OTHER PROPERTIES Worksheet

This worksheet is a placeholder intended to gather property data and references for properties other than thermal or transport properties that already have data worksheets in DSEF. One example would be to have a worksheet for mechanical properties such as Young's Modulus, compressive strength, thermal expansion coefficients, etc. The data from such a worksheet could then be passed to ARIA or DIABLO to run thermal-mechanical analysis.

The THERMAL-FEM Worksheet

The THERMAL-FEM worksheet is a placeholder to interface with other Finite Element Model (FEM) thermal analysis codes, such as TOPAZ or DIABLO from LLNL, ARIA from SNL, SINDAG from ANL, etc. It is meant to be able to pass required inputs for those codes by pulling the problem/case definition information from other worksheets in DSEF.

This worksheet could function the way that the THERMAL-ANALYTICAL worksheet does to pass information to an external FEM code. It is expected that use of such codes would also include some post-processing of data to write the results back to the THERMAL-ANALYTICAL OUTPUT worksheet

14. References

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(Greenberg 2012a). Harris R. Greenberg, Montu Sharma, Mark Sutton, and Alethia V. Barnwell, *Repository Near-Field Thermal Modeling Update Including Analysis of Open Mode Design Concepts*, LLNL-TR-572252, Aug 2012

(Greenberg 2012b). Harris R. Greenberg, Montu Sharma and Mark Sutton, *Investigations on Repository Near-Field Thermal Modeling,* LLNL-TR-491099-Rev-2, November 2012

(Greenberg 2013a). H.R. Greenberg, J. A. Blink, and T. A. Buscheck, *Repository Layout and Required Ventilation Trade Studies in Clay/Shale using the DSEF Thermal Analytical Model,* LLNL-TR-638880, June 12, 2013.

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(Hardin 2012a). E. Hardin, T. Hadgu, D. Clayton; R. Howard; H. R. Greenberg, J. Blink, M. Sharma, M. Sutton, J. Carter, M. DuPont and P. Rodwell, *Design Concepts/Thermal Load Management (FY11/12) Summary Report*, FCRD-UFD-2012-00219, August 2012

(Hardin 2012b). E. Hardin, T. Hadgu, D. Clayton; R. Howard; H. R. Greenberg, J. Blink, M. Sharma, M. Sutton, J. Carter, M. DuPont and P. Rodwell, *Repository Reference Disposal Concepts and Thermal Load Management Analysis*, FCRD-UFD-2012-00219, Rev. 2, November 2012

(Sutton 2011). Mark Sutton, James A. Blink, Massimiliano Fratoni, Harris R. Greenberg, William G. Halsey and Thomas J. Wolery, *Disposal Systems Evaluation Framework Version 1.0* Progress Report, June 2011.

Appendix A – Setting up Excel to Allow the DSEF Macros to Work

In order for the Form controls in DSEF to work you must enable macros. If you weren't prompted to ENABLE MACROS when you first started DSEF, and the Form controls do not appear to be working, the steps outlined in this Appendix should resolve the problem.

Please follow Figures A.1 through A.7 and the steps outlined below:

Figure A-1– The FILE menu choices
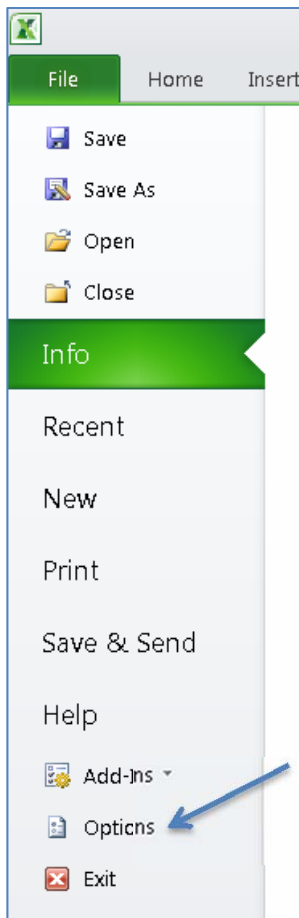
- Figure A.1 - Click on the FILE menu
- Under HELP, select   OPTIONS
- Figure A.2 shows the OPTIONS menu,
- Select the TRUST CENTER option
- Figure A.3 shows the TRUST CENTER button
- Click on the TRUST CENTER SETTINGS button
- Figure A.4 shows the TRUST CENTER options
- You need to select settings for
  - Macros
  - Message bar
- Suggested settings are shown in Figures A.5 – A.7

Appendix A

Figure A-2 – The OPTIONS menu choices
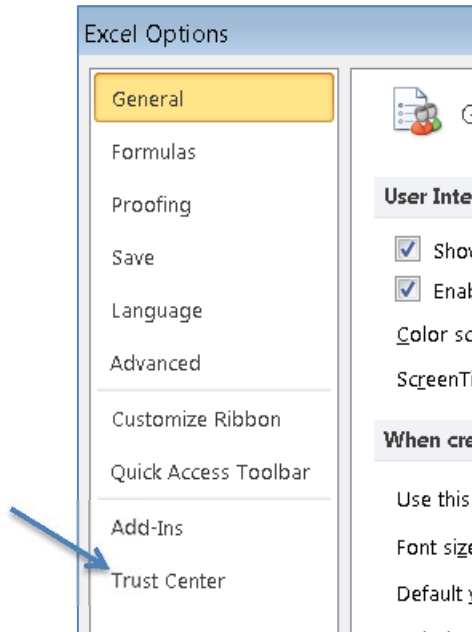
Figure A-3 – Select Trust Center Settings
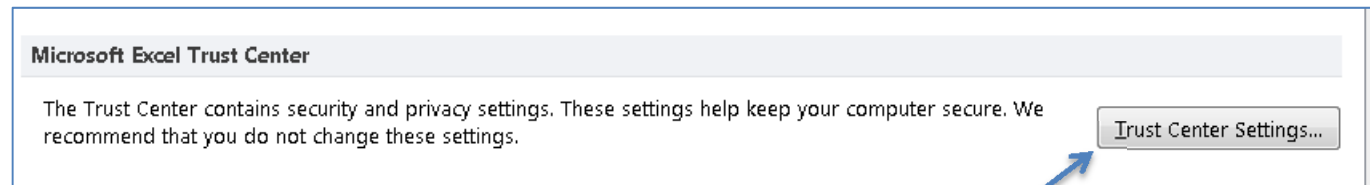
Figure A-4 – Trust Center Settings
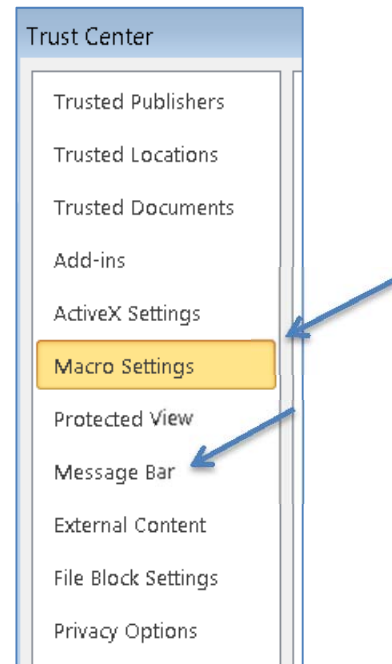
Figure A-5 – Prompt before enabling all controls with minimal restrictions
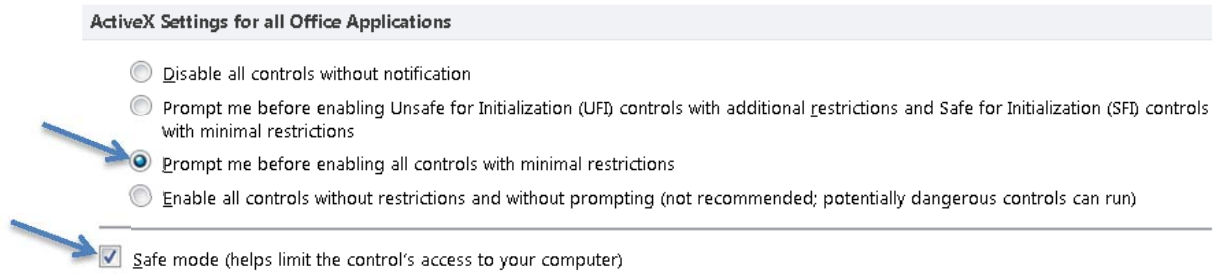
Figure A-6 – Macro settings
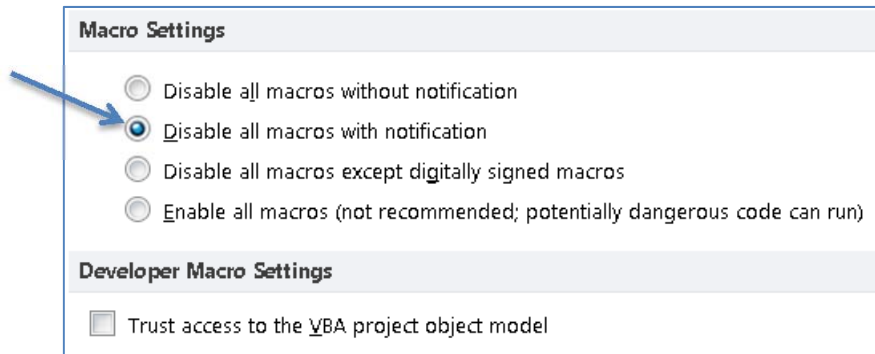
Figure A-7 – Message bar settings
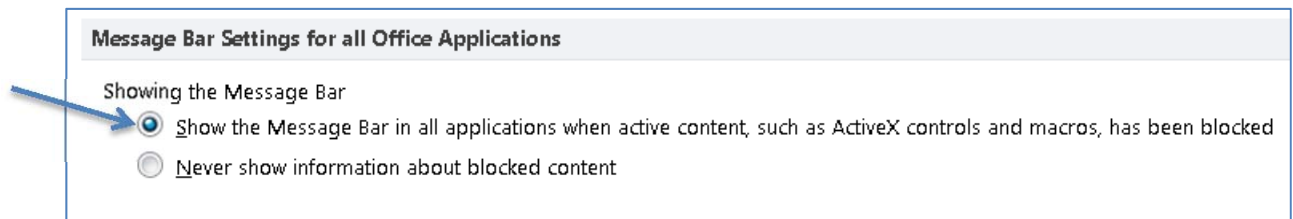
Appendix B – The Mathcad Thermal-Analytical Component of DSEF

This appendix contains PDF pages of the two DSEF Version 3.0 Mathcad thermal-analytical models that receive input from the THERMAL-ANALYTICAL worksheet, and return transient and peak summary data to the THERMAL-ANALYTICAL OUTPUT worksheet in DSEF. The basic Mathcad thermal-analytical model was benchmarked against two different finite-element model (FEM) computer codes by ANL and by SNL. The benchmarking analyses are documented in Sections G.6.1 and G.6.2 of Greenberg 2012b respectively.

Section B.1 describes the use of the Mathcad thermal-analytical models, and their interface with the DSEF Excel spreadsheet.

Section B.2 documents the update to the parametric study analysis model documented in the DSEF Version 2.1 User Manual to add the capability to perform iterative analyses to determine required ventilation time. This one model can perform either parametric study case analyses when the input data sets the mode to "Parametric", or individual case and iterative convergence modeling when the mode is set to "Single". Section B.2 shows an example of a parametric study set of analysis cases.

Section B.3 documents the additional programming added to the parametric study analysis model to perform iterative analysis to determine required ventilation time necessary to meet input temperature constraint values for the drift wall (which is easily modified to apply the temperature constraint at other locations as well). This model was used to perform the analyses documented in Greenberg 2012a.

Section B.4 documents a new DSEF Version 3.0 Mathcad model that allows temperature and time-dependent thermal properties within the EBS layers of the model. The particular PDF file and Mathcad document example applies these to salt for temperature-dependent thermal conductivity and time-dependent crushed salt porosity to model consolidation of the crushed salt layer with time and heat. The data for the time-dependent crushed salt consolidation comes from a finite element model in Hardin 2012b (Figure C-5). This model provides proof-of-principle that the thermal-analytical model can accommodate more complex thermal property modeling than the constant properties assumed in models and analysis using earlier versions of DSEF. The thermal results of this new model have a better fit to the FEM model results for the 12-PWR 40-GWd/MT burnup waste stream with 50 years of surface storage documented in Hardin 2012b than was possible with previous analyses using constant salt properties in the EBS (see Greenberg 2012b, Section G.6.2).

With different temperature or time-depending functions, this methodology could be used to model moisture dependent properties covering dryout or re-wetting effects in other media. This would require other data or analysis to set the basic input functions, but then the benefits of the analytical-model approach could be applied to a broader class of problems.

B.1 Using the Mathcad models in conjunction with the DSEF Excel file

The Mathcad file and the DSEF Excel file need to be in the same directory to facilitate the data transfer. Before Mathcad can read the Excel file, the Excel file must be closed. By default the Mathcad DSEF file has the calculation mode set to manual, and the variable "Write_OK" is set to "No". This allows the user to make adjustments and look at results prior to writing them back to the DSEF Excel file. To calculate a screen at a time as the user pages through the Mathcad file, press F9 or use the Mathcad TOOLS – CALCULATE menu to select CALCULATE NOW, alternatively the user can calculate the entire document by pressing CTRL-F9 or selecting the menu option TOOLS – CALCULATE - CALCULATE WORKSHEET. After reviewing the results in MathCad, set the variable "Write_OK" to "Yes" and recalculate the Mathcad document to write the results back to the Excel file in the THERMAL-ANALYTICAL OUTPUT worksheet. To preserve a record of the full Mathcad calculation, the user should print the file to a PDF file for future reference.

Working with the Mathcad component of DSEF – here are some key pointers for using the Mathcad file:

- Connecting to the DSEF Excel component – on the first page (page 1 of 21 of the PDF listing) assign the file name of the Excel file you want to work with to the variable "file".

- The calculation mode setting in Mathcad – the calculation mode setting in the Mathcad component is set to "Manual" (under the Mathcad TOOLS menu selection). This gives the user more control when working with a large model, and also allows you to set variables that will turn on or delay writing back to the DSEF Excel file until you are ready. Pressing the F9 key, or using the Mathcad menu to select "Calculate Now" will process only the currently visible screen and variables, so you can work your way slowly through the file and see the data, section-by-section as it is being read in from the THERMAL-ANALYTICAL worksheet. Either pressing CTRL-F9, or using the menu to select "Calculate Worksheet" will initiate a complete calculation of the entire file.

- Writing the results back to the THERMAL-ANALYTICAL OUTPUT worksheet – on the first page of the PDF listing, use the variable "Write_OK" to "Yes" if you are ready to immediately write your calculated results back to the Excel file, or to "No" if you want to examine the results first. Setting the variable to "No" allows you to make changes in Mathcad to some of the input variables if you want to make adjustments to refine your design case to reach some desired goal. For example, if you wanted to find the required ventilation time to meet a given design constraint, you might want to adjust the ventilation time until the goal was met, and then go back and set "Write_OK" to "Yes".

- Speeding up the calculations – on the bottom of page 11 of 21 in the PDF file, there are two variables "Counter" and "Step". These variables set the number of time-steps and the size of the time-step in the main calculation loop for the transient calculations. If you are doing a large number of parametric study cases, or covering a long time period, you may first want to set a large time-step to quickly get a ball-park answer, and then later

rerun the case with a smaller time-step after you have adjusted some variables in your design case to try to optimize your results.

- Additional graphics in the Mathcad file – the Mathcad file includes a number of plots for working with the analysis that are not currently returned to the DSEF Excel component. These include a plot of the thermal resistance versus radius of the EBS layers before and after backfill is installed (see pages 5 and 6 of the PDF file), and a plot of the thermal gradients within the EBS at the time of the waste package peak temperature and the drift wall peak temperature (see page 19 of 21 in the PDF file).

- Selectively overriding input variables – After a variable has been assigned a value, either by reading it in from the DSEF Excel component or within the Mathcad component itself, the user can override the value and provide a new assignment. Mathcad notes the re-assignment by underlining the variable and displaying a message on mouse-over of the variable as you work. Care should be taken when re-assigning variables. The user is advised to make any re-assignments at the point where the variable is first assigned, so that the changes are easily identified. The notes section of the INPUTS CHECKLIST in the DSEF Excel component is the place to note any such changes that remain in effect when the final analysis results are returned to the Excel file.

- Printing the Mathcad Output – it should be noted that saving the Mathcad file after an analysis does not save the results, it just saves the problem setup and variables. To see the results again the Mathcad worksheet must be completely recalculated. This is not a problem for short calculations. However, for longer more complex calculations, or if you want to keep a record of intermediate design "test cases", it is recommended that the user print the fully evaluated results to a PDF file or to a printer for traceability, and to create records for QA/QC purposes. The current Mathcad component has a header that lists the Mathcad file name.

B.2 The Mathcad parametric analysis and iterative convergence model – parametric study example

Step 13 on the DSEF INPUTS worksheet allows the user to either select a "single" calculation mode that uses all of the input data for the reference case defined in Steps 1 through 12, or to select a "parametric" study calculation mode. Figure 12 shows the options available for parametric studies, where the basic inputs have been set, but the user can then define up to 10 data values for one of six possible parameters – waste package spacing, drift spacing, storage time, ventilation duration, rock thermal conductivity, and backfill thermal conductivity. The Mathcad model documented in this section is essentially the same as that documented in the Version 2.1 User Manual for running parametric study cases when "parametric" is selected as the study mode. The model looks slightly different because of the additional capabilities discussed in Section B.3, and because "collapsible" regions have been added to the Mathcad document to speed up review of results when using the iterative model discussed in Section B.3. The collapsible region boundaries appear as lines going across the entire page, with a drop-down arrow at the left-hand edge of the line.

The specific parametric study example case was taken from Greenberg 2012b, and is Case 500-1 in that report, which corresponds to DSEF Case Library case number 427. It is a parametric study of waste package spacing (with 10 values ranging from 15 to 24 m) for a large 32-PWR waste package having 40-GWd/MT burnup, with a drift spacing of 70 m, surface storage of 50 years, and 100 years of ventilation in a clay/shale repository design. As the last figure in the analysis shows, a waste package spacing of 23 m is required to achieve a maximum drift wall temperature of 100°C. Greenberg 2012b included analysis of thermal gradients into the host rock outside the drift wall by varying the depth of Compliance Point 2 (CP2), and in this example run CP2 = 1 m.

The program loop for the iterative convergence model appears on page 19 of 23 of the example output, but there are no results shown on pages 20 and 21 of 23, since the variable Iterate_OK = "No", and thus the iterative model was not used.

DSEF R3.0 parametric and iterative model with collapsable areas - for rapid iteration.

Values over-written from DSEF Excel file to create case include: Drift_spacing, TC and t_{vent}.

Allow output transients to be written back to DSEF FILE

$Case\_name := "500-1"$

Variables for repository symmetry and extent:

$Write\_OK := "YES"$

$N_{drifts} := 4$ $N_{adj} := 4$

REQUIRED REPOSITORY INPUT DATA (from DSEF):

$file := "DSEF\ R3.0\_2013Aug12\_HRG-Clay\_UOX-40,CP2=1m,DS70,Vent100,WP\ param\_Case-500-1.xlsm"$

$sheet := "Thermal-Analytical!"$

DATA FOR ITERATION ON TEMPERATURE ACCEPTACE CRITERIAA:

READ DSEF INPUT FILE

$TC := 100$ $T_{criteria} := (TC + 273.15) \cdot K = 373.15\,K$ $T_{criteria} = 100 \cdot °C$

Input 1 = Operating Mode (enclosed or open)

$t_{convergence} := 1 \cdot yr$ CONVERGE CRITERIA FOR REQUIRED VENTILATION TIME IN YEARS

$Input\_1 := READEXCEL(file, concat(sheet, "A5:B5"))$

$Input\_1 = ("MODE = Open\ or\ Enclosed:"\quad "Open")$ $Mode := Input\_1_{1,2} = "Open"$

SET THE VARIABLE ITERATE_OK TO "NO" TO TURN OFF THE AUTOMATIC CONVERGENCE CALCULATION, AND MANUALLY RESET IT TO "YES" IF YOU WANT TO FINE TUNE YOUR ANSWER:

$Input\_2 := READEXCEL(file, concat(sheet, "A7:B16"))$ **Input 2 = Case Definitions**

$ITERATE\_OK := "NO""$

Input 3 = Ventilation Parameters (for Open Modes)

$$Input\_2 = \begin{pmatrix} "Host\ Media" & "Clay" \\ "Rock\ thermal\ conductivity,\ W/m\text{-}K" & 1.75 \\ "Rock\ thermal\ diffusivity,\ m2/sec" & 6.45 \times 10^{-7} \\ "Repository\ Depth,\ m" & 500 \\ "Surface\ temperature,\ °C" & 15 \\ "Geothermal\ gradient,\ °C/km" & 25 \\ "Ambient\ temperature\ at\ depth,\ °C" & 27.5 \\ "Waste\ Package\ (axial)\ spacing,\ m" & 20 \\ "Drift\ /\ Borehole\ (lateral)\ spacing,\ m" & 70 \\ "Surface\ storage\ time,\ y" & 50 \end{pmatrix}$$

$Input\_3 := READEXCEL(file, concat(sheet, "e7:f11"))$

$$Input\_3 = \begin{pmatrix} "Ventilation\ Duration,\ yr" & 100 \\ "Unventilated\ Closure\ Duration\ (Backfill\ Installation),\ yr" & 10 \\ "Ventilation\ Thermal\ Efficiency,\ \%" & 0.75 \\ "Rock\ Wall\ Emissivity" & 0.9 \\ "Waste\ Package\ Emissivity" & 0.6 \end{pmatrix}$$

$RT\_name := Input\_2_{1,2} = "Clay"$

$t_{vent} := if\left[(Mode = "Enclosed"), 0, Input\_3_{1,2}\right] \cdot yr = 100 \cdot yr$

$Kth := Input\_2_{2,2} \cdot \dfrac{W}{m \cdot K} = 1.75 \dfrac{m \cdot kg}{K \cdot s^3}$

$t_{backfill} := if\left[(Mode = "Enclosed"), 0, Input\_3_{2,2}\right] \cdot yr = 10 \cdot yr$

$V_{eff} := if\left[(Mode = "Enclosed"), 0, Input\_3_{3,2}\right] = 0.75$

$\alpha := Input\_2_{3,2} \cdot \dfrac{m^2}{s} = 6.45 \times 10^{-7} \dfrac{m^2}{s}$

$\varepsilon_{wall} := if\left[(Mode = "Enclosed"), .9, Input\_3_{4,2}\right] = 0.9$

$\text{WP\_depth} := \text{Input\_2}_{4,2} \cdot m = 500\,m$

$\varepsilon_{WP} := \text{if}\left[(\text{Mode} = \text{"Enclosed"}), .6, \text{Input\_3}_{5,2}\right] = 0.6$

$T_{surface} := \left(\text{Input\_2}_{5,2} + 273.15\right) \cdot K = 288.15\,K$

$\text{geothermal\_gradient} := \text{Input\_2}_{6,2}\frac{K}{km} = 0.025\frac{K}{m}$

<mark>OVER-RIDE VENTILATION DURATION</mark>

$T_{ambient} := \left(\text{Input\_2}_{7,2} + 273.15\right) \cdot K = 300.65\,K$

$\text{WP\_spacing} := \text{Input\_2}_{8,2} \cdot m = 20\,m$

<mark>OVER-RIDE DRIFT AND/OR WASTE PACKAGE SPACING</mark>

$\text{Drift\_spacing} := \text{Input\_2}_{9,2} \cdot m = 70\,m$

$t_{store} := \text{Input\_2}_{10,2} \cdot yr = 50 \cdot yr$

$t_{operate} := \left(t_{store} + t_{vent}\right) = 150 \cdot yr$

<mark>T_OPERATE = T_STORE + T_VENTILATE</mark>

$t_{closure} := t_{operate} + t_{backfill} = 160 \cdot yr$

<mark>TCLOSURE = TOPERATE + TIME TO BACKFILL</mark>

Input 4 = ENGINEERED BARRIER SYSTEM DATA:

$\text{Input\_4} := \text{READEXCEL}(file, concat(sheet, "A20:F27"))$

Input 5 = COMPLIANCE POINT 2 INPUT DATA

$\text{Input\_5} := \text{READEXCEL}(file, concat(sheet, "C32"))$

$\text{Input\_4} = \begin{pmatrix} \text{"Waste Form Outer Radius, m"} & 0.535 & \text{"N/A"} & 0.535 & \text{"UOX-40"} & \text{"N/A"} \\ \text{"Canister"} & 0 & 0.535 & 0.535 & \text{"None"} & \text{"N/A"} \\ \text{"Waste Package"} & 0.11 & 0.535 & 0.645 & \text{"Carbon Steel"} & \text{"N/A"} \\ \text{"Buffer"} & 0 & 0.645 & 0.645 & \text{"None"} & \text{"N/A"} \\ \text{"Envelope"} & 0 & 0.645 & 0.645 & \text{"None"} & \text{"N/A"} \\ \text{"Backfill"} & 1.58 & 0.645 & 2.225 & \text{"70\% Bentonite 30\% Sand"} & 1.2 \\ \text{"Liner"} & 0.025 & 2.225 & 2.25 & \text{"Steel"} & 46 \\ \text{"Host Rock Inner Radius, m ----{>}"} & \text{NaN} & 2.25 & \text{NaN} & \text{NaN} & \text{NaN} \end{pmatrix}$

$\text{Input\_5} = (3.25)$

$r_{CP2} := \text{Input\_5}_1 \cdot m = 3.25\,m$

$r_{DW} := \text{Input\_4}_{8,3} \cdot m = 2.25\,m$

$r_{WP} := \text{Input\_4}_{3,4} \cdot m = 0.645\,m$

$\text{EBS\_name}_1 := \text{Input\_4}_{7,1} = \text{"Liner"}$

$\text{EBS\_material}_1 := \text{Input\_4}_{7,5} = \text{"Steel"}$

$\text{thickness}_1 := \text{Input\_4}_{7,2} \cdot m = 0.025\,m$

$r_1 := \text{Input\_4}_{7,4} \cdot m = 2.25\,m$

$k1 := \text{Input\_4}_{7,6} = 46$

$k_1 := \text{if}\left[(k1 = \text{"N/A"}), 0, k1\right] \cdot \frac{W}{m \cdot K} = 46 \cdot \frac{W}{m \cdot K}$

$EBS_name_2 := Input_46_{,1} = $ "Backfill" $EBS_material_2 := Input_46_{,5} = $ "70% Bentonite 30% Sand"

$thickness_2 := Input\_46_{,2} \cdot m = 1.58\,m$ $r_2 := Input\_46_{,4} \cdot m = 2.225\,m$

$k2 := Input\_46_{,6} = 1.2$

$k_2 := if\,[(k2 = "N/A"),0,k2] \cdot \dfrac{W}{m \cdot K} = 1.2 \cdot \dfrac{W}{m \cdot K}$

$k_{radiation} := if\left[(Mode = "Enclosed"),k_2,0\right] = 0 \cdot \dfrac{W}{m \cdot K}$

$EBS_name_3 := Input_45_{,1} = $ "Envelope" $EBS_material_3 := Input_45_{,5} = $ "None"

$thickness_3 := Input\_45_{,2} \cdot m = 0\,m$ $r_3 := Input\_45_{,4} \cdot m = 0.645\,m$

$k3 := Input_45_{,6} = $ "N/A"

$k_3 := if\,[(k3 = "N/A"),0,k3] \cdot \dfrac{W}{m \cdot K} = 0 \cdot \dfrac{W}{m \cdot K}$

$EBS_name_4 := Input_44_{,1} = $ "Buffer" $EBS_material_4 := Input_44_{,5} = $ "None"

$thickness_4 := Input\_44_{,2} \cdot m = 0\,m$ $r_4 := Input\_44_{,4} \cdot m = 0.645\,m$

$k4 := Input_44_{,6} = $ "N/A"

$k_4 := if\,[(k4 = "N/A"),0,k4] \cdot \dfrac{W}{m \cdot K} = 0 \cdot \dfrac{W}{m \cdot K}$

==Define the total thermal resistance between the rock wall and the waste package surface based on a heat flux per unit area, it is then applied to a heat flux is per unit length adjusting to area per unit length and q_L (W/m):==

$r_{WP} = 0.645\,m$ $r_4 = 0.645\,m$ $r_3 = 0.645\,m$ $r_2 = 2.225\,m$ $r_1 = 2.25\,m$ $r_{DW} = 2.25\,m$

$R_1(k_1) := if\left[\left[thickness_1 = 0 \lor (k1 = "N/A")\right],0,\dfrac{r_{DW}}{k_1} \cdot ln\left(\dfrac{r_1}{r_2}\right)\right]$ $R_1(k_1) = 5.465 \times 10^{-4} \cdot \dfrac{m^2 \cdot K}{W}$ ==Thermal resistance==

$EBS_name_1 = $ "Liner" $EBS_material_1 = $ "Steel"

==ADDED CORRECTION FOR PARAMETRIC $t_{closure}$ replaced $t_{closure}$ with ($t_{operate} + t_{backfill}$)==   ==Revised R_2 to make it an explicit function of $t_{operate}$ and $t_{backfill}$.==

$R_2(k_2,t,t_{operate},t_{backfill}) := \begin{vmatrix} kk \leftarrow k_{radiation} \cdot \left[t < \left(t_{operate} + t_{backfill}\right)\right] + k_2 \cdot \left[t \geq \left(t_{operate} + t_{backfill}\right)\right] \\ return\;\; if\left[\left[\left(thickness_2 = 0\right) \lor (kk = 0)\right],0,\dfrac{r_{DW}}{kk} \cdot ln\left(\dfrac{r_2}{r_3}\right)\right] \end{vmatrix}$ $\dfrac{r_{DW}}{k_2} \cdot ln\left(\dfrac{r_2}{r_3}\right) = 2.322 \cdot \dfrac{m^2 \cdot K}{W}$

$\text{EBS\_name}_2 = \text{"Backfill"} \qquad \text{EBS\_material}_2 = \text{"70\% Bentonite 30\% Sand"}$

$$R_2\left(k_2, 5 \cdot yr, 300 \cdot yr, 10 \cdot yr\right) = 0 \cdot \frac{m^2 \cdot K}{W} \qquad R_2\left(k_2, 1000 \cdot yr, 300 \cdot yr, 10 \cdot yr\right) = 2.321741 \cdot \frac{m^2 \cdot K}{W}$$

$$R_3\left(k_3\right) := \text{if}\left[\left[\text{thickness}_3 = 0 \vee (k3 = \text{"N/A"})\right], 0, \frac{r_{DW}}{k_3} \cdot \ln\left(\frac{r_3}{r_4}\right)\right] \qquad R_3\left(k_3\right) = 0 \cdot \frac{m^2 \cdot K}{W}$$

$\text{EBS\_name}_3 = \text{"Envelope"} \qquad \text{EBS\_material}_3 = \text{"None"}$

$$R_4\left(k_4\right) := \text{if}\left[\left[\text{thickness}_4 = 0 \vee (k4 = \text{"N/A"})\right], 0, \frac{r_{DW}}{k_4} \cdot \ln\left(\frac{r_4}{r_{WP}}\right)\right] \qquad R_4\left(k_4\right) = 0 \cdot \frac{m^2 \cdot K}{W}$$

$\text{EBS\_name}_4 = \text{"Buffer"} \qquad \text{EBS\_material}_4 = \text{"None"}$

$$R_{Total}\left(t, k_1, k_2, k_3, k_4\right) := R_1\left(k_1\right) + R_2\left(k_2, t, t_{operate}, t_{backfill}\right) + R_3\left(k_3\right) + R_4\left(k_4\right) \qquad \text{==Total thermal resistance between wall and waste package==}$$

$$t_{backfill} = 10 \cdot yr \qquad t_{operate} = 150 \cdot yr$$

$$R_{continuous}\left(t, r, k_1, k_2, k_3, k_4\right) := \begin{array}{|l}
kk_2 \leftarrow k_{radiation} \cdot \left[t < \left(t_{operate} + t_{backfill}\right)\right] + k_2 \cdot \left[t \geq \left(t_{operate} + t_{backfill}\right)\right] \\[2mm]
R \leftarrow R_1\left(k_1\right) + R_2\left(k_2, t, t_{operate}, t_{backfill}\right) + R_3\left(k_3\right) + \text{if}\left[\left[\left(\text{thickness}_4 = 0\right) \vee (k4 = \text{"N/A"})\right], 0, \frac{r_{DW}}{k_4} \cdot \ln\left(\frac{r_4}{r}\right)\right] \ \text{if} \ r \leq r_4 \wedge r \geq r_{WP} \\[2mm]
R \leftarrow R_1\left(k_1\right) + R_2\left(k_2, t, t_{operate}, t_{backfill}\right) + \text{if}\left[\left[\left(\text{thickness}_3 = 0\right) \vee (k3 = \text{"N/A"})\right], 0, \frac{r_{DW}}{k_3} \cdot \ln\left(\frac{r_3}{r}\right)\right] \ \text{if} \ r \leq r_3 \wedge r > r_4 \\[2mm]
R \leftarrow R_1\left(k_1\right) + \text{if}\left[\left[\left(\text{thickness}_2 = 0\right) \vee kk_2 = 0\right], 0, \frac{r_{DW}}{kk_2} \cdot \ln\left(\frac{r_2}{r}\right)\right] \ \text{if} \ r \leq r_2 \wedge r \geq r_3 \\[2mm]
R \leftarrow \text{if}\left[\left[\left(\text{thickness}_1 = 0\right) \vee (k1 = \text{"N/A"})\right], 0, \frac{r_{DW}}{k_1} \cdot \ln\left(\frac{r_1}{r}\right)\right] \ \text{if} \ r \leq r_{DW} \wedge r \geq r_2 \\[2mm]
R \leftarrow \text{"Invalid Radius"} \quad \text{otherwise} \\[2mm]
\text{return } R
\end{array}$$

$$R_{continuous}\left(5 \cdot yr, r_{WP}, k_1, k_2, k_3, k_4\right) = 5.465 \times 10^{-4} \frac{K \cdot s^3}{kg} \qquad R_{continuous}\left(1000 \cdot yr, r_{WP}, k_1, k_2, k_3, k_4\right) = 2.322288 \frac{K \cdot s^3}{kg}$$

Early Time - Thermal Resistance From Rock Wall to r

Thermal Resistance (m^2-K/W) vs Radial Location Within the EBS (m)

— Thermal resistance prior to closure

$r_{DW} = 2.25\,m$

$r_1 = 2.25\,m$ $EBS_name_1 = $ "Liner" $EBS_material_1 = $ "Steel"

$r_2 = 2.225\,m$ <mark>Note that for "open modes", the backfill hasn't been emplaced at early time</mark>

$r_3 = 0.645\,m$ $EBS_name_3 = $ "Envelope" $EBS_material_3 = $ "None"

$r_4 = 0.645\,m$ $EBS_name_4 = $ "Buffer" $EBS_material_4 = $ "None"

$r_{WP} = 0.645\,m$

$$R_1(k_1) = 5.465 \times 10^{-4} \cdot \frac{m^2 \cdot K}{W} \qquad R_2(k_2, 5 \cdot yr, t_{operate}, t_{backfill}) = 0 \cdot \frac{m^2 \cdot K}{W} \qquad R_3(k_3) = 0 \cdot \frac{m^2 \cdot K}{W} \qquad R_4(k_4) = 0 \cdot \frac{m^2 \cdot K}{W}$$

$$R_{Total}(50yr, k_1, k_2, k_3, k_4) = 5.465 \times 10^{-4} \cdot \frac{m^2 \cdot K}{W}$$

Late Time - Thermal Resistance From Rock Wall to r

Thermal Resistance (m^2-K/W) vs Radial Location Within the EBS (m)

— Thermal resistance prior to closure

$r_{DW} = 2.25\,m$

$r_1 = 2.25\,m$ $EBS_name_1 = $ "Liner" $EBS_material_1 = $ "Steel"

$r_2 = 2.225\,m$ $EBS_name_2 = $ "Backfill" $EBS_material_2 = $ "70% Bentonite 30% Sand"

$r_3 = 0.645\,m$ $EBS_name_3 = $ "Envelope" $EBS_material_3 = $ "None"

$r_4 = 0.645\,m$ $EBS_name_4 = $ "Buffer" $EBS_material_4 = $ "None"

$r_{WP} = 0.645\,m$

$$R_1(k_1) = 5.465 \times 10^{-4} \cdot \frac{m^2 \cdot K}{W} \qquad R_2(k_2, t_{closure}, t_{operate}, t_{backfill}) = 2.322 \cdot \frac{m^2 \cdot K}{W} \qquad R_3(k_3) = 0 \cdot \frac{m^2 \cdot K}{W}$$

$$R_{Total}(1000yr, k_1, k_2, k_3, k_4) = 2.322 \cdot \frac{m^2 \cdot K}{W}$$

INPUT 6 = WASTE FORM DATA

$\text{Input\_6} := \text{READEXCEL}(\text{file}, \text{concat}(\text{sheet}, "A35:B38"))$

$$\text{Input\_6} = \begin{pmatrix} \text{"Waste form short name"} & \text{"UOX-40"} \\ \text{"Waste form type"} & \text{"Assembly"} \\ \text{"Waste package capacity"} & 32 \\ \text{"Waste package length, m"} & 5 \end{pmatrix}$$

$\text{WF\_name} := \text{Input\_6}_{1,2} = \text{"UOX-40"}$

$\text{WF\_type} := \text{Input\_6}_{2,2} = \text{"Assembly"}$

$\text{WP\_cap} := \text{Input\_6}_{3,2} = 32$

Outside of the liner	Outside of the backfill	Outside of the envelope	Outside of the buffer

$\text{WP\_length} := \text{Input\_6}_{4,2} \cdot \text{m} = 5\,\text{m}$

$A_1 := 2 \cdot \pi \cdot r_1 \cdot \text{WP\_length} = 70.69\,\text{m}^2$

$A_2 := 2 \cdot \pi \cdot r_2 \cdot \text{WP\_length} = 69.9\,\text{m}^2$

$A_3 := 2 \cdot \pi \cdot r_3 \cdot \text{WP\_length} = 20.26\,\text{m}^2$

$A_4 := 2 \cdot \pi \cdot r_4 \cdot \text{WP\_length} = 20.26\,\text{m}^2$

$A_{DW} := 2 \cdot \pi \cdot r_{DW} \cdot \text{WP\_length} = 70.686\,\text{m}^2$

$A_{WP} := 2 \cdot \pi \cdot r_{WP} \cdot \text{WP\_length} = 20.263\,\text{m}^2$

CONSIDER THE ALTERNATE DESIGN CASE OF AN "OPEN MODE" DESIGN, WITH A CEMENTITIOUS LINER, BUT ONLY AIR BETWEEN THE LINER AND THE WASTE PACKAGE FOR THE FIRST 300 YEARS. ASSUME NO VENTILATION FOR 300 YEARS, AND THEN BACKFILL AT CLOSURE.

CALCULATE THE EQUIVALENT THERMAL RESISTANCE OF THE AIR GAP USING A LINEARIZED RADIATION HEAT TRANSFER COEFFICIENT. BASE THE COEFFICIENT ON THE ROCK WALL TEMPERATURE AT THE DRIFT, AND THE EQUIVALENT WASTE PACKAGE TEMPERATURE NECESSARY TO MOVE THE HEAT GENERATED AT THE WASTE PACKAGE AT ANY GIVEN TIME. THE EQUATION FOR THE RADIATION HEAT TRANSFER COEFFICIENT IS FROM INCROPERA AND DEWITT.

$A_{wall} := \text{WP\_length} \cdot 2 \cdot \pi \cdot r_{DW} = 70.686\,\text{m}^2$

Stefan Boltzmann constant $\sigma := 5.670 \cdot 10^{-8} \cdot \dfrac{\text{W}}{\text{m}^2 \cdot \text{K}^4}$

The basis for the rock and waste package emissivity assumed is F. P. Incropera and D.P. DeWitt, *Fundamentals of Heat and Mass Transfer*, 4th Edition, 1996, Table A-11, which shows a range of 0.88 to 0.93 is adapted from hemispherical emissivity of rock at around 300 K. This range is corroborated by the "Heat Transmission" section of Perry's Chemical Engineers Handbook, 6th Edition, 1984 (Table 10-17, pages 10-51 to 10-52) for normal emissivity of rough silica and rough fused quartz, ranging from 0.8 to 0.93. The waste package surface is assumed to be covered with dust and dirt. The emissivity values to the left were specified in DSEF, and should be changed there if necessary.

Waste Package emissivity $\varepsilon_{WP} = 0.6$

Rock wall or cementitious liner emissivity $\varepsilon_{wall} = 0.9$

Reference for radiation heat transfer coefficient, h_{rad}, is from Incropera and DeWitt, Table 13.3 for concentric infinite cylinders (based on the inner surface as the heat source), and is also referenced in the YMP *Ventilation Model and Analysis Report*, ANL-EBS-MD-000030 REV 04, Oct. 2004, page 6-8.

$$h_{rad\_infinite}(r_i, r_o, \varepsilon_i, \varepsilon_o) := \dfrac{\sigma}{\dfrac{1}{\varepsilon_i} + \left(\dfrac{1 - \varepsilon_o}{\varepsilon_o}\right) \cdot \dfrac{r_i}{r_o}}$$

$h_{rad\_infinite}(r_{WP}, r_{DW}, \varepsilon_{WP}, \varepsilon_{wall}) = 3.338 \times 10^{-8} \cdot \dfrac{\text{W}}{\text{m}^2\,\text{K}^4}$

Usage is Q in watts = h*A_i*(T_i^4 - T_o^4)

For radiation between the liner and the envelope (both metal surfaces) use r_2 and r_3, and assume the same emissivity for both surfaces.

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$$Q_{rad\_infinite}(r_i, r_o, \varepsilon_i, \varepsilon_o, L, T_{cold}, T_{hot}) := h_{rad\_infinite}(r_i, r_o, \varepsilon_i, \varepsilon_o) \cdot (2 \cdot \pi \cdot r_i \cdot L) (T_{hot}^4 - T_{cold}^4)$$

$$Q_{rad\_infinite}(r_3, r_2, \varepsilon_{WP}, \varepsilon_{wall}, WP\_length, 300 \cdot K, 600 \cdot K) = 8.217 \times 10^4 \, W$$

$$Q_{L\_rad\_infinite}(r_i, r_o, \varepsilon_i, \varepsilon_o, T_{cold}, T_{hot}) := h_{rad\_infinite}(r_i, r_o, \varepsilon_i, \varepsilon_o) \cdot (2 \cdot \pi \cdot r_i) (T_{hot}^4 - T_{cold}^4)$$

$$Q_{L\_rad\_infinite}(r_3, r_2, \varepsilon_{WP}, \varepsilon_{wall}, 300 \cdot K, 600 \cdot K) = 1.643 \times 10^4 \, \frac{W}{m}$$

Heat transfer by radiation from NIRAS/ONDRAF December 2005 Report: Eef Weetjens and Xavier Sillen; *Thermal analysis of the Supercontainer concept 2D axisymmetric heat transport calculations,* Section 6.4.3. Pg 34, equation 29.

$$Q_{L\_infinite}(r_i, r_o, \varepsilon_i, \varepsilon_o, T_{cold}, T_{hot}) := \frac{2\pi\sigma \cdot (T_{hot}^4 - T_{cold}^4)}{\dfrac{1 - \varepsilon_i}{\varepsilon_i \cdot r_i} + \dfrac{1}{r_i} + \dfrac{1 - \varepsilon_o}{\varepsilon_o \cdot r_o}}$$

$$Q_{L\_infinite}(r_3, r_2, \varepsilon_{WP}, \varepsilon_{wall}, 300 \cdot K, 600 \cdot K) = 1.643 \times 10^4 \cdot \frac{W}{m}$$

This is the same as the Incropera and DeWitt result, $Q_{L\_rad\_infinite}$

Comparision of thermal radiation across a gap to conduction after the gap has been filled with backfill material.

$$Q_{L\_conduction\_comparison}(r_i, r_o, T_{cold}, T_{hot}) := \frac{2 \cdot \pi \cdot r_o}{\dfrac{r_{DW}}{k_2} \cdot \ln\left(\dfrac{r_o}{r_i}\right)} \cdot (T_{hot} - T_{cold})$$

$$Q_{L\_conduction\_comparison}(r_3, r_2, 300 \cdot K, 600 \cdot K) = 1.806 \times 10^3 \cdot \frac{W}{m}$$

$$Q_{ratio}(r_i, r_o, \varepsilon_i, \varepsilon_o, T_{cold}, T_{hot}) := \frac{Q_{L\_infinite}(r_i, r_o, \varepsilon_i, \varepsilon_o, T_{cold}, T_{hot})}{Q_{L\_conduction\_comparison}(r_i, r_o, T_{cold}, T_{hot})}$$

$$Q_{ratio}(r_3, r_2, \varepsilon_{WP}, \varepsilon_{wall}, 300 \cdot K, 600 \cdot K) = 9.097$$

INPUT 7 = PARAMETRIC STUDY VARIABLE INPUT DATA

$$Input\_7 := READEXCEL(file, concat(sheet, "F29:F41"))$$

$$Cases := Input\_7_1 = 10$$

$$Parameter := Input\_7_2 = "WP \ Spacing"$$

$$Parameter\_units := Input\_7_3 = "m"$$

$$ij := 1 .. Cases$$

$$Parameter\_data_{ij} := Input\_7_{ij+3}$$

$$Parameter\_description_{ij} := \begin{cases} "Single \ Base \ Case" & if \ Cases = 1 \\ concat[num2str[Input\_7_{(ij+3)}], ", \ ", Input\_7_3] & otherwise \end{cases}$$

$$Input\_7 =$$

	1
1	10
2	"WP Spacing"
3	"m"
4	15
5	16
6	17
7	18
8	19
9	20
10	21
11	22
12	23
13	24

$$Parameter\_data =$$

	1
1	15
2	16
3	17
4	18
5	19
6	20
7	21
8	22
9	23
10	24

$$Parameter\_description =$$

	1
1	"15, m"
2	"16, m"
3	"17, m"
4	"18, m"
5	"19, m"
6	"20, m"
7	"21, m"
8	"22, m"
9	"23, m"
10	"24, m"

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<mark>**INPUT 8 = DECAY HEAT INPUT DATA PER UNIT SOURCE (ASSEMBLY OR CANISTER):**</mark>

$\text{Input\_8\_size} := \text{READEXCEL}(\text{file}, \text{concat}(\text{sheet}, \text{"C43"}))$ $\text{Input\_8\_size}_1 = 58$ $\text{Decay\_heat\_range} := \text{concat}\left[\text{"A43:B"}, \text{num2str}\left(\left(\text{Input\_8\_size}_1 + 42\right)\right)\right] = \text{"A43:B100"}$

$\text{Input\_8} := \text{READEXCEL}(\text{file}, \text{concat}(\text{sheet}, \text{Decay\_heat\_range}))$

$\text{Time\_out\_of\_Reactor} := \text{Input\_8}^{\langle 1 \rangle} \cdot \text{yr}$ $\text{Decay\_Heat\_per\_Cnt} := \text{Input\_8}^{\langle 2 \rangle} \cdot \text{W}$

$\text{Input\_8} =$

	1	2
1	5	$1.028 \cdot 10^3$
2	5.1	$1.011 \cdot 10^3$
3	5.5	949.125
4	5.75	916.671
5	6	887.984
6	8	742.948
7	10	670.028
8	11.5	634.239
9	15	576.929
10	20	...

$\text{Time\_out\_of\_Reactor} =$

	1
1	5
2	5.1
3	5.5
4	5.75
5	6
6	8
7	10
8	11.5
9	15
10	...

$\cdot \text{yr}$

$\text{Decay\_Heat\_per\_Cnt} =$

	1
1	$1.028 \cdot 10^3$
2	$1.011 \cdot 10^3$
3	949.125
4	916.671
5	887.984
6	742.948
7	670.028
8	634.239
9	576.929
10	...

W

$Q(t) := \text{interp}(\text{cspline}(\text{Time\_out\_of\_Reactor}, \text{Decay\_Heat\_per\_Cnt}), \text{Time\_out\_of\_Reactor}, \text{Decay\_Heat\_per\_Cnt}, t)$

Ventilation efficiency for open systems is $\boxed{V_{\text{eff}} = 0.75}$ between t_{store} and t_{operate}

<mark>FUNCTION DEFINITION FOR ONE OUTPUT FILE</mark>

<mark>**FORMULAS FOR CALCULATING THE TRANSIENT DRIFT WALL TEMPERATURE:**</mark>

<mark>Central waste package:</mark>

$$Q_{\text{L\_wp}}\left(t, t_{\text{store}}, t_{\text{operate}}, \text{WP\_cap}\right) := \frac{Q(t) \cdot \text{WP\_cap}}{\text{WP\_length}} \cdot \left[1 - 1 \cdot \left(t \leq t_{\text{store}}\right)\right] \cdot \left[1 - V_{\text{eff}} \cdot \left(t \leq t_{\text{operate}}\right)\right]$$

$$Q_{\text{L\_wp}}\left(55 \cdot \text{yr}, t_{\text{store}}, t_{\text{operate}}, 12\right) = 177.365 \cdot \frac{\text{W}}{\text{m}}$$

Note - added r_{DW} as a function parameter to allow calculations at additional compliance points inside the rock, where r_{DW} would be replaced with new radius value.

$$DW\_T\_finite\_line\left(t, r_{DW}, y, t_{store}, t_{operate}, WP\_cap, Kth, \alpha\right) := \left[\int_0^t \frac{Q_{L\_wp}\left(\tau, t_{store}, t_{operate}, WP\_cap\right)}{8 \cdot (\pi \cdot Kth) \cdot (t - \tau)} \cdot e^{\frac{-\left(r_{DW}^2\right)}{4 \cdot \alpha \cdot (t-\tau)}} \cdot \left[\operatorname{erf}\left[\frac{1}{2} \cdot \frac{\left(y + \frac{WP\_length}{2}\right)}{\sqrt{\alpha \cdot (t - \tau)}}\right] - \operatorname{erf}\left[\frac{1}{2} \cdot \frac{\left(y - \frac{WP\_length}{2}\right)}{\sqrt{\alpha \cdot (t - \tau)}}\right]\right] d\tau\right]$$

Adjacent drifts:

$$Q_{L\_avg}\left(t, t_{store}, t_{operate}, WP\_cap, WP\_spacing\right) := \frac{Q(t) \cdot WP\_cap}{WP\_spacing} \cdot \left[1 - 1 \cdot \left(t \le t_{store}\right)\right] \cdot \left[1 - V_{eff} \cdot \left(t \le t_{operate}\right)\right]$$

Note - added r_{DW} as a function parameter to allow calculations at additional compliance points inside the rock, where r_{DW} would be replaced with new radius value.

$$DW\_T\_drifts\left(t, r_{DW}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha\right) := 2 \left[\sum_{id = 1}^{N_{drifts}} \int_0^t \frac{Q_{L\_avg}\left(\tau, t_{store}, t_{operate}, WP\_cap, WP\_spacing\right)}{4 \cdot (\pi \cdot Kth) \cdot (t - \tau)} \cdot e^{\frac{-\left[(r_{DW})^2 + (id \cdot Drift\_spacing)^2\right]}{4 \cdot \alpha \cdot (t-\tau)}} d\tau\right]$$

Adjacent waste packages:

$$Q_{wp}\left(t, t_{store}, t_{operate}, WP\_cap\right) := Q(t) \, WP\_cap \cdot \left[1 - 1 \cdot \left(t \le t_{store}\right)\right] \cdot \left[1 - V_{eff} \cdot \left(t \le t_{operate}\right)\right]$$

Note - added r_{DW} as a function parameter to allow calculations at additional compliance points inside the rock, where r_{DW} would be replaced with new radius value.

$$DW\_T\_adjacent\_pkgs\left(t, r_{DW}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Kth, \alpha\right) := 2 \left[\sum_{ip = 1}^{N_{adj}} \int_0^t \frac{Q_{wp}\left(\tau, t_{store}, t_{operate}, WP\_cap\right)}{8 \cdot Kth \cdot \sqrt{\alpha} \cdot \pi^{1.5} \cdot (t - \tau)^{1.5}} \cdot e^{\frac{-\left[r_{DW}^2 + (ip \cdot WP\_spacing)^2\right]}{4\alpha \cdot (t-\tau)}} d\tau\right]$$

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OutfileName := file = "DSEF R3.0_2013Aug12_HRG-Clay_UOX-40_CP2=1m,DS70,Vent100,WP param_Case-500-1.xlsm"

Out_sheet := "Thermal-Analytical Output!"

Cases = 10   Read in from Thermal-Analytical sheet in DSEF (Inputs_7)

$i := 1 .. Cases$

$$\text{Parameter\_vector}_i := \begin{cases} \text{"Base Case"} & \text{if } \text{Cases} = 1 \\ \text{concat}(\text{Parameter}, " ", \text{Parameter\_description}_i) & \text{otherwise} \end{cases}$$

$$\text{Parameter\_vector} = \begin{array}{c|c} & 1 \\ \hline 1 & \text{"WP Spacing 15, m"} \\ 2 & \text{"WP Spacing 16, m"} \\ 3 & \text{"WP Spacing 17, m"} \\ 4 & \text{"WP Spacing 18, m"} \\ 5 & \text{"WP Spacing 19, m"} \\ 6 & \text{"WP Spacing 20, m"} \\ 7 & \text{"WP Spacing 21, m"} \\ 8 & \text{"WP Spacing 22, m"} \\ 9 & \text{"WP Spacing 23, m"} \\ 10 & \text{"WP Spacing 24, m"} \end{array}$$

$$\text{heading1}_i := \begin{pmatrix} \text{concat}("Parameter value: ", \text{Parameter\_vector}_i) \\ "" \\ "" \\ "" \\ "" \\ "" \\ "" \\ "" \\ "" \\ "" \end{pmatrix}$$

$$\text{heading2} := \begin{pmatrix} \text{"TooR (yr)"} \\ \text{"Wall } \Delta\text{T Central Line Src"} \\ \text{"Wall } \Delta\text{T Adj Drifts"} \\ \text{"Wall } \Delta\text{T Adj Pkgs"} \\ \text{"Compliance Point 2, C"} \\ \text{"Rock Wall Temp, C"} \\ \text{"EBS 1 inner Temp, C"} \\ \text{"EBS 2 inner Temp, C"} \\ \text{"EBS 3 inner Temp, C"} \\ \text{"Waste Pkg Temp, C"} \end{pmatrix}$$

$\text{heading1}_i := \text{heading1}_i^T \qquad \text{heading2} := \text{heading2}^T$

$\text{Title\_array}_i := \text{stack}(\text{heading1}_i, \text{heading2})$

$$\text{Title\_array}_2 = \begin{array}{c|c|c|c|c|c} & 1 & 2 & 3 & 4 & 5 \\ \hline 1 & \text{ter value: WP Spacing 16, m"} & "" & "" & "" & "" \\ 2 & \text{"TooR (yr)"} & \text{"Wall } \Delta\text{T Central Line Src"} & \text{"Wall } \Delta\text{T Adj Drifts"} & \text{"Wall } \Delta\text{T Adj Pkgs"} & \ldots \end{array}$$

$\text{length}(\text{Parameter\_data}) = 10$

$r_{DW} = 2.25 \, \text{m}$ $t_{store} = 50 \cdot \text{yr}$

$r_{CP2} = 3.25 \, \text{m}$ $t_{operate} = 150 \cdot \text{yr}$

$t_{vent} = 100 \cdot \text{yr}$

$t_{closure} = 160 \cdot \text{yr}$

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$\text{Counter} := 200 \qquad \text{Step} := 5 \qquad \text{time\_after\_emplacement\_analzyed} := (\text{Counter} \cdot \text{Step} \cdot \text{yr}) + t_{store} = 1050 \cdot yr$

$\text{outdata}\left(r_{DW}, r_{CP2}, t_{store}, t_{operate}, \text{WP\_cap}, \text{WP\_spacing}, \text{Drift\_spacing}, \text{Kth}, \alpha, k_1, k_2, k_3, k_4\right) :=$

$\text{for } i \in 1 .. \text{Counter} + 1$

$tt_i \leftarrow \text{Step} \cdot i \cdot yr + t_{store} - \text{Step} \cdot 1yr$

$kk_2 \leftarrow k_{radiation} \cdot \left[tt_i < \left(t_{operate} + t_{backfill}\right)\right] + k_2 \cdot \left[tt_i \geq \left(t_{operate} + t_{backfill}\right)\right]$

$\text{Wall\_deltaT\_finite\_line}_i \leftarrow \text{DW\_T\_finite\_line}\left(tt_i, r_{DW}, 0, t_{store}, t_{operate}, \text{WP\_cap}, \text{Kth}, \alpha\right)$

$\text{Wall\_deltaT\_drifts}_i \leftarrow \text{DW\_T\_drifts}\left(tt_i, r_{DW}, t_{store}, t_{operate}, \text{WP\_cap}, \text{WP\_spacing}, \text{Drift\_spacing}, \text{Kth}, \alpha\right)$

$\text{Wall\_deltaT\_adj\_pkgs}_i \leftarrow \text{DW\_T\_adjacent\_pkgs}\left(tt_i, r_{DW}, t_{store}, t_{operate}, \text{WP\_cap}, \text{WP\_spacing}, \text{Kth}, \alpha\right)$

$\text{Wall\_T}_i \leftarrow T_{ambient} + \text{Wall\_deltaT\_finite\_line}_i + \text{Wall\_deltaT\_drifts}_i + \text{Wall\_deltaT\_adj\_pkgs}_i$

$\text{CP2\_deltaT\_finite\_line}_i \leftarrow \text{DW\_T\_finite\_line}\left(tt_i, r_{CP2}, 0, t_{store}, t_{operate}, \text{WP\_cap}, \text{Kth}, \alpha\right)$

$\text{CP2\_deltaT\_drifts}_i \leftarrow \text{DW\_T\_drifts}\left(tt_i, r_{CP2}, t_{store}, t_{operate}, \text{WP\_cap}, \text{WP\_spacing}, \text{Drift\_spacing}, \text{Kth}, \alpha\right)$

$\text{CP2\_deltaT\_adj\_pkgs}_i \leftarrow \text{DW\_T\_adjacent\_pkgs}\left(tt_i, r_{CP2}, t_{store}, t_{operate}, \text{WP\_cap}, \text{WP\_spacing}, \text{Kth}, \alpha\right)$

$\text{CP2\_T}_i \leftarrow T_{ambient} + \text{CP2\_deltaT\_finite\_line}_i + \text{CP2\_deltaT\_drifts}_i + \text{CP2\_deltaT\_adj\_pkgs}_i$

$Q_i \leftarrow Q_{L\_wp}\left(tt_i, t_{store}, t_{operate}, \text{WP\_cap}\right)$

$\text{EBS\_1}_i \leftarrow \text{Wall\_T}_i + \dfrac{Q_i}{2 \cdot \pi \cdot r_{DW}} \cdot R_1\left(k_1\right)$

$\text{EBS\_2}_i \leftarrow \left| \begin{array}{l} \text{EBS\_1}_i + \dfrac{Q_i}{2 \cdot \pi \cdot r_{DW}} \cdot R_2\left(kk_2, tt_i, t_{operate}, t_{backfill}\right) \quad \text{if } kk_2 \neq 0 \cdot \dfrac{W}{m \cdot K} \\[2em] \left[\left[\dfrac{Q_i}{h_{rad\_infinite}\left(r_3, r_2, \varepsilon_{WP}, \varepsilon_{wall}\right) \cdot 2 \cdot \pi \cdot r_3} + \left(\text{EBS\_1}_i\right)^4\right]^{\frac{1}{4}}\right] \quad \text{otherwise} \end{array} \right.$

$\text{EBS\_3}_i \leftarrow \text{EBS\_2}_i + \dfrac{Q_i}{2 \cdot \pi \cdot r_{DW}} \cdot R_3\left(k_3\right)$

$\text{WP\_T}_i \leftarrow \text{EBS\_3}_i + \dfrac{Q_i}{2 \cdot \pi \cdot r_{DW}} \cdot R_4\left(k_4\right)$

$T1_i \leftarrow \text{CP2\_T}_i - 273.15K$

$T2_i \leftarrow \text{Wall\_T}_i - 273.15K$

$T3_i \leftarrow \text{EBS\_1}_i - 273.15K$

$T4_i \leftarrow \text{EBS\_2}_i - 273.15K$

$T5_i \leftarrow \text{EBS\_3}_i - 273.15K$

$T6_i \leftarrow \text{WP\_T}_i - 273.15K$

$\text{Data\_array} \leftarrow \text{augment}\left(tt \cdot \dfrac{1}{yr}, \text{Wall\_deltaT\_finite\_line} \cdot \dfrac{1}{K}, \text{Wall\_deltaT\_drifts} \cdot \dfrac{1}{K}, \text{Wall\_deltaT\_adj\_pkgs} \cdot \dfrac{1}{K}, T1 \cdot \dfrac{1}{K}, T2 \cdot \dfrac{1}{K}, T3 \cdot \dfrac{1}{K}, T4 \cdot \dfrac{1}{K}, T5 \cdot \dfrac{1}{K}, T6 \cdot \dfrac{1}{K}\right)$

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$jjj := 1 .. Cases$ 　　　　$Cases = 10$

$X_{jjj} := Parameter\_data_{jjj}$ 　　　　$Parameter = \text{"WP Spacing"}$

$$Temp\_array_{jjj} := \begin{array}{ll} outdata\left(r_{DW}, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha, k_1, k_2, k_3, k_4\right) & \text{if } Parameter = \text{"Single"} \\ outdata\left(r_{DW}, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, X_{jjj} \cdot m, Kth, \alpha, k_1, k_2, k_3, k_4\right) & \text{if } Parameter = \text{"Drift Spacing"} \\ outdata\left(r_{DW}, r_{CP2}, t_{store}, t_{operate}, WP\_cap, X_{jjj} \cdot m, Drift\_spacing, Kth, \alpha, k_1, k_2, k_3, k_4\right) & \text{if } Parameter = \text{"WP Spacing"} \\ outdata\left(r_{DW}, r_{CP2}, X_{jjj} \cdot yr, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha, k_1, k_2, k_3, k_4\right) & \text{if } Parameter = \text{"Storage Time"} \\ outdata\left(r_{DW}, r_{CP2}, t_{store}, t_{store} + X_{jjj} \cdot yr, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha, k_1, k_2, k_3, k_4\right) & \text{if } Parameter = \text{"Ventilation Duration"} \\ outdata\left(r_{DW}, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, X_{jjj} \cdot \frac{W}{m \cdot K}, \alpha, k_1, k_2, k_3, k_4\right) & \text{if } Parameter = \text{"Rock Conductivity"} \\ outdata\left(r_{DW}, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha, k_1, X_{jjj} \cdot \frac{W}{m \cdot K}, k_3, k_4\right) & \text{if } Parameter = \text{"Backfill Conductivity"} \\ \text{"Undefined"} & \text{otherwise} \end{array}$$

$File\_array_{jjj} := stack\left(Title\_array_{jjj}, Temp\_array_{jjj}\right)$

$File\_array_1 =$

	1	2	3	4	5	6
1	"Parameter value: WP Spacing 15, m"	""	""	""	""	""
2	"TooR (yr)"	"Wall ΔT Central Line Src"	"Wall ΔT Adj Drifts"	"Wall ΔT Adj Pkgs"	"Compliance Point 2, C"	"Rock Wall Temp, C"
3	50	0	0	0	27.5	27.5
4	55	35.579	$6.058 \cdot 10^{-6}$	4.514	56.729	67.593
5	60	34.943	$5.304 \cdot 10^{-3}$	7.492	59.778	69.94
6	65	33.507	0.055	9.174	60.687	70.236
7	70	31.898	0.188	10.203	60.822	69.789
8	75	30.316	0.402	10.841	60.618	69.059
9	80	28.814	0.677	11.225	60.25	68.216
10	85	27.416	0.992	11.436	59.808	67.344
11	90	26.118	1.328	11.527	59.325	66.473
12	95	24.936	1.671	11.531	58.841	65.638
13	100	23.83	2.016	11.479	58.349	64.826
14	105	22.827	2.354	11.387	57.878	64.068
15	110	21.9	2.682	11.252	57.41	63.334
16	115	21.059	2.999	11.117	56.99	...

$iii := 1 .. 10$

$\text{Peak\_array}_{jjj, iii} := \max\left[\left[\left(\text{Temp\_array}_{jjj}\right)^{\langle iii \rangle}\right]\right]$

$\text{Peak\_array}_{1,2} = 59.322$

	1
1	27.5
2	67.593
3	69.94
4	70.236
5	69.789
6	69.059
7	68.216
8	67.344
9	66.473
10	65.638
11	64.826
12	64.068
13	63.334
14	62.675
15	62.09
16	...

$\left(\text{Temp\_array}_1\right)^{\langle 6 \rangle} =$

$\text{Time\_array} := \left(\text{Temp\_array}_1\right)^{\langle 1 \rangle}$

$\text{Peak\_T}(m, n) := \max\left[\left(\text{Temp\_array}_m\right)^{\langle n \rangle}\right]$

$\text{Peak\_T}(1, 5) = 102.266$

$\text{Peak\_time}(m, n) := \text{lookup}\left[\text{Peak\_T}(m, n), \left(\text{Temp\_array}_m\right)^{\langle n \rangle}, \text{Time\_array}\right]$

$\text{Peak\_time}(1, 5) = (315)$

$\text{Time\_array} =$

	1
1	50
2	55
3	60
4	65
5	70
6	75
7	80
8	85
9	90
10	95
11	100
12	105
13	110
14	115
15	120
16	...

Initialize the peak value data array:

$i := 1 .. 6 \qquad j := 1 .. 20$

$\text{Peak\_values}_{i,j} := ""$

$$\text{Peak\_values} = \begin{pmatrix} "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \end{pmatrix}$$

Fill in the peak temperatures and times:

$mj := 1 .. \text{Cases} \qquad nn := 1 .. 6$

$\text{Peak\_values}_{nn, mj \cdot 2 - 1} := \text{Peak\_T}(mj, nn + 4)$

$\text{Peak\_values}_{nn, mj \cdot 2} := \text{Peak\_time}(mj, nn + 4)_1$

$t_{vent} = 100 \cdot yr$

$\text{Parameter\_vector}^T =$

	1	2
1	"WP Spacing 15, m"	...

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$$\text{Peak\_values} = \begin{pmatrix} 102.266 & 315 & 99.137 & 285 & 96.413 & 285 & 93.988 & 285 & 91.828 & 260 & 89.914 & 250 & 88.231 & 235 & 86.66 & 235 & 85.276 & 230 & 84.019 & 230 \\ 115.262 & 210 & 112.287 & 205 & 109.734 & 190 & 107.536 & 190 & 105.602 & 185 & 103.927 & 185 & 102.391 & 185 & 101.064 & 180 & 99.912 & 175 & 98.88 & 175 \\ 115.285 & 210 & 112.311 & 205 & 109.759 & 190 & 107.561 & 190 & 105.628 & 185 & 103.952 & 185 & 102.417 & 185 & 101.09 & 180 & 99.939 & 175 & 98.907 & 175 \\ 231.735 & 160 & 229.391 & 160 & 227.373 & 160 & 225.623 & 160 & 224.095 & 160 & 222.753 & 160 & 221.567 & 160 & 220.514 & 160 & 219.576 & 160 & 218.736 & 160 \\ 231.735 & 160 & 229.391 & 160 & 227.373 & 160 & 225.623 & 160 & 224.095 & 160 & 222.753 & 160 & 221.567 & 160 & 220.514 & 160 & 219.576 & 160 & 218.736 & 160 \\ 231.735 & 160 & 229.391 & 160 & 227.373 & 160 & 225.623 & 160 & 224.095 & 160 & 222.753 & 160 & 221.567 & 160 & 220.514 & 160 & 219.576 & 160 & 218.736 & 160 \end{pmatrix}$$

$$\text{Peak\_Wall\_T} := \left(\text{Peak\_values}^{\langle 1 \rangle}\right)_2 = 115.262$$

▼

$\text{outsheet} := \text{"Thermal-Analytical Output!"}$

$\text{rows}(\text{Temp\_array}_1) = 201 \qquad \text{rows}(\text{File\_array}_1) = 203 \qquad\qquad$ Transient output starting row in DSEF on the Thermal-= 60

$\text{start\_row} := 100 \quad \text{end\_row} := \text{start\_row} + \text{rows}(\text{Temp\_array}_1) - 1 = 300 \qquad$ NOTE - USE File_array to write to stand-alone Excel files, and Temp_array to write back to the DSEF Excel file.

$$\text{transient\_case\_cols} := \begin{pmatrix} \text{"A"} & \text{"J"} \\ \text{"L"} & \text{"U"} \\ \text{"W"} & \text{"AF"} \\ \text{"AH"} & \text{"AQ"} \\ \text{"AS"} & \text{"BB"} \\ \text{"BD"} & \text{"BM"} \\ \text{"BO"} & \text{"BX"} \\ \text{"BZ"} & \text{"CI"} \\ \text{"CK"} & \text{"CT"} \\ \text{"CV"} & \text{"DE"} \end{pmatrix}$$

To write the transients for each case horizontally instead of vertically, the following location array includes 10 columns for each case with one column separating the cases.

$\text{iw} := 1 .. \text{Cases}$

$\text{start\_row} = 100 \qquad\qquad\qquad \text{end\_row} = 300$

$\text{transient\_write\_range}_{\text{iw}} := \text{concat}\left[\text{outsheet}, \left(\text{transient\_case\_cols}^{\langle 1 \rangle}\right)_{\text{iw}}, \text{num2str}(\text{start\_row}), \text{":"}, \left(\text{transient\_case\_cols}^{\langle 2 \rangle}\right)_{\text{iw}}, \text{num2str}(\text{end\_row})\right]$

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$\text{transient\_write\_range}_2 = \text{"Thermal-Analytical Output!L100:U300"}$ $\text{peaks\_write\_range} := \text{concat}(\text{outsheet}, \text{"C6:V11"}) = \text{"Thermal-Analytical Output!C6:V11"}$

$$\text{transient\_write\_range} = \begin{pmatrix} \text{"Thermal-Analytical Output!A100:J300"} \\ \text{"Thermal-Analytical Output!L100:U300"} \\ \text{"Thermal-Analytical Output!W100:AF300"} \\ \text{"Thermal-Analytical Output!AH100:AQ300"} \\ \text{"Thermal-Analytical Output!AS100:BB300"} \\ \text{"Thermal-Analytical Output!BD100:BM300"} \\ \text{"Thermal-Analytical Output!BO100:BX300"} \\ \text{"Thermal-Analytical Output!BZ100:CI300"} \\ \text{"Thermal-Analytical Output!CK100:CT300"} \\ \text{"Thermal-Analytical Output!CV100:DE300"} \end{pmatrix}$$

$\text{Transient\_size} := (\text{Counter} \quad \text{Step})$ $\text{Transient\_size} = (200 \quad 5)$ $\text{Transient\_size\_range} := \text{concat}(\text{outsheet}, \text{"B92:C92"}) = \text{"Thermal-Analytical Output!B92:C92"}$

Make writing an output file optional $t_{vent} = 100 \cdot yr$

$\text{Write\_file} := \text{Write\_OK} = \text{"YES"}$ $\text{OutfileName} = \text{"DSEF R3.0\_2013Aug12\_HRG-Clay\_UOX-40\_CP2=1m,DS70,Vent100,WP param\_Case-500-1.xlsm"}$

$\text{write\_the\_peaks}(\text{Write\_file}) := \begin{vmatrix} \text{write\_it} \leftarrow \begin{vmatrix} \text{WRITEEXCEL}(\text{Peak\_values}, \text{OutfileName}, \text{peaks\_write\_range}) & \text{if } (\text{Write\_file} = \text{"Yes"}) \vee (\text{Write\_file} = \text{"YES"}) \\ \text{"File written"} \end{vmatrix} \\ \text{write\_it} \leftarrow \text{"No file written"} \quad \text{otherwise} \end{vmatrix}$

$\text{write\_the\_peaks}(\text{Write\_file}) = \text{"File written"}$

$\text{write\_the\_transient\_size}(\text{Write\_file}) := \begin{vmatrix} \text{write\_it} \leftarrow \begin{vmatrix} \text{WRITEEXCEL}(\text{Transient\_size}, \text{OutfileName}, \text{Transient\_size\_range}) & \text{if } (\text{Write\_file} = \text{"Yes"}) \vee (\text{Write\_file} = \text{"YES"}) \\ \text{"File written"} \end{vmatrix} \\ \text{write\_it} \leftarrow \text{"No file written"} \quad \text{otherwise} \end{vmatrix}$

$\text{write\_the\_transient\_size}(\text{Write\_file}) = \text{"File written"}$

$\text{Write\_file} := \text{Write\_OK} = \text{"YES"}$ $\text{Cases} = 10$

$\text{iww} := 1 .. \text{Cases}$ NOTE - USE File_array to write to stand-alone Excel files, and Temp_array to write back to the DSEF Excel file.

$\text{write\_the\_transients}(jj) := \begin{vmatrix} \text{write\_array} \leftarrow \text{Temp\_array}_{jj} \\ \text{write\_it} \leftarrow \begin{vmatrix} \text{WRITEEXCEL}(\text{write\_array}, \text{OutfileName}, \text{transient\_write\_range}_{jj}) & \text{if } (\text{Write\_file} = \text{"Yes"}) \vee (\text{Write\_file} = \text{"YES"}) \\ \text{"File written"} \end{vmatrix} \\ \text{write\_it} \leftarrow \text{"No file written"} \quad \text{otherwise} \end{vmatrix}$

$$\text{write\_the\_transients(iww)} = \begin{pmatrix} \text{"File written"} \\ \text{"File written"} \\ \text{"File written"} \\ \text{"File written"} \\ \text{"File written"} \\ \text{"File written"} \\ \text{"File written"} \\ \text{"File written"} \\ \text{"File written"} \\ \text{"File written"} \end{pmatrix}$$

$\text{Plot\_case} := 6$ 　　　　　Select parametric study case to plot (default plot is for case 1)

$\text{WP\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 10 \rangle}\right]$ 　　$\text{EBS3\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 9 \rangle}\right]$ 　　$\text{EBS2\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 8 \rangle}\right]$ 　　$\text{EBS1\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 7 \rangle}\right]$ 　　$\text{Wall\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 6 \rangle}\right]$

$\text{CP2\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 5 \rangle}\right]$ 　　$\text{Delta\_WPs\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 4 \rangle}\right]$ 　　$\text{Delta\_drifts\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 3 \rangle}\right]$ 　　$\text{Delta\_central\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 2 \rangle}\right]$

Temperature Transients

Parameter Study: Plot_case = 6
Parameter_vector$_{Plot\_case}$ = "WP Spacing 20, m"

Base Case Description:
RT_name = "Clay"
WF_name = "UOX-40"
WP_cap = 32
WP_spacing = 20 m
Drift_spacing = 70 m
r_{DW} = 2.25 m r_{CP2} = 3.25 m
t_{store} = 50·yr t_{vent} = 100·yr

Temperature (°C)

Time out of Reactor (yr)

──── Waste Package Surface Temperature
······ EBS3 Temperature
– – – EBS2 Temperature
–·–·– EBS1 Temperature
──── Drift Wall Temperature
------- Compliance point 2 Temperature

Contributions to the Wall Temperature

Parameter Study: Plot_case = 6
Parameter_vector$_{Plot\_case}$ = "WP Spacing 20, m"

Temperature (°C)

Time out of Reactor (yr)

──── Rock Wall Temperature (total)
······ Adjacent Waste Packages
– – – Adjacent Drifts / Boreholes
–·–·– Central Line Source

$$T_{EBS}\left(r, t, Wall\_T, k_1, k_2, k_3, k_4\right) := Wall\_T \cdot K + \frac{Q_{L\_wp}\left(t, t_{store}, t_{operate}, WP\_cap\right)}{2 \cdot \pi \cdot r_{DW}} \cdot R_{continuous}\left(t, r, k_1, k_2, k_3, k_4\right)$$

$$Q_{L\_wp}\left(110 \cdot yr, t_{store}, t_{operate}, WP\_cap\right) = 255.7 \cdot \frac{W}{m}$$

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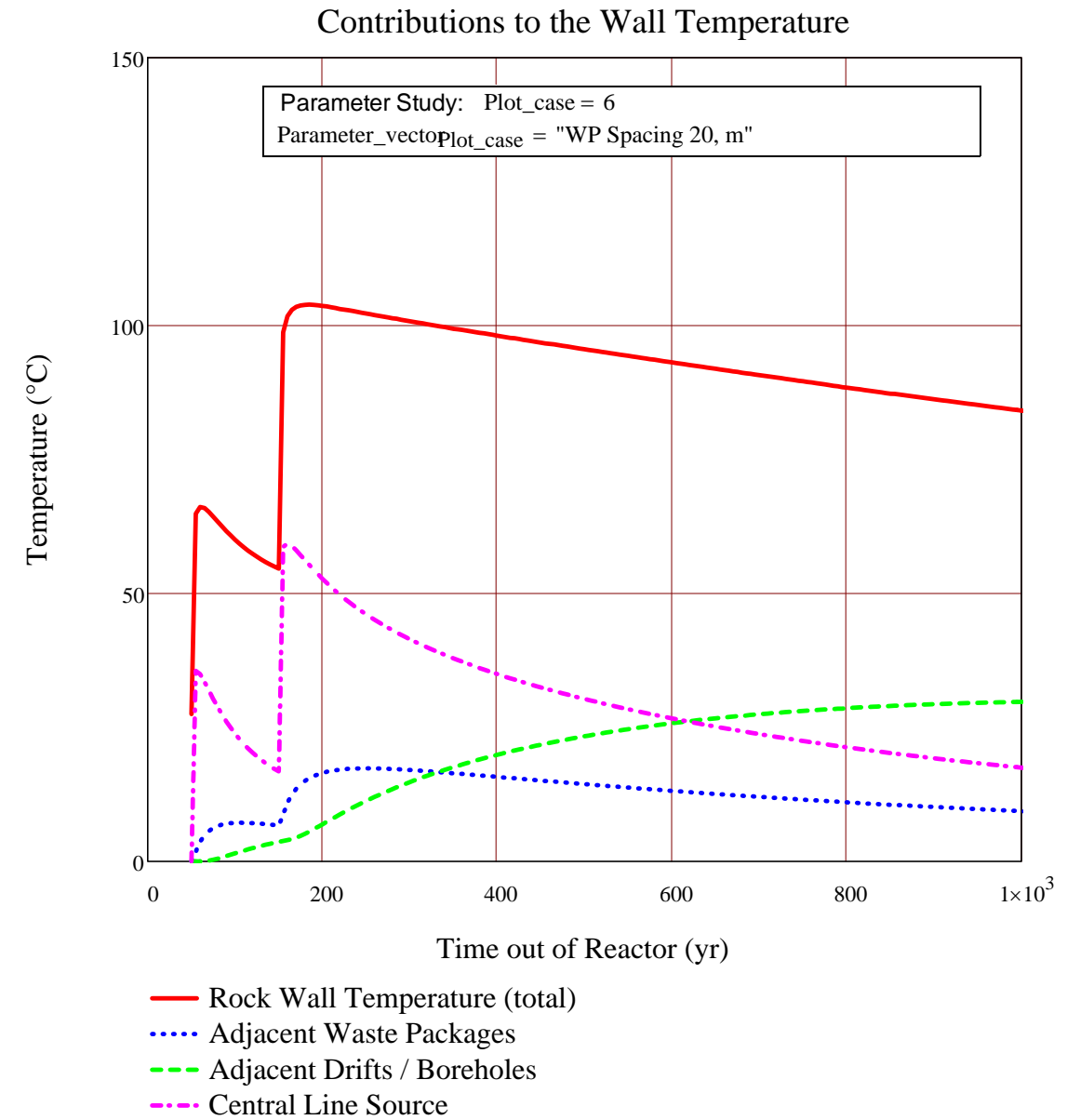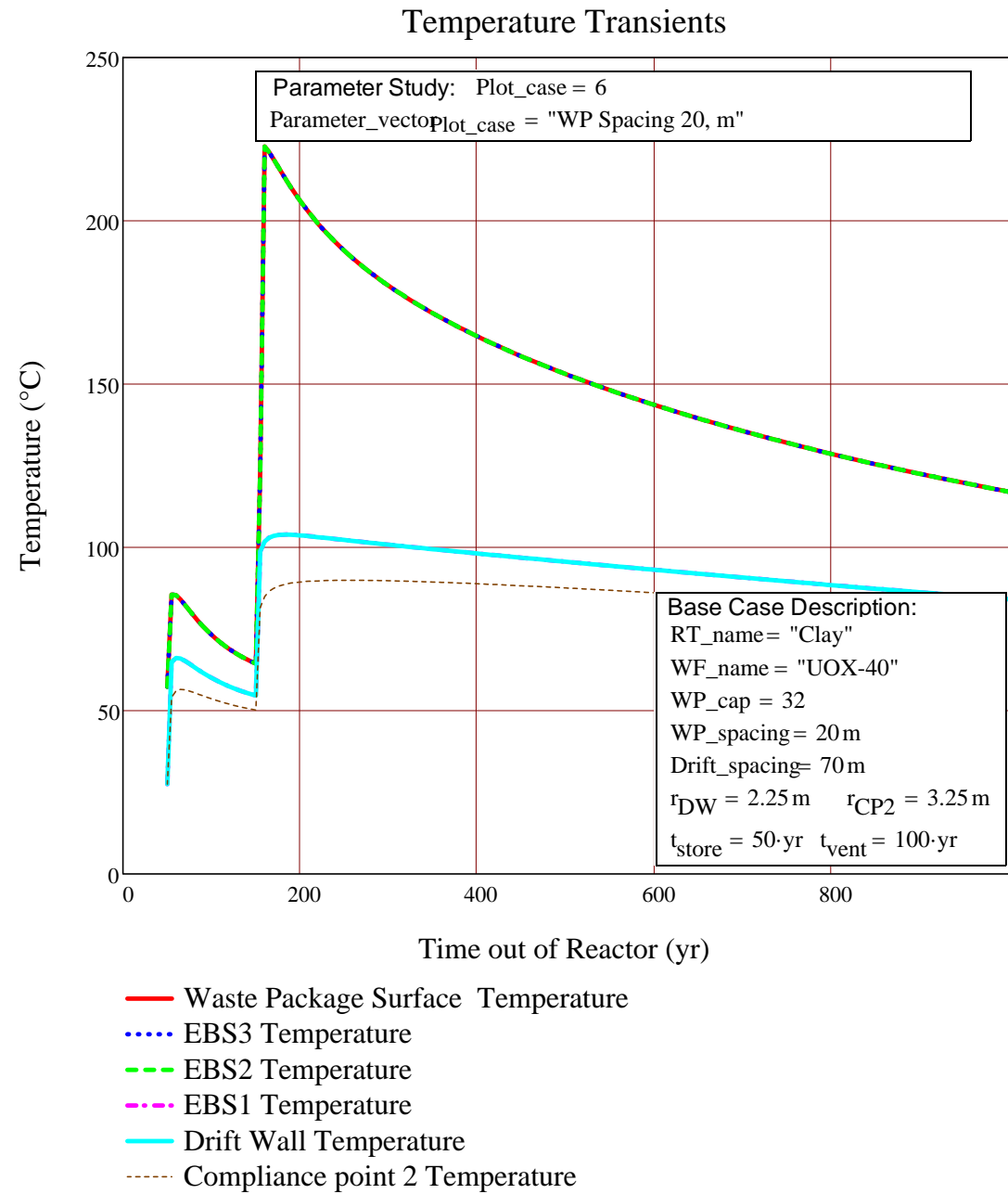
$\text{tt\_rw} := \left[(\text{Peak\_values})^{\langle \text{Plot\_case}\cdot 2\rangle}\right]_2 = 185$

$\text{Wall\_T\_at\_tt\_rw} := \left[(\text{Peak\_values})^{\langle \text{Plot\_case}\cdot 2 - 1\rangle}\right]_2 = 103.927$

$\text{WP\_T\_at\_tt\_wp} := \left[(\text{Peak\_values})^{\langle \text{Plot\_case}\cdot 2 - 1\rangle}\right]_6 = 222.753$

$\text{tt\_wp} := \left[(\text{Peak\_values})^{\langle \text{Plot\_case}\cdot 2\rangle}\right]_6 = 160$

$\text{Wall\_T\_at\_tt\_wp} := \left[(\text{Temp\_array}_{\text{Plot\_case}})^{\langle 6\rangle}\right]_{\frac{\left(\text{tt\_wp} - \frac{t_{\text{store}}}{yr}\right)}{\text{Step}}} = 98.739$

$\text{WP\_T\_at\_tt\_rw} := \left[(\text{Temp\_array}_{\text{Plot\_case}})^{\langle 10\rangle}\right]_{\frac{\left(\text{tt\_rw} - \frac{t_{\text{store}}}{yr}\right)}{\text{Step}}} = 214.369$

Temperature Gradient in the EBS

Parameter Study: Plot_case = 6
Parameter_vector$_{\text{Plot\_case}}$ = "WP Spacing 20, m"

Base Case Description:
RT_name = "Clay"
WP_spacing = 20 m
Drift_spacing = 70 m
WP_cap = 32
t_{store} = 50·yr

Rock wall ------>

<-- Waste Package Surface

Temperature (°C)

Radial Location in the EBS (m)

—— Gradient at the time of the Waste Package Peak T
····· Gradient at the time of the Rock Wall Peak T

OVERRIDE COUNTER AND STEP SIZE TO GET FINER CONVERGENCE ON THE ANSWER

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$t_{vent} = 100 \cdot yr$ OPTIONALLY OVERRIDE VENTILATION TIME TO SHORTEN ITERATION CONVERGENCE

ITERATE_OK := "No" $t_{convergence} = 1 \cdot yr$

$t_{required\_storage}(t_{operate}, T_{criteria}, t_{convergence}) :=$

$\quad time_{OK} \leftarrow t_{operate} - t_{convergence}$

$\quad Peak\_Wall\_T_{check} \leftarrow (Peak\_Wall\_T + 273.15) \cdot K$

$\quad time_{OK} \leftarrow t_{operate} \quad if \ Peak\_Wall\_T_{check} \leq T_{criteria}$

$\quad while \ Peak\_Wall\_T_{check} > T_{criteria}$

$\qquad time_{OK} \leftarrow time_{OK} + t_{convergence}$

$\qquad calc_{array} \leftarrow outdata(r_{DW}, r_{CP2}, t_{store}, time_{OK}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha, k_1, k_2, k_3, k_4)$

$\qquad Peak\_Wall\_T_{check} \leftarrow \left(max\left(calc_{array}^{\langle 6 \rangle} \right) + 273.15 \right) \cdot K$

$\quad return \begin{pmatrix} \dfrac{time_{OK}}{yr} \\ \dfrac{Peak\_Wall\_T_{check} - 273.15K}{K} \\ outdata(r_{DW}, r_{CP2}, t_{store}, time_{OK}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha, k_1, k_2, k_3, k_4) \end{pmatrix}$

$Final\_array := \begin{vmatrix} t_{required\_storage}(t_{operate}, T_{criteria}, t_{convergence}) & if \ ITERATE\_OK = "YES" \\ "No\ Iteration\ Performed" & otherwise \end{vmatrix}$

$t_{operate\_required} := Final\_array_1 \ yr \ = \blacksquare \cdot yr$

$t_{vent\_required} := t_{operate\_required} - t_{store} = \blacksquare \cdot yr$ <mark>REQUIRED VENTILATION TIME NEEDED TO MEET $T_{criteria} = 100 \cdot °C$</mark>

$Peak\_Wall\_T_{check} := (Final\_array_2 + 273.15) \cdot K = \blacksquare \cdot °C$

$\text{Result} := \text{stack}\left(\text{Title\_array}_1, \text{Final\_array}_3\right)$ ==NOTE THAT THIS SECTION WILL BE BLANK IF NO ITERATIVE ANALYSIS IS PERFORMED (Iterate_OK = "No"==

$\text{Result} = \blacksquare$

$\text{Time\_array} := \left(\text{Final\_array}_3\right)^{\langle 1 \rangle}$

$\text{Peak\_Temp(n)} := \max\left[\left(\text{Final\_array}_3\right)^{\langle n \rangle}\right]$ $\text{Peak\_Temp(6)} = \blacksquare$

$\text{Peak\_t(n)} := \text{lookup}\left[\text{Peak\_Temp(n)}, \left(\text{Final\_array}_3\right)^{\langle n \rangle}, \text{Time\_array}\right]$ $\text{Peak\_t(6)}_1 \cdot \text{yr} = \blacksquare \cdot \text{yr}$

$\text{nn} := 5 \,.. \, 10$ $\text{Peak\_results}_{nn-4, 1} := \text{Peak\_Temp(nn)}$ $\text{Peak\_results}_{nn-4, 2} := \text{Peak\_t(nn)}_1$

CP2	, time of peak
Peak Wall T,	time of peak
Peak EBS 1,	time of peak
Peak EBS 2,	time of peak
Peak EBS 3,	time of peak
Waste Pkg T,	time of peak

$\text{Peak\_results} = \blacksquare$

$\text{Array\_row\_at\_Wall\_T\_peak} := \text{match}\left[\text{Peak\_Temp(6)}, \left(\text{Final\_array}_3\right)^{\langle 6 \rangle}\right]_1 = \blacksquare$

$\text{CP2\_at\_Wall\_T\_pk\_t} := \left[\left(\text{Final\_array}_3\right)^{\langle 5 \rangle}\right]_{\text{Array\_row\_at\_Wall\_T\_peak}} = \blacksquare$

$\text{Ceintral\_WP\_delta} := \left[\left(\text{Final\_array}_3\right)^{\langle 2 \rangle}\right]_{\text{Array\_row\_at\_Wall\_T\_peak}} = \blacksquare$

$\text{Adj\_Drift\_delta} := \left[\left(\text{Final\_array}_3\right)^{\langle 3 \rangle}\right]_{\text{Array\_row\_at\_Wall\_T\_peak}} = \blacksquare$

$$\text{Adj\_WP\_delta} := \left[\left(\text{Final\_array}_3 \right)^{\langle 4 \rangle} \right]_{\text{Array\_row\_at\_Wall\_T\_peak}} = \blacksquare$$

$$\text{Result\_Vector} := \left(\frac{\text{WP\_spacing}}{\text{m}} \quad \text{TC} \quad \frac{\text{Drift\_spacing}}{\text{m}} \quad \text{Peak\_results}_{6,1} \quad \text{Peak\_results}_{6,2} \quad \text{Peak\_results}_{2,1} \quad \text{Peak\_results}_{2,2} \quad \text{CP2\_at\_Wall\_T\_pk\_t} \quad \frac{t_{\text{vent\_required}}}{\text{yr}} \quad \text{Ceintral\_WP\_delta} \quad \text{Adj\_Drift\_delta} \quad \text{Adj\_WP\_delta} \right)$$

$$\text{Result\_headings} := \left(\text{"WP Spacing"} \quad \text{"Temp Criteria"} \quad \text{"Drift Spacing"} \quad \text{"Peak WP T"} \quad \text{"Time of WP Peak"} \quad \text{"Peak Wall T"} \quad \text{"Time of Wall Peak"} \quad \text{"Peak CP2 T"} \quad \text{"Ventilation time"} \quad \text{"Central WP delta"} \quad \text{"Adj Drift delta"} \quad \text{"Adj WP delta"} \right)$$

$$\text{Result\_Vector} = \blacksquare$$ This is the result vector for transcription to the Excel case results tracking file

$$\text{RV} := \text{augment}\left(\text{Result\_headings}^{\text{T}}, \text{Result\_Vector}^{\text{T}} \right) \qquad T_{\text{ambient}} = 27.5 \cdot °\text{C}$$ Contribution percentages at time of peak wall temperature

$$\text{Percent\_central\_WP\_delta} := \frac{\text{Ceintral\_WP\_delta}}{\text{Peak\_Temp}(6) - \dfrac{\left(T_{\text{ambient}} - 273.15 \cdot \text{K} \right)}{\text{K}}} \cdot 100 = \blacksquare$$

$$\text{Percent\_adj\_Drift\_delta} := \frac{\text{Adj\_Drift\_delta}}{\text{Peak\_Temp}(6) - \dfrac{\left(T_{\text{ambient}} - 273.15 \cdot \text{K} \right)}{\text{K}}} \cdot 100 = \blacksquare$$

$$\text{RV} = \blacksquare$$

$$\text{Percent\_adj\_WP\_delta} := \frac{\text{Adj\_WP\_delta}}{\text{Peak\_Temp}(6) - \dfrac{\left(T_{\text{ambient}} - 273.15 \cdot \text{K} \right)}{\text{K}}} \cdot 100 = \blacksquare$$

$$\text{Percent\_central\_WP\_delta} + \text{Percent\_adj\_WP\_delta} + \text{Percent\_adj\_Drift\_delta} = \blacksquare$$

Plot temperature results as a function of parameter data

$ip := 1 .. Cases$

$Peak\_WP\_T_{ip} := \left(Peak\_values^{\langle ip \cdot 2 - 1 \rangle}\right)_6$ $Peak\_EBS3\_T_{ip} := \left(Peak\_values^{\langle ip \cdot 2 - 1 \rangle}\right)_5$ $Peak\_EBS2\_T_{ip} := \left(Peak\_values^{\langle ip \cdot 2 - 1 \rangle}\right)_4$ $Peak\_EBS1\_T_{ip} := \left(Peak\_values^{\langle ip \cdot 2 - 1 \rangle}\right)_3$

$$Peak\_WP\_T = \begin{pmatrix} 231.735 \\ 229.391 \\ 227.373 \\ 225.623 \\ 224.095 \\ 222.753 \\ 221.567 \\ 220.514 \\ 219.576 \\ 218.736 \end{pmatrix}$$

$$Peak\_EBS3\_T = \begin{pmatrix} 231.735 \\ 229.391 \\ 227.373 \\ 225.623 \\ 224.095 \\ 222.753 \\ 221.567 \\ 220.514 \\ 219.576 \\ 218.736 \end{pmatrix}$$

$$Peak\_EBS2\_T = \begin{pmatrix} 231.735 \\ 229.391 \\ 227.373 \\ 225.623 \\ 224.095 \\ 222.753 \\ 221.567 \\ 220.514 \\ 219.576 \\ 218.736 \end{pmatrix}$$

$$Peak\_EBS1\_T = \begin{pmatrix} 115.285 \\ 112.311 \\ 109.759 \\ 107.561 \\ 105.628 \\ 103.952 \\ 102.417 \\ 101.09 \\ 99.939 \\ 98.907 \end{pmatrix}$$

$Peak\_Wall\_T_{ip} := \left(Peak\_values^{\langle ip \cdot 2 - 1 \rangle}\right)_2$ $Peak\_CP2\_T_{ip} := \left(Peak\_values^{\langle ip \cdot 2 - 1 \rangle}\right)_1$

$$Peak\_Wall\_T = \begin{pmatrix} 115.262 \\ 112.287 \\ 109.734 \\ 107.536 \\ 105.602 \\ 103.927 \\ 102.391 \\ 101.064 \\ 99.912 \\ 98.88 \end{pmatrix}$$

$$Peak\_CP2\_T = \begin{pmatrix} 102.266 \\ 99.137 \\ 96.413 \\ 93.988 \\ 91.828 \\ 89.914 \\ 88.231 \\ 86.66 \\ 85.276 \\ 84.019 \end{pmatrix}$$

$$Parameter\_data = \begin{pmatrix} 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \\ 21 \\ 22 \\ 23 \\ 24 \end{pmatrix}$$

$$Parameter\_vector = \begin{pmatrix} \text{"WP Spacing 15, m"} \\ \text{"WP Spacing 16, m"} \\ \text{"WP Spacing 17, m"} \\ \text{"WP Spacing 18, m"} \\ \text{"WP Spacing 19, m"} \\ \text{"WP Spacing 20, m"} \\ \text{"WP Spacing 21, m"} \\ \text{"WP Spacing 22, m"} \\ \text{"WP Spacing 23, m"} \\ \text{"WP Spacing 24, m"} \end{pmatrix}$$

Peak Temperatures versus Parameter Study Data

Parameter Study
Parameter = "WP Spacing"
Parameter_units= "m"

Base Case Description:
$RT\_name=$ "Clay"
$WF\_name=$ "UOX-40"
$WP\_cap = 32$
$WP\_spacing= 20\,m$
$Drift\_spacing= 70\,m$
$r_{DW} = 2.25\,m$
$t_{store} = 50 \cdot yr$

Legend:
— Waste Package Surface Temperaturee
---- EBS_3 Temperature
---- EBS_2 Temperature
---- EBS_1 Temperature
— Rock Wall Temperature
---- Compliance Point 2 Temperature
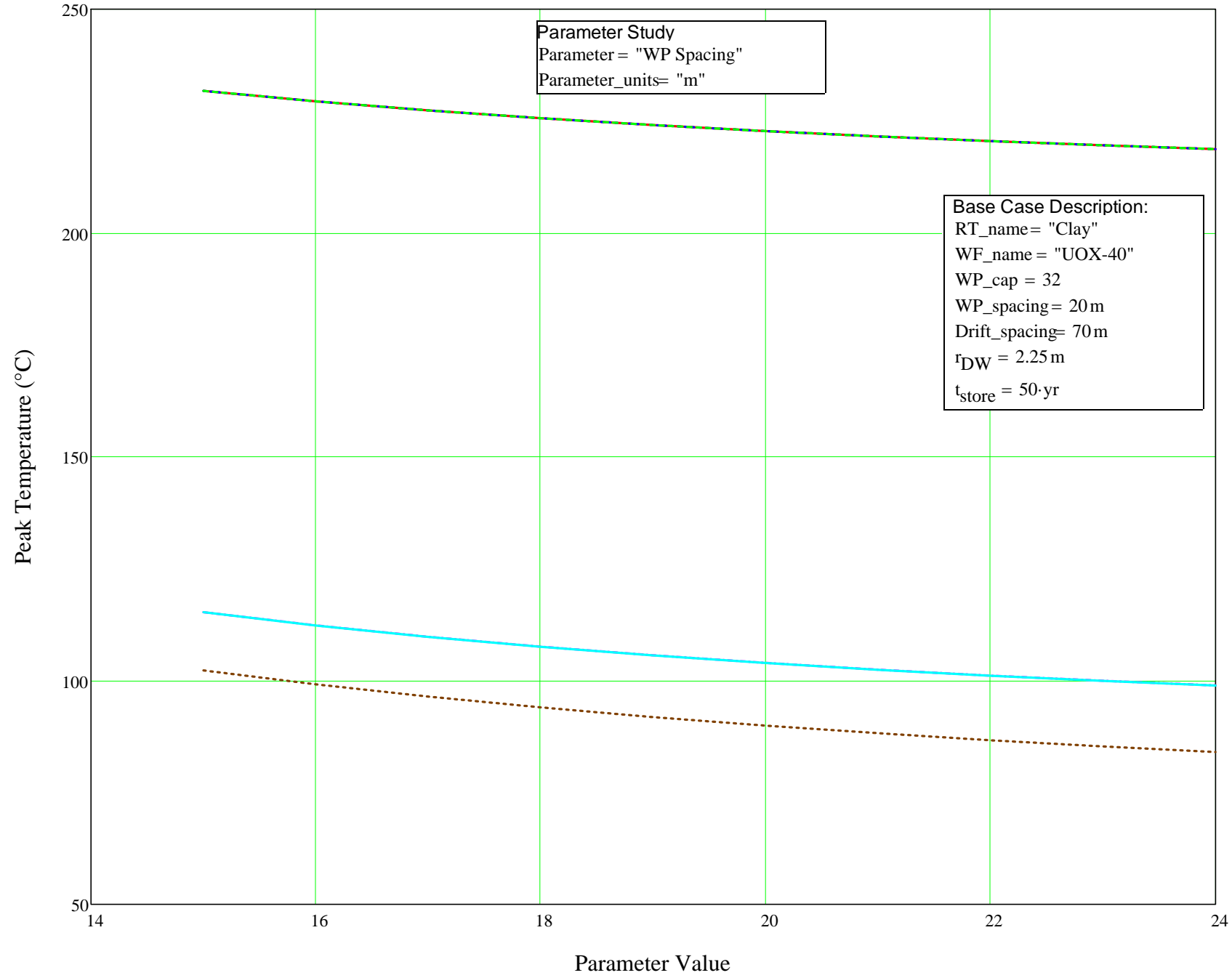
B.3 The Mathcad parametric analysis and iterative convergence model – iterative convergence example

As noted in Section B.2, the iterative convergence programming loop started on page 19 of 23 of the Mathcad document. However, to perform an iterative convergence analysis to determine required ventilation time, a number of input variables must be set. First, the "Parameter" variable passed from the DSEF Excel file must be set to "Single". Then the two critical variables of the iterative convergence study – the initial guess for required ventilation time (t_{vent}), and the target temperature criterion (TC) are set locally in the Mathcad document itself.

The next variable to be set turns the iterative loop on or keeps it off, and it is recommended to keep it initially off (Iterate_OK = "No") unless, based on previous analysis in the Case Library, you already have a reasonable guess for the required ventilation time. This is recommended since a single non-iterative analysis with the Mathcad thermal-analytical model should take around 15 to 30 seconds. If the initial guess is a poor one and if the step size is small and close convergence is being required, then the iterative mode could take a long time to run. Before setting Iterate_OK to "Yes", make sure the starting ventilation time results in a temperature that is above the temperature acceptance value. If you start with a ventilation time that already meets the acceptance criterion, then the convergence loop will just return the same starting ventilation time since it is already acceptable.

The example PDF file in this appendix set the temperature acceptance criterion at the drift wall of a clay/shale repository analysis at TC = 100°C. To speed up the iterative calculation process there are also three new input variables "Counter", "Step", and "Convergence" that allow initially larger and few calculation steps to quickly converge an analysis, and then optionally to make more smaller steps to cover the same time span but a more detailed transient if desired.

This specific example is from Greenberg 2013a, and is report case 225-19 (DSEF Case Library case number 342) and represents a required ventilation time calculation for a 21-PWR waste package with 40 GWd/MT burnup in a clay/shale repository, with a layout design of 30 m drift spacing and 20 m waste package spacing, to meet a temperature acceptance criterion of 100°C at the drift wall. The result presented originally was taken within 0.5 degrees and gave 100.1°C with 125 years of ventilation. To check more accurately and assure the temperature is below 100°C, the iterative convergence was turned on using Iterate_OK:="YES". In this case, we knew the answer, but just to demonstrate the convergence loop, we started the case off with a guess of t_{vent} = 120 years. The result showed that with 127 years of ventilation, we get a drift wall temperature of 99.93°C (shown on page 19 of 23 in the PDF printout).

Note that the last figure on page 23 of 23 is blank, since it is reserved to show parametric study results and this was a "Single" analysis.

DSEF R3.0 parametric and iterative model with collapsed areas - for rapid iteration.

Values over-written from DSEF Excel file to create case include: Drift_spacing, TC and t_{vent}.

Allow output transients to be written back to DSEF FILE

Case_name := "500-1"

Variables for repository symmetry and extent:

Write_OK := "YES"

N_{drifts} := 4 N_{adj} := 4

REQUIRED REPOSITORY INPUT DATA (from DSEF):

file := "DSEF R3.0_2013Aug12_HRG-Clay_UOX-40_Iterative convergence example_Case-225-19.xlsm"

sheet := "Thermal-Analytical!"   DATA FOR ITERATION ON TEMPERATURE ACCEPTACE CRITERIAA:

READ DSEF INPUT FILE

TC := 100 $T_{criteria}$:= (TC + 273.15)·K = 373.15 K $T_{criteria}$ = 100·°C

Input 1 = Operating Mode (enclosed or open)

$t_{convergence}$:= 1·yr   CONVERGE CRITERIA FOR REQUIRED VENTILATION TIME IN YEARS

Input_1 := READEXCEL(file, concat(sheet, "A5:B5"))

Input_1 = ("MODE = Open or Enclosed:" "Open")   Mode := $Input\_1_{1,2}$ = "Open"

SET THE VARIABLE ITERATE_OK TO "NO" TO TURN OFF THE AUTOMATIC CONVERGENCE CALCULATION, AND MANUALLY RESET IT TO "YES" IF YOU WANT TO FINE TUNE YOUR ANSWER:

Input_2 := READEXCEL(file, concat(sheet, "A7:B16")) **Input 2 = Case Definitions**

ITERATE_OK := "YES""

Input 3 = Ventilation Parameters (for Open Modes)

Input_3 := READEXCEL(file, concat(sheet, "e7:f11"))

$$Input\_2 = \begin{pmatrix} \text{"Host Media"} & \text{"Clay"} \\ \text{"Rock thermal conductivity, W/m-K"} & 1.75 \\ \text{"Rock thermal diffusivity, m2/sec"} & 6.45 \times 10^{-7} \\ \text{"Repository Depth, m"} & 500 \\ \text{"Surface temperature, °C"} & 15 \\ \text{"Geothermal gradient, °C/km"} & 25 \\ \text{"Ambient temperature at depth, °C"} & 27.5 \\ \text{"Waste Package (axial) spacing, m"} & 20 \\ \text{"Drift / Borehole (lateral) spacing, m"} & 30 \\ \text{"Surface storage time, y"} & 50 \end{pmatrix}$$

$$Input\_3 = \begin{pmatrix} \text{"Ventilation Duration, yr"} & 125 \\ \text{"Unventilated Closure Duration (Backfill Installation), yr"} & 10 \\ \text{"Ventilation Thermal Efficiency, %"} & 0.75 \\ \text{"Rock Wall Emissivity"} & 0.9 \\ \text{"Waste Package Emissivity"} & 0.6 \end{pmatrix}$$

RT_name := $Input\_2_{1,2}$ = "Clay"

t_{vent} := if$\left[(Mode = \text{"Enclosed"}), 0, Input\_3_{1,2}\right]$·yr = 125·yr

Kth := $Input\_2_{2,2} \cdot \dfrac{W}{m \cdot K} = 1.75 \dfrac{m \cdot kg}{K \cdot s^3}$

$t_{backfill}$:= if$\left[(Mode = \text{"Enclosed"}), 0, Input\_3_{2,2}\right]$·yr = 10·yr

V_{eff} := if$\left[(Mode = \text{"Enclosed"}), 0, Input\_3_{3,2}\right]$ = 0.75

α := $Input\_2_{3,2} \cdot \dfrac{m^2}{s} = 6.45 \times 10^{-7} \dfrac{m^2}{s}$

ε_{wall} := if$\left[(Mode = \text{"Enclosed"}), .9, Input\_3_{4,2}\right]$ = 0.9

$\text{WP\_depth} := \text{Input\_2}_{4,2} \cdot m = 500\,m$

$\varepsilon_{WP} := \text{if}\left[(\text{Mode} = \text{"Enclosed"}), .6, \text{Input\_3}_{5,2}\right] = 0.6$

$T_{surface} := \left(\text{Input\_2}_{5,2} + 273.15\right) \cdot K = 288.15\,K$

$\text{geothermal\_gradient} := \text{Input\_2}_{6,2} \dfrac{K}{km} = 0.025 \dfrac{K}{m}$

OVER-RIDE VENTILATION DURATION

$t_{vent} := 120 \cdot yr$

$T_{ambient} := \left(\text{Input\_2}_{7,2} + 273.15\right) \cdot K = 300.65\,K$

$\text{WP\_spacing} := \text{Input\_2}_{8,2} \cdot m = 20\,m$

OVER-RIDE DRIFT AND/OR WASTE PACKAGE SPACING

$\text{Drift\_spacing} := \text{Input\_2}_{9,2} \cdot m = 30\,m$

$t_{store} := \text{Input\_2}_{10,2} \cdot yr = 50 \cdot yr$

$t_{operate} := \left(t_{store} + t_{vent}\right) = 170 \cdot yr$ T_OPERATE = T_STORE + T_VENTILATE

$t_{closure} := t_{operate} + t_{backfill} = 180 \cdot yr$ TCLOSURE = TOPERATE + TIME TO BACKFILL

Input 4 = ENGINEERED BARRIER SYSTEM DATA:

$\text{Input\_4} := \text{READEXCEL}(\text{file}, \text{concat}(\text{sheet}, \text{"A20:F27"}))$

Input 5 = COMPLIANCE POINT 2 INPUT DATA

$\text{Input\_5} := \text{READEXCEL}(\text{file}, \text{concat}(\text{sheet}, \text{"C32"}))$

$$\text{Input\_4} = \begin{pmatrix} \text{"Waste Form Outer Radius, m"} & 0.535 & \text{"N/A"} & 0.535 & \text{"UOX-40"} & \text{"N/A"} \\ \text{"Canister"} & 0 & 0.535 & 0.535 & \text{"None"} & \text{"N/A"} \\ \text{"Waste Package"} & 0.11 & 0.535 & 0.645 & \text{"Carbon Steel"} & \text{"N/A"} \\ \text{"Buffer"} & 0 & 0.645 & 0.645 & \text{"None"} & \text{"N/A"} \\ \text{"Envelope"} & 0 & 0.645 & 0.645 & \text{"None"} & \text{"N/A"} \\ \text{"Backfill"} & 1.58 & 0.645 & 2.225 & \text{"70\% Bentonite 30\% Sand"} & 1.2 \\ \text{"Liner"} & 0.025 & 2.225 & 2.25 & \text{"Steel"} & 46 \\ \text{"Host Rock Inner Radius, m ----$>$"} & \text{NaN} & 2.25 & \text{NaN} & \text{NaN} & \text{NaN} \end{pmatrix}$$

$\text{Input\_5} = (5.25)$

$r_{CP2} := \text{Input\_5}_1 \cdot m = 5.25\,m$

$r_{DW} := \text{Input\_4}_{8,3} \cdot m = 2.25\,m$

$r_{WP} := \text{Input\_4}_{3,4} \cdot m = 0.645\,m$

$\text{EBS\_name}_1 := \text{Input\_4}_{7,1} = \text{"Liner"}$

$\text{EBS\_material}_1 := \text{Input\_4}_{7,5} = \text{"Steel"}$

$\text{thickness}_1 := \text{Input\_4}_{7,2} \cdot m = 0.025\,m$

$r_1 := \text{Input\_4}_{7,4} \cdot m = 2.25\,m$

$k1 := \text{Input\_4}_{7,6} = 46$

$k_1 := \text{if}\left[(k1 = \text{"N/A"}), 0, k1\right] \cdot \dfrac{W}{m \cdot K} = 46 \cdot \dfrac{W}{m \cdot K}$

$EBS\_name_2 := Input\_46_{,1} = \text{"Backfill"}$ $\qquad$ $EBS\_material_2 := Input\_46_{,5} = \text{"70\% Bentonite 30\% Sand"}$

$thickness_2 := Input\_46_{,2} \cdot m = 1.58\,m$ $\qquad$ $r_2 := Input\_46_{,4} \cdot m = 2.225\,m$

$k2 := Input\_46_{,6} = 1.2$

$\qquad k_2 := if\,[(k2 = \text{"N/A"}),0,k2] \cdot \dfrac{W}{m \cdot K} = 1.2 \cdot \dfrac{W}{m \cdot K}$

$\qquad\qquad k_{radiation} := if\left[(Mode = \text{"Enclosed"}),k_2,0\right] = 0 \cdot \dfrac{W}{m \cdot K}$

$EBS\_name_3 := Input\_45_{,1} = \text{"Envelope"}$ $\qquad$ $EBS\_material_3 := Input\_45_{,5} = \text{"None"}$

$thickness_3 := Input\_45_{,2} \cdot m = 0\,m$ $\qquad$ $r_3 := Input\_45_{,4} \cdot m = 0.645\,m$

$k3 := Input\_45_{,6} = \text{"N/A"}$

$\qquad k_3 := if\,[(k3 = \text{"N/A"}),0,k3] \cdot \dfrac{W}{m \cdot K} = 0 \cdot \dfrac{W}{m \cdot K}$

$EBS\_name_4 := Input\_44_{,1} = \text{"Buffer"}$ $\qquad$ $EBS\_material_4 := Input\_44_{,5} = \text{"None"}$

$thickness_4 := Input\_44_{,2} \cdot m = 0\,m$ $\qquad$ $r_4 := Input\_44_{,4} \cdot m = 0.645\,m$

$k4 := Input\_44_{,6} = \text{"N/A"}$

$\qquad k_4 := if\,[(k4 = \text{"N/A"}),0,k4] \cdot \dfrac{W}{m \cdot K} = 0 \cdot \dfrac{W}{m \cdot K}$

Define the total thermal resistance between the rock wall and the waste package surface based on a heat flux per unit area, it is then applied to a heat flux is per unit length adjusting to area per unit length and q_L (W/m):

$r_{WP} = 0.645\,m$ $\qquad$ $r_4 = 0.645\,m$ $\qquad$ $r_3 = 0.645\,m$ $\qquad$ $r_2 = 2.225\,m$ $\qquad$ $r_1 = 2.25\,m$ $\qquad$ $r_{DW} = 2.25\,m$

$R_1(k_1) := if\left[\left[thickness_1 = 0 \lor (k1 = \text{"N/A"})\right],0,\dfrac{r_{DW}}{k_1} \cdot ln\left(\dfrac{r_1}{r_2}\right)\right]$ $\qquad$ $R_1(k_1) = 5.465 \times 10^{-4} \cdot \dfrac{m^2 \cdot K}{W}$ $\qquad$ Thermal resistance

$EBS\_name_1 = \text{"Liner"}$ $\qquad$ $EBS\_material_1 = \text{"Steel"}$

ADDED CORRECTION FOR PARAMETRIC $t_{closure}$ replaced $t_{closure}$ with $(t_{operate} + t_{backfill})$ $\qquad$ Revised R_2 to make it an explicit function of $t_{operate}$ and $t_{backfill}$.

$R_2(k_2,t,t_{operate},t_{backfill}) := \left| \begin{array}{l} kk \leftarrow k_{radiation} \cdot \left[t < (t_{operate} + t_{backfill})\right] + k_2 \cdot \left[t \geq (t_{operate} + t_{backfill})\right] \\[2mm] return\ \ if\left[\left[(thickness_2 = 0) \lor (kk = 0)\right],0,\dfrac{r_{DW}}{kk} \cdot ln\left(\dfrac{r_2}{r_3}\right)\right] \end{array} \right.$ $\qquad$ $\dfrac{r_{DW}}{k_2} \cdot ln\left(\dfrac{r_2}{r_3}\right) = 2.322 \cdot \dfrac{m^2 \cdot K}{W}$

Mathcad Component of DSEF 3.0 $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ Page 3 of 23

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Mathcad DSEF 3.0 parametric and iterative model - example for User's Manual.xmcd

$\text{EBS\_name}_2 = \text{"Backfill"} \qquad \text{EBS\_material}_2 = \text{"70\% Bentonite 30\% Sand"}$

$$R_2\left(k_2, 5 \cdot yr, 300 \cdot yr, 10 \cdot yr\right) = 0 \cdot \frac{m^2 \cdot K}{W} \qquad R_2\left(k_2, 1000 \cdot yr, 300 \cdot yr, 10 \cdot yr\right) = 2.321741 \cdot \frac{m^2 \cdot K}{W}$$

$$R_3\left(k_3\right) := \text{if}\left[\left[\text{thickness}_3 = 0 \vee (k3 = \text{"N/A"})\right], 0, \frac{r_{DW}}{k_3} \cdot \ln\left(\frac{r_3}{r_4}\right)\right] \qquad R_3\left(k_3\right) = 0 \cdot \frac{m^2 \cdot K}{W}$$

$\text{EBS\_name}_3 = \text{"Envelope"} \qquad \text{EBS\_material}_3 = \text{"None"}$

$$R_4\left(k_4\right) := \text{if}\left[\left[\text{thickness}_4 = 0 \vee (k4 = \text{"N/A"})\right], 0, \frac{r_{DW}}{k_4} \cdot \ln\left(\frac{r_4}{r_{WP}}\right)\right] \qquad R_4\left(k_4\right) = 0 \cdot \frac{m^2 \cdot K}{W}$$

$\text{EBS\_name}_4 = \text{"Buffer"} \qquad \text{EBS\_material}_4 = \text{"None"}$

$$R_{Total}\left(t, k_1, k_2, k_3, k_4\right) := R_1\left(k_1\right) + R_2\left(k_2, t, t_{operate}, t_{backfill}\right) + R_3\left(k_3\right) + R_4\left(k_4\right) \qquad$$ <mark>Total thermal resistance between wall and waste package</mark>

$$t_{backfill} = 10 \cdot yr \qquad t_{operate} = 170 \cdot yr$$

$$R_{continuous}\left(t, r, k_1, k_2, k_3, k_4\right) := \left|
\begin{array}{l}
kk_2 \leftarrow k_{radiation} \cdot \left[t < \left(t_{operate} + t_{backfill}\right)\right] + k_2 \cdot \left[t \geq \left(t_{operate} + t_{backfill}\right)\right] \\[6pt]
R \leftarrow R_1\left(k_1\right) + R_2\left(k_2, t, t_{operate}, t_{backfill}\right) + R_3\left(k_3\right) + \text{if}\left[\left[\left(\text{thickness}_4 = 0\right) \vee (k4 = \text{"N/A"})\right], 0, \frac{r_{DW}}{k_4} \cdot \ln\left(\frac{r_4}{r}\right)\right] \quad \text{if } r \leq r_4 \wedge r \geq r_{WP} \\[6pt]
R \leftarrow R_1\left(k_1\right) + R_2\left(k_2, t, t_{operate}, t_{backfill}\right) + \text{if}\left[\left[\left(\text{thickness}_3 = 0\right) \vee (k3 = \text{"N/A"})\right], 0, \frac{r_{DW}}{k_3} \cdot \ln\left(\frac{r_3}{r}\right)\right] \quad \text{if } r \leq r_3 \wedge r > r_4 \\[6pt]
R \leftarrow R_1\left(k_1\right) + \text{if}\left[\left[\left(\text{thickness}_2 = 0\right) \vee kk_2 = 0\right], 0, \frac{r_{DW}}{kk_2} \cdot \ln\left(\frac{r_2}{r}\right)\right] \quad \text{if } r \leq r_2 \wedge r \geq r_3 \\[6pt]
R \leftarrow \text{if}\left[\left[\left(\text{thickness}_1 = 0\right) \vee (k1 = \text{"N/A"})\right], 0, \frac{r_{DW}}{k_1} \cdot \ln\left(\frac{r_1}{r}\right)\right] \quad \text{if } r \leq r_{DW} \wedge r \geq r_2 \\[6pt]
R \leftarrow \text{"Invalid Radius"} \quad \text{otherwise} \\[6pt]
\text{return } R
\end{array}
\right.$$

$$R_{continuous}\left(5 \cdot yr, r_{WP}, k_1, k_2, k_3, k_4\right) = 5.465 \times 10^{-4} \frac{K \cdot s^3}{kg} \qquad R_{continuous}\left(1000 \cdot yr, r_{WP}, k_1, k_2, k_3, k_4\right) = 2.322288 \frac{K \cdot s^3}{kg}$$

Mathcad Component of DSEF 3.0

Early Time - Thermal Resistance From Rock Wall to r

Thermal resistance prior to closure

$r_{DW} = 2.25\,m$

$r_1 = 2.25\,m$ $\qquad$ EBS_name$_1$ = "Liner" $\qquad$ EBS_material$_1$ = "Steel"

$r_2 = 2.225\,m$ <mark>Note that for "open modes", the backfill hasn't been emplaced at early time</mark>

$r_3 = 0.645\,m$ $\qquad$ EBS_name$_3$ = "Envelope" $\quad$ EBS_material$_3$ = "None"

$r_4 = 0.645\,m$ $\qquad$ EBS_name$_4$ = "Buffer" $\quad$ EBS_material$_4$ = "None"

$r_{WP} = 0.645\,m$

$$R_1\left(k_1\right) = 5.465\times 10^{-4}\cdot\frac{m^2\cdot K}{W} \qquad R_2\left(k_2,5\cdot yr,t_{operate},t_{backfill}\right) = 0\cdot\frac{m^2\cdot K}{W} \qquad R_3\left(k_3\right) = 0\cdot\frac{m^2\cdot K}{W} \qquad R_4\left(k_4\right) = 0\cdot\frac{m^2\cdot K}{W}$$

$$R_{Total}\left(50yr,k_1,k_2,k_3,k_4\right) = 5.465\times 10^{-4}\cdot\frac{m^2\cdot K}{W}$$

Late Time - Thermal Resistance From Rock Wall to r

Thermal resistance prior to closure

$r_{DW} = 2.25\,m$

$r_1 = 2.25\,m$ $\qquad$ EBS_name$_1$ = "Liner" $\qquad$ EBS_material$_1$ = "Steel"

$r_2 = 2.225\,m$ $\qquad$ EBS_name$_2$ = "Backfill" $\qquad$ EBS_material$_2$ = "70% Bentonite 30% Sand"

$r_3 = 0.645\,m$ $\qquad$ EBS_name$_3$ = "Envelope" $\qquad$ EBS_material$_3$ = "None"

$r_4 = 0.645\,m$ $\qquad$ EBS_name$_4$ = "Buffer" $\qquad$ EBS_material$_4$ = "None"

$r_{WP} = 0.645\,m$

$$R_1\left(k_1\right) = 5.465\times 10^{-4}\cdot\frac{m^2\cdot K}{W} \qquad R_2\left(k_2,t_{closure},t_{operate},t_{backfill}\right) = 2.322\cdot\frac{m^2\cdot K}{W} \qquad R_3\left(k_3\right) = 0\cdot\frac{m^2\cdot K}{W}$$

$$R_{Total}\left(1000yr,k_1,k_2,k_3,k_4\right) = 2.322\cdot\frac{m^2\cdot K}{W}$$

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<mark>INPUT 6 = WASTE FORM DATA</mark>

$\text{Input\_6} := \text{READEXCEL}(\text{file}, \text{concat}(\text{sheet}, "A35:B38"))$

$$\text{Input\_6} = \begin{pmatrix} \text{"Waste form short name"} & \text{"UOX-40"} \\ \text{"Waste form type"} & \text{"Assembly"} \\ \text{"Waste package capacity"} & 21 \\ \text{"Waste package length, m"} & 5 \end{pmatrix}$$

$\text{WF\_name} := \text{Input\_6}_{1,2} = \text{"UOX-40"}$

$\text{WF\_type} := \text{Input\_6}_{2,2} = \text{"Assembly"}$

$\text{WP\_cap} := \text{Input\_6}_{3,2} = 21$

Outside of the liner Outside of the backfill Outside of the envelope Outside of the buffer

$\text{WP\_length} := \text{Input\_6}_{4,2} \cdot \text{m} = 5\,\text{m}$ $A_1 := 2 \cdot \pi \cdot r_1 \cdot \text{WP\_length} = 70.69\,\text{m}^2$ $A_2 := 2 \cdot \pi \cdot r_2 \cdot \text{WP\_length} = 69.9\,\text{m}^2$ $A_3 := 2 \cdot \pi \cdot r_3 \cdot \text{WP\_length} = 20.26\,\text{m}^2$ $A_4 := 2 \cdot \pi \cdot r_4 \cdot \text{WP\_length} = 20.26\,\text{m}^2$

$A_{DW} := 2 \cdot \pi \cdot r_{DW} \cdot \text{WP\_length} = 70.686\,\text{m}^2$ $A_{WP} := 2 \cdot \pi \cdot r_{WP} \cdot \text{WP\_length} = 20.263\,\text{m}^2$

CONSIDER THE ALTERNATE DESIGN CASE OF AN "OPEN MODE" DESIGN, WITH A CEMENTITIOUS LINER, BUT ONLY AIR BETWEEN THE LINER AND THE WASTE PACKAGE FOR THE FIRST 300 YEARS. ASSUME NO VENTILATION FOR 300 YEARS, AND THEN BACKFILL AT CLOSURE.

CALCULATE THE EQUIVALENT THERMAL RESISTANCE OF THE AIR GAP USING A LINEARIZED RADIATION HEAT TRANSFER COEFFICIENT. BASE THE COEFFICIENT ON THE ROCK WALL TEMPERATURE AT THE DRIFT, AND THE EQUIVALENT WASTE PACKAGE TEMPERATURE NECESSARY TO MOVE THE HEAT GENERATED AT THE WASTE PACKAGE AT ANY GIVEN TIME. THE EQUATION FOR THE RADIATION HEAT TRANSFER COEFFICIENT IS FROM INCROPERA AND DEWITT.

$A_{wall} := \text{WP\_length} \cdot 2 \cdot \pi \cdot r_{DW} = 70.686\,\text{m}^2$

Stefan Boltzmann constant $\sigma := 5.670 \cdot 10^{-8} \cdot \dfrac{W}{m^2 \cdot K^4}$ The basis for the rock and waste package emissivity assumed is F. P. Incropera and D.P. DeWitt, *Fundamentals of Heat and Mass Transfer*, 4th Edition, 1996, Table A-11, which shows a range of 0.88 to 0.93 is adapted from hemispherical emissivity of rock at around 300 K. This range is corroborated by the "Heat Transmission" section of Perry's Chemical Engineers Handbook, 6th Edition, 1984 (Table 10-17, pages 10-51 to 10-52) for normal emissivity of rough silica and rough fused quartz, ranging from 0.8 to 0.93. The waste package surface is assumed to be covered with dust and dirt. The emissivity values to the left were specified in DSEF, and should be changed there if necessary.

<mark>Waste Package emissivity</mark> $\varepsilon_{WP} = 0.6$

<mark>Rock wall or cementitious liner emissivity</mark> $\varepsilon_{wall} = 0.9$

Reference for radiation heat transfer coefficient, h_{rad}, is from Incropera and DeWitt, Table 13.3 for concentric infinite cylinders (based on the inner surface as the heat source), and is also referenced in the YMP *Ventilation Model and Analysis Report*, ANL-EBS-MD-000030 REV 04, Oct. 2004, page 6-8.

$$h_{rad\_infinite}(r_i, r_o, \varepsilon_i, \varepsilon_o) := \dfrac{\sigma}{\dfrac{1}{\varepsilon_i} + \left(\dfrac{1 - \varepsilon_o}{\varepsilon_o}\right) \cdot \dfrac{r_i}{r_o}}$$ $h_{rad\_infinite}(r_{WP}, r_{DW}, \varepsilon_{WP}, \varepsilon_{wall}) = 3.338 \times 10^{-8} \cdot \dfrac{W}{m^2\,K^4}$ For radiation between the liner and the envelope (both metal surfaces) use r_2 and r_3, and assume the same emissivity for both surfaces.

Usage is Q in watts = $h \cdot A_i \cdot (T_i{}^4 - T_o{}^4)$

Mathcad DSEF 3.0 parametric and iterative model - example for User's Manual.xmcd

$$Q_{rad\_infinite}\left(r_i, r_o, \varepsilon_i, \varepsilon_o, L, T_{cold}, T_{hot}\right) := h_{rad\_infinite}\left(r_i, r_o, \varepsilon_i, \varepsilon_o\right) \cdot \left(2 \cdot \pi \cdot r_i \cdot L\right)\left(T_{hot}^4 - T_{cold}^4\right)$$

$$Q_{rad\_infinite}\left(r_3, r_2, \varepsilon_{WP}, \varepsilon_{wall}, WP\_length, 300 \cdot K, 600 \cdot K\right) = 8.217 \times 10^4 \, W$$

$$Q_{L\_rad\_infinite}\left(r_i, r_o, \varepsilon_i, \varepsilon_o, T_{cold}, T_{hot}\right) := h_{rad\_infinite}\left(r_i, r_o, \varepsilon_i, \varepsilon_o\right) \cdot \left(2 \cdot \pi \cdot r_i\right)\left(T_{hot}^4 - T_{cold}^4\right)$$

$$Q_{L\_rad\_infinite}\left(r_3, r_2, \varepsilon_{WP}, \varepsilon_{wall}, 300 \cdot K, 600 \cdot K\right) = 1.643 \times 10^4 \cdot \frac{W}{m}$$

Heat transfer by radiation from NIRAS/ONDRAF December 2005 Report: Eef Weetjens and Xavier Sillen; *Thermal analysis of the Supercontainer concept 2D axisymmetric heat transport calculations,* Section 6.4.3. Pg 34, equation 29.

$$Q_{L\_infinite}\left(r_i, r_o, \varepsilon_i, \varepsilon_o, T_{cold}, T_{hot}\right) := \frac{2\pi\sigma \cdot \left(T_{hot}^4 - T_{cold}^4\right)}{\dfrac{1-\varepsilon_i}{\varepsilon_i \cdot r_i} + \dfrac{1}{r_i} + \dfrac{1-\varepsilon_o}{\varepsilon_o \cdot r_o}}$$

$$Q_{L\_infinite}\left(r_3, r_2, \varepsilon_{WP}, \varepsilon_{wall}, 300 \cdot K, 600 \cdot K\right) = 1.643 \times 10^4 \cdot \frac{W}{m}$$

This is the same as the Incropera and DeWitt result, $Q_{L\_rad\_infinite}$

Comparision of thermal radiation across a gap to conduction after the gap has been filled with backfill material.

$$Q_{L\_conduction\_comparison}\left(r_i, r_o, T_{cold}, T_{hot}\right) := \frac{2 \cdot \pi \cdot r_o}{\dfrac{r_{DW}}{k_2} \cdot \ln\left(\dfrac{r_o}{r_i}\right)} \cdot \left(T_{hot} - T_{cold}\right)$$

$$Q_{L\_conduction\_comparison}\left(r_3, r_2, 300 \cdot K, 600 \cdot K\right) = 1.806 \times 10^3 \cdot \frac{W}{m}$$

$$Q_{ratio}\left(r_i, r_o, \varepsilon_i, \varepsilon_o, T_{cold}, T_{hot}\right) := \frac{Q_{L\_infinite}\left(r_i, r_o, \varepsilon_i, \varepsilon_o, T_{cold}, T_{hot}\right)}{Q_{L\_conduction\_comparison}\left(r_i, r_o, T_{cold}, T_{hot}\right)}$$

$$Q_{ratio}\left(r_3, r_2, \varepsilon_{WP}, \varepsilon_{wall}, 300 \cdot K, 600 \cdot K\right) = 9.097$$

INPUT 7 = PARAMETRIC STUDY VARIABLE INPUT DATA

$\text{Input\_7} := \text{READEXCEL}(\text{file}, \text{concat}(\text{sheet}, \text{"F29:F41"}))$

$\text{Cases} := \text{Input\_7}_1 = 1$

$\text{Parameter} := \text{Input\_7}_2 = \text{"Single"}$

$\text{Parameter\_units} := \text{Input\_7}_3 = \text{"None"}$

	0
0	1
1	"Single"
2	"None"
3	""
4	""
5	""
6	""
7	""
8	""
9	""
10	""
11	""
12	""

$\text{Input\_7} =$

$ij := 1 .. \text{Cases}$

$\text{Parameter\_data}_{ij} := \text{Input\_7}_{ij+3}$

$\text{Parameter\_data} = (\text{""})$

$$\text{Parameter\_description}_{ij} := \begin{vmatrix} \text{"Single Base Case"} & \text{if } \text{Cases} = 1 \\ \text{concat}\left[\text{num2str}\left[\text{Input\_7}_{(ij+3)}\right], \text{", "}, \text{Input\_7}_3\right] & \text{otherwise} \end{vmatrix}$$

$\text{Parameter\_description} = (\text{"Single Base Case"})$

INPUT 8 = DECAY HEAT INPUT DATA PER UNIT SOURCE (ASSEMBLY OR CANISTER):

$\text{Input\_8\_size} := \text{READEXCEL}(\text{file}, \text{concat}(\text{sheet}, \text{"C43"}))$ $\quad$ $\text{Input\_8\_size}_1 = 58$ $\quad$ $\text{Decay\_heat\_range} := \text{concat}\left[\text{"A43:B"}, \text{num2str}\left(\left(\text{Input\_8\_size}_1 + 42\right)\right)\right] = \text{"A43:B100"}$

$\text{Input\_8} := \text{READEXCEL}(\text{file}, \text{concat}(\text{sheet}, \text{Decay\_heat\_range}))$

$\text{Time\_out\_of\_Reactor} := \text{Input\_8}^{\langle 1 \rangle} \cdot \text{yr}$ $\qquad$ $\text{Decay\_Heat\_per\_Cnt} := \text{Input\_8}^{\langle 2 \rangle} \cdot \text{W}$

$\text{Input\_8} =$

	0	1
0	5	$1.028 \cdot 10^3$
1	5.1	$1.011 \cdot 10^3$
2	5.5	949.125
3	5.75	916.671
4	6	887.984
5	8	742.948
6	10	670.028
7	11.5	634.239
8	15	576.929
9	20	...

$\text{Time\_out\_of\_Reactor} =$

	0
0	5
1	5.1
2	5.5
3	5.75
4	6
5	8
6	10
7	11.5
8	15
9	...

$\cdot \text{yr}$

$\text{Decay\_Heat\_per\_Cnt} =$

	0
0	$1.028 \cdot 10^3$
1	$1.011 \cdot 10^3$
2	949.125
3	916.671
4	887.984
5	742.948
6	670.028
7	634.239
8	576.929
9	...

W

$Q(t) := \text{interp}(\text{cspline}(\text{Time\_out\_of\_Reactor}, \text{Decay\_Heat\_per\_Cnt}), \text{Time\_out\_of\_Reactor}, \text{Decay\_Heat\_per\_Cnt}, t)$

Ventilation efficiency for open systems is $\boxed{V_{\text{eff}} = 0.75}$ between t_{store} and t_{operate}

FUNCTION DEFINITION FOR ONE OUTPUT FILE

FORMULAS FOR CALCULATING THE TRANSIENT DRIFT WALL TEMPERATURE:

Central waste package:

$$Q_{\text{L\_wp}}\left(t, t_{\text{store}}, t_{\text{operate}}, \text{WP\_cap}\right) := \frac{Q(t) \cdot \text{WP\_cap}}{\text{WP\_length}} \cdot \left[1 - 1 \cdot \left(t \le t_{\text{store}}\right)\right] \cdot \left[1 - V_{\text{eff}} \cdot \left(t \le t_{\text{operate}}\right)\right]$$

$$Q_{\text{L\_wp}}\left(55 \cdot \text{yr}, t_{\text{store}}, t_{\text{operate}}, 12\right) = 177.365 \cdot \frac{\text{W}}{\text{m}}$$

Note - added r_{DW} as a function parameter to allow calculations at additional compliance points inside the rock, where r_{DW} would be replaced with new radius value.

$$DW\_T\_finite\_line\left(t, r_{DW}, y, t_{store}, t_{operate}, WP\_cap, Kth, \alpha\right) := \left[\int_0^t \frac{Q_{L\_wp}\left(\tau, t_{store}, t_{operate}, WP\_cap\right)}{8 \cdot (\pi \cdot Kth) \cdot (t - \tau)} \cdot e^{\frac{-\left(r_{DW}^2\right)}{4 \cdot \alpha \cdot (t-\tau)}} \cdot \left[erf\left[\frac{1}{2} \cdot \frac{\left(y + \frac{WP\_length}{2}\right)}{\sqrt{\alpha \cdot (t - \tau)}}\right] - erf\left[\frac{1}{2} \cdot \frac{\left(y - \frac{WP\_length}{2}\right)}{\sqrt{\alpha \cdot (t - \tau)}}\right]\right] d\tau\right]$$

Adjacent drifts:

$$Q_{L\_avg}\left(t, t_{store}, t_{operate}, WP\_cap, WP\_spacing\right) := \frac{Q(t) \cdot WP\_cap}{WP\_spacing} \cdot \left[1 - 1 \cdot \left(t \le t_{store}\right)\right] \cdot \left[1 - V_{eff} \cdot \left(t \le t_{operate}\right)\right]$$

Note - added r_{DW} as a function parameter to allow calculations at additional compliance points inside the rock, where r_{DW} would be replaced with new radius value.

$$DW\_T\_drifts\left(t, r_{DW}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha\right) := 2 \left[\sum_{id=1}^{N_{drifts}} \int_0^t \frac{Q_{L\_avg}\left(\tau, t_{store}, t_{operate}, WP\_cap, WP\_spacing\right)}{4 \cdot (\pi \cdot Kth) \cdot (t - \tau)} \cdot e^{\frac{-\left[(r_{DW})^2 + (id \cdot Drift\_spacing)^2\right]}{4 \cdot \alpha \cdot (t-\tau)}} d\tau\right]$$

Adjacent waste packages:

$$Q_{wp}\left(t, t_{store}, t_{operate}, WP\_cap\right) := Q(t) \, WP\_cap \cdot \left[1 - 1 \cdot \left(t \le t_{store}\right)\right] \cdot \left[1 - V_{eff} \cdot \left(t \le t_{operate}\right)\right]$$

Note - added r_{DW} as a function parameter to allow calculations at additional compliance points inside the rock, where r_{DW} would be replaced with new radius value.

$$DW\_T\_adjacent\_pkgs\left(t, r_{DW}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Kth, \alpha\right) := 2 \left[\sum_{ip=1}^{N_{adj}} \int_0^t \frac{Q_{wp}\left(\tau, t_{store}, t_{operate}, WP\_cap\right)}{8 \cdot Kth \cdot \sqrt{\alpha} \cdot \pi^{1.5} \cdot (t - \tau)^{1.5}} \cdot e^{\frac{-\left[r_{DW}^2 + (ip \cdot WP\_spacing)^2\right]}{4\alpha \cdot (t-\tau)}} d\tau\right]$$

Mathcad DSEF 3.0 parametric and iterative model - example for User's Manual.xmcd

OutfileName := file = "DSEF R3.0_2013Aug12_HRG-Clay_UOX-40_Iterative convergence example_Case-225-19.xlsm"

Out_sheet := "Thermal-Analytical Output!"

This section specifies the column headings for output sensitivity studies

Cases = 1   Read in from Thermal-Analytical sheet in DSEF (Inputs_7)

$i := 1 .. Cases$

$\text{Parameter\_vector}_i := \begin{vmatrix} \text{"Base Case"} & \text{if Cases} = 1 \\ \text{concat}(\text{Parameter}, " ", \text{Parameter\_description}_i) & \text{otherwise} \end{vmatrix}$

$\text{Parameter\_vector} = (\text{"Base Case"})$

$\text{heading1}_i := \begin{pmatrix} \text{concat}(\text{"Parameter value: "}, \text{Parameter\_vector}_i) \\ "" \\ "" \\ "" \\ "" \\ "" \\ "" \\ "" \\ "" \\ "" \\ "" \end{pmatrix}$

$\text{heading2} := \begin{pmatrix} \text{"TooR (yr)"} \\ \text{"Wall } \Delta T \text{ Central Line Src"} \\ \text{"Wall } \Delta T \text{ Adj Drifts"} \\ \text{"Wall } \Delta T \text{ Adj Pkgs"} \\ \text{"Compliance Point 2, C"} \\ \text{"Rock Wall Temp, C"} \\ \text{"EBS 1 inner Temp, C"} \\ \text{"EBS 2 inner Temp, C"} \\ \text{"EBS 3 inner Temp, C"} \\ \text{"Waste Pkg Temp, C"} \end{pmatrix}$

$\text{heading1}_i := \text{heading1}_i{}^T \qquad \text{heading2} := \text{heading2}^T$

$\text{Title\_array}_i := \text{stack}(\text{heading1}_i, \text{heading2})$

$\text{Title\_array}_2 = \blacksquare$

$\text{length}(\text{Parameter\_data}) = 1$

$r_{DW} = 2.25\,m$

$r_{CP2} = 5.25\,m$

$t_{store} = 50 \cdot yr$

$t_{operate} = 170 \cdot yr$

$t_{closure} = 180 \cdot yr$

$t_{vent} = 120 \cdot yr$

Changed j vector to Parameter_data, Inserted row 2
in row 5 changed to $k_{radiation}$ and k_2 from k_2 and $k_{backfill}$
row 8 changed WP_space$_j$ to WP_spacing.

Removed loop on "j", added r_{DW} into DW_T functions.

Note for enclosed modes $k_{radiation} = k_2$

Mathcad Component of DSEF 3.0

Mathcad DSEF 3.0 parametric and iterative model - example for User's Manual.xmcd

$Counter := 200$ $Step := 5$ $\text{time\_after\_emplacement\_analzyed} := (Counter \cdot Step \cdot yr) + t_{store} = 1050 \cdot yr$

$$\text{outdata}\left(r_{DW}, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha, k_1, k_2, k_3, k_4\right) :=$$

for $i \in 1 .. Counter + 1$

$tt_i \leftarrow Step \cdot i \cdot yr + t_{store} - Step \cdot 1yr$

$kk_2 \leftarrow k_{radiation} \cdot \left[tt_i < \left(t_{operate} + t_{backfill}\right) \right] + k_2 \cdot \left[tt_i \geq \left(t_{operate} + t_{backfill}\right) \right]$

$Wall\_deltaT\_finite\_line_i \leftarrow DW\_T\_finite\_line\left(tt_i, r_{DW}, 0, t_{store}, t_{operate}, WP\_cap, Kth, \alpha\right)$

$Wall\_deltaT\_drifts_i \leftarrow DW\_T\_drifts\left(tt_i, r_{DW}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha\right)$

$Wall\_deltaT\_adj\_pkgs_i \leftarrow DW\_T\_adjacent\_pkgs\left(tt_i, r_{DW}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Kth, \alpha\right)$

$Wall\_T_i \leftarrow T_{ambient} + Wall\_deltaT\_finite\_line_i + Wall\_deltaT\_drifts_i + Wall\_deltaT\_adj\_pkgs_i$

$CP2\_deltaT\_finite\_line_i \leftarrow DW\_T\_finite\_line\left(tt_i, r_{CP2}, 0, t_{store}, t_{operate}, WP\_cap, Kth, \alpha\right)$

$CP2\_deltaT\_drifts_i \leftarrow DW\_T\_drifts\left(tt_i, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha\right)$

$CP2\_deltaT\_adj\_pkgs_i \leftarrow DW\_T\_adjacent\_pkgs\left(tt_i, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Kth, \alpha\right)$

$CP2\_T_i \leftarrow T_{ambient} + CP2\_deltaT\_finite\_line_i + CP2\_deltaT\_drifts_i + CP2\_deltaT\_adj\_pkgs_i$

$Q_i \leftarrow Q_{L\_wp}\left(tt_i, t_{store}, t_{operate}, WP\_cap\right)$

$EBS\_1_i \leftarrow Wall\_T_i + \dfrac{Q_i}{2 \cdot \pi \cdot r_{DW}} \cdot R_1\left(k_1\right)$

$EBS\_2_i \leftarrow \left| \begin{array}{l} EBS\_1_i + \dfrac{Q_i}{2 \cdot \pi \cdot r_{DW}} \cdot R_2\left(kk_2, tt_i, t_{operate}, t_{backfill}\right) \quad \text{if } kk_2 \neq 0 \cdot \dfrac{W}{m \cdot K} \\[2em] \left[\left[\dfrac{Q_i}{h_{rad\_infinite}\left(r_3, r_2, \varepsilon_{WP}, \varepsilon_{wall}\right) \cdot 2 \cdot \pi \cdot r_3} + \left(EBS\_1_i\right)^4 \right]^{\frac{1}{4}} \right] \quad \text{otherwise} \end{array} \right.$

$EBS\_3_i \leftarrow EBS\_2_i + \dfrac{Q_i}{2 \cdot \pi \cdot r_{DW}} \cdot R_3\left(k_3\right)$

$WP\_T_i \leftarrow EBS\_3_i + \dfrac{Q_i}{2 \cdot \pi \cdot r_{DW}} \cdot R_4\left(k_4\right)$

$T1_i \leftarrow CP2\_T_i - 273.15K$

$T2_i \leftarrow Wall\_T_i - 273.15K$

$T3_i \leftarrow EBS\_1_i - 273.15K$

$T4_i \leftarrow EBS\_2_i - 273.15K$

$T5_i \leftarrow EBS\_3_i - 273.15K$

$T6_i \leftarrow WP\_T_i - 273.15K$

$Data\_array \leftarrow augment\left(tt \cdot \dfrac{1}{yr}, Wall\_deltaT\_finite\_line \cdot \dfrac{1}{K}, Wall\_deltaT\_drifts \cdot \dfrac{1}{K}, Wall\_deltaT\_adj\_pkgs \cdot \dfrac{1}{K}, T1 \cdot \dfrac{1}{K}, T2 \cdot \dfrac{1}{K}, T3 \cdot \dfrac{1}{K}, T4 \cdot \dfrac{1}{K}, T5 \cdot \dfrac{1}{K}, T6 \cdot \dfrac{1}{K}\right)$

Mathcad DSEF 3.0 parametric and iterative model - example for User's Manual.xmcd

$jjj := 1 .. Cases \qquad Cases = 1$

$X_{jjj} := Parameter\_data_{jjj} \qquad Parameter = "Single"$

$Temp\_array_{jjj} :=$

$\Big|\ outdata\big(r_{DW}, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha, k_1, k_2, k_3, k_4\big)$ if $Parameter = "Single"$

$outdata\big(r_{DW}, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, X_{jjj} \cdot m, Kth, \alpha, k_1, k_2, k_3, k_4\big)$ if $Parameter = "Drift\ Spacing"$

$outdata\big(r_{DW}, r_{CP2}, t_{store}, t_{operate}, WP\_cap, X_{jjj} \cdot m, Drift\_spacing, Kth, \alpha, k_1, k_2, k_3, k_4\big)$ if $Parameter = "WP\ Spacing"$

$outdata\big(r_{DW}, r_{CP2}, X_{jjj} \cdot yr, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha, k_1, k_2, k_3, k_4\big)$ if $Parameter = "Storage\ Time"$

$outdata\big(r_{DW}, r_{CP2}, t_{store}, t_{store} + X_{jjj} \cdot yr, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha, k_1, k_2, k_3, k_4\big)$ if $Parameter = "Ventilation\ Duration"$

$outdata\Big(r_{DW}, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, X_{jjj} \cdot \frac{W}{m \cdot K}, \alpha, k_1, k_2, k_3, k_4\Big)$ if $Parameter = "Rock\ Conductivity"$

$outdata\Big(r_{DW}, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha, k_1, X_{jjj} \cdot \frac{W}{m \cdot K}, k_3, k_4\Big)$ if $Parameter = "Backfill\ Conductivity"$

$"Undefined"$ otherwise

$File\_array_{jjj} := stack\big(Title\_array_{jjj}, Temp\_array_{jjj}\big)$

$File\_array_1 =$

	0	1	2	3	4	5
0	"Parameter value: Base Case"	""	""	""	""	""
1	"TooR (yr)"	"Wall ΔT Central Line Src"	"Wall ΔT Adj Drifts"	"Wall ΔT Adj Pkgs"	"Compliance Point 2, C"	"Rock Wall Temp, C"
2	50	0	0	0	27.5	27.5
3	55	23.349	0.269	1.181	38.116	52.299
4	60	22.931	1.341	2.422	40.833	54.195
5	65	21.989	2.532	3.206	42.678	55.227
6	70	20.933	3.643	3.728	43.983	55.804
7	75	19.895	4.644	4.085	44.978	56.124
8	80	18.909	5.536	4.332	45.748	56.278
9	85	17.992	6.332	4.501	46.352	56.325
10	90	17.14	7.042	4.612	46.831	56.294
11	95	16.364	7.675	4.681	47.21	56.22
12	100	15.639	8.245	4.719	47.518	56.103
13	105	14.98	8.756	4.735	47.767	55.972
14	110	14.372	9.214	4.728	47.957	55.814
15	115	13.82	9.628	4.71	48.116	...

Mathcad DSEF 3.0 parametric and iterative model - example for User's Manual.xmcd

$iii := 1 .. 10$

$Peak\_array_{jjj, iii} := max\left[\left[\left(Temp\_array_{jjj}\right)^{\langle iii \rangle}\right]\right]$

$Peak\_array_{1,2} = 35.526$

$\left(Temp\_array_1\right)^{\langle 6 \rangle} =$

	0
0	27.5
1	52.299
2	54.195
3	55.227
4	55.804
5	56.124
6	56.278
7	56.325
8	56.294
9	56.22
10	56.103
11	55.972
12	55.814
13	55.658
14	55.508
15	...

$Time\_array := \left(Temp\_array_1\right)^{\langle 1 \rangle}$

$Peak\_T(m, n) := max\left[\left(Temp\_array_m\right)^{\langle n \rangle}\right]$

$Peak\_T(1, 5) = 88.663$

$Peak\_time(m, n) := lookup\left[Peak\_T(m, n), \left(Temp\_array_m\right)^{\langle n \rangle}, Time\_array\right]$

$Peak\_time(1, 5) = (475)$

$Time\_array =$

	0
0	50
1	55
2	60
3	65
4	70
5	75
6	80
7	85
8	90
9	95
10	100
11	105
12	110
13	115
14	120
15	...

Initialize the peak value data array:

$i := 1 .. 6 \qquad j := 1 .. 20$

$Peak\_values_{i, j} := ""$

$$Peak\_values = \begin{pmatrix} "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \end{pmatrix}$$

Fill in the peak temperatures and times:

$mj := 1 .. Cases \qquad nn := 1 .. 6$

$Peak\_values_{nn, mj \cdot 2 - 1} := Peak\_T(mj, nn + 4)$

$Peak\_values_{nn, mj \cdot 2} := Peak\_time(mj, nn + 4)_1$

$t_{vent} = 120 \cdot yr$

$Parameter\_vector^T = (\text{"Base Case"})$

Mathcad DSEF 3.0 parametric and iterative model - example for User's Manual.xmcd

$$\text{Peak\_values} = \begin{pmatrix} 88.663 & 475 & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ 100.744 & 385 & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ 100.755 & 385 & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ 157.563 & 195 & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ 157.563 & 195 & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ 157.563 & 195 & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \end{pmatrix}$$

$$\text{Peak\_Wall\_T} := \left(\text{Peak\_values}^{\langle 1 \rangle} \right)_2 = 100.744$$

outsheet := "Thermal-Analytical Output!"

$\text{rows}(\text{Temp\_array}_1) = 201 \qquad \text{rows}(\text{File\_array}_1) = 203$ Transient output starting row in DSEF on the Thermal-= 60

$\text{start\_row} := 100 \quad \text{end\_row} := \text{start\_row} + \text{rows}(\text{Temp\_array}_1) - 1 = 300$ NOTE - USE File_array to write to stand-alone Excel files, and Temp_array to write back to the DSEF Excel file.

$$\text{transient\_case\_cols} := \begin{pmatrix} "A" & "J" \\ "L" & "U" \\ "W" & "AF" \\ "AH" & "AQ" \\ "AS" & "BB" \\ "BD" & "BM" \\ "BO" & "BX" \\ "BZ" & "CI" \\ "CK" & "CT" \\ "CV" & "DE" \end{pmatrix}$$

To write the transients for each case horizontally instead of vertically, the following location array includes 10 columns for each case with one column separating the cases.

iw := 1 .. Cases

start_row = 100   end_row = 300

$\text{transient\_write\_range}_{iw} := \text{concat}\left[\text{outsheet}, \left(\text{transient\_case\_cols}^{\langle 1 \rangle} \right)_{iw}, \text{num2str}(\text{start\_row}), ":", \left(\text{transient\_case\_cols}^{\langle 2 \rangle} \right)_{iw}, \text{num2str}(\text{end\_row}) \right]$

Mathcad DSEF 3.0 parametric and iterative model - example for User's Manual.xmcd

$\text{transient\_write\_range}_2 = \text{"Thermal-Analytical Output!L100:U300"}$ $\text{peaks\_write\_range} := \text{concat}(\text{outsheet}, \text{"C6:V11"}) = \text{"Thermal-Analytical Output!C6:V11"}$

$\text{transient\_write\_range} = (\text{"Thermal-Analytical Output!A100:J300"})$

$\text{Transient\_size} := (\text{Counter} \quad \text{Step})$ $\text{Transient\_size} = (200 \quad 5)$ $\text{Transient\_size\_range} := \text{concat}(\text{outsheet}, \text{"B92:C92"}) = \text{"Thermal-Analytical Output!B92:C92"}$

Make writing an output file optional $t_{vent} = 120 \cdot \text{yr}$

$\text{OutfileName} = \text{"DSEF R3.0\_2013Aug12\_HRG-Clay\_UOX-40\_Iterative convergence example\_Case-225-19.xlsm"}$

$\text{Write\_file} := \text{Write\_OK} = \text{"YES"}$

$$\text{write\_the\_peaks}(\text{Write\_file}) := \begin{vmatrix} \text{write\_it} \leftarrow \begin{vmatrix} \text{WRITEEXCEL}(\text{Peak\_values}, \text{OutfileName}, \text{peaks\_write\_range}) & \text{if } (\text{Write\_file} = \text{"Yes"}) \vee (\text{Write\_file} = \text{"YES"}) \\ \text{"File written"} \end{vmatrix} \\ \text{write\_it} \leftarrow \text{"No file written"} \quad \text{otherwise} \end{vmatrix}$$

$\text{write\_the\_peaks}(\text{Write\_file}) = \text{"File written"}$

$$\text{write\_the\_transient\_size}(\text{Write\_file}) := \begin{vmatrix} \text{write\_it} \leftarrow \begin{vmatrix} \text{WRITEEXCEL}(\text{Transient\_size}, \text{OutfileName}, \text{Transient\_size\_range}) & \text{if } (\text{Write\_file} = \text{"Yes"}) \vee (\text{Write\_file} = \text{"YES"}) \\ \text{"File written"} \end{vmatrix} \\ \text{write\_it} \leftarrow \text{"No file written"} \quad \text{otherwise} \end{vmatrix}$$

$\text{write\_the\_transient\_size}(\text{Write\_file}) = \text{"File written"}$

$\text{Write\_file} := \text{Write\_OK} = \text{"YES"}$ $\text{Cases} = 1$

$\text{iww} := 1 .. \text{Cases}$ NOTE - USE File_array to write to stand-alone Excel files, and Temp_array to write back to the DSEF Excel file.

$$\text{write\_the\_transients}(jj) := \begin{vmatrix} \text{write\_array} \leftarrow \text{Temp\_array}_{jj} \\ \text{write\_it} \leftarrow \begin{vmatrix} \text{WRITEEXCEL}(\text{write\_array}, \text{OutfileName}, \text{transient\_write\_range}_{jj}) & \text{if } (\text{Write\_file} = \text{"Yes"}) \vee (\text{Write\_file} = \text{"YES"}) \\ \text{"File written"} \end{vmatrix} \\ \text{write\_it} \leftarrow \text{"No file written"} \quad \text{otherwise} \end{vmatrix}$$

$\text{write\_the\_transients}(\text{iww}) = (\text{"File written"})$

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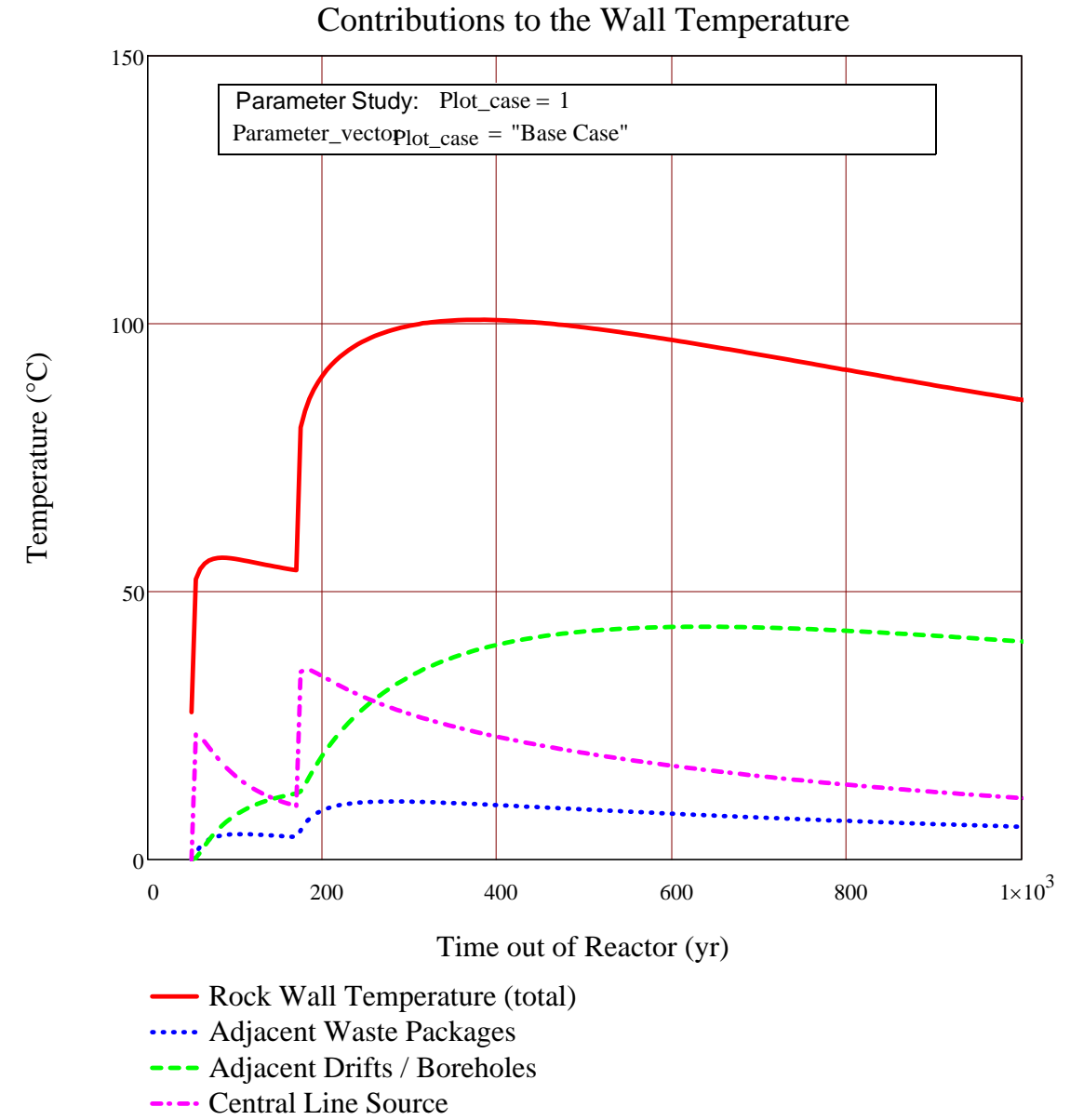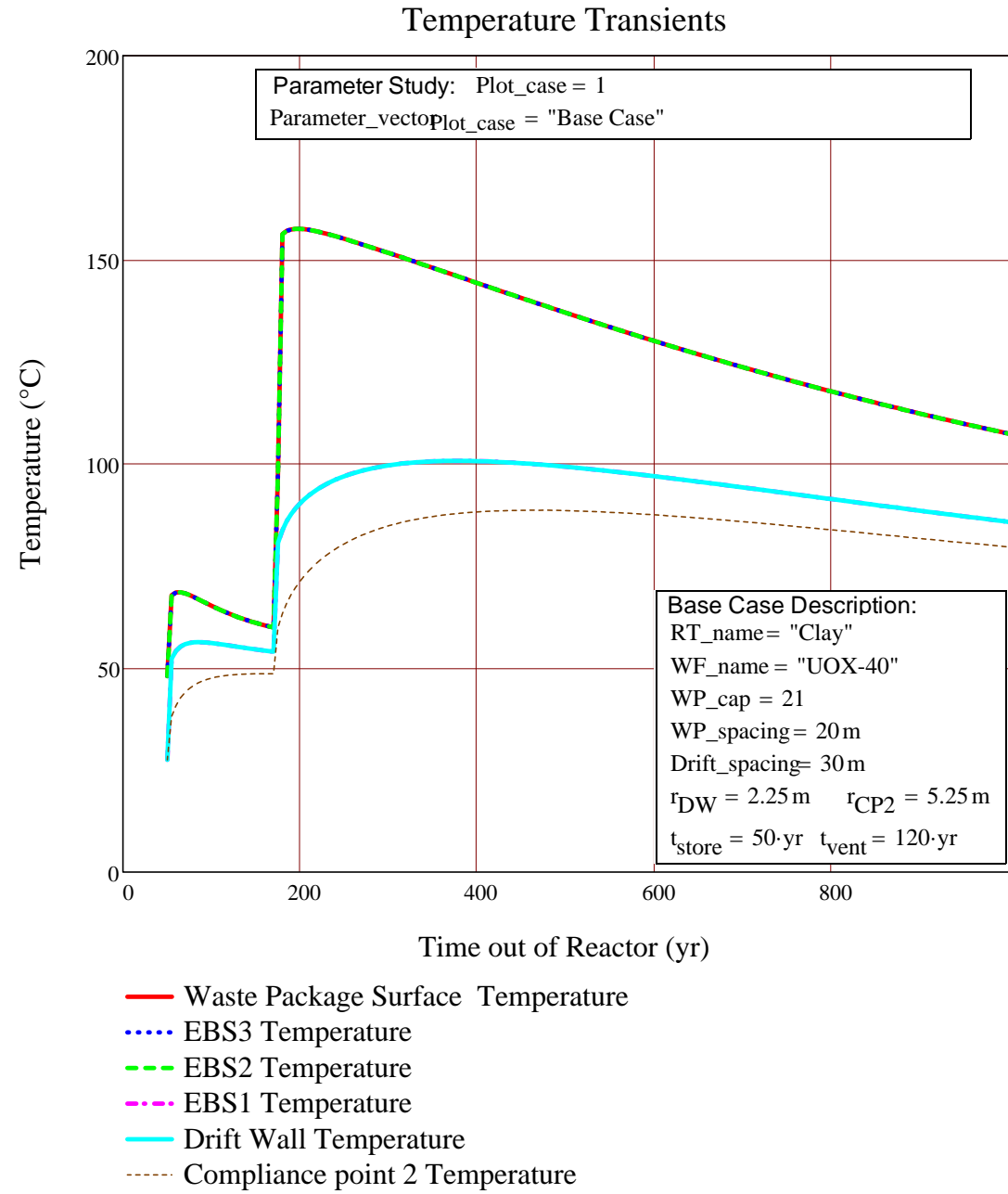
$\text{Plot\_case} := 1$ Select parametric study case to plot (default plot is for case 1)

$\text{WP\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}} \right)^{\langle 10 \rangle} \right]$ $\text{EBS3\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}} \right)^{\langle 9 \rangle} \right]$ $\text{EBS2\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}} \right)^{\langle 8 \rangle} \right]$ $\text{EBS1\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}} \right)^{\langle 7 \rangle} \right]$ $\text{Wall\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}} \right)^{\langle 6 \rangle} \right]$

$\text{CP2\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}} \right)^{\langle 5 \rangle} \right]$ $\text{Delta\_WPs\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}} \right)^{\langle 4 \rangle} \right]$ $\text{Delta\_drifts\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}} \right)^{\langle 3 \rangle} \right]$ $\text{Delta\_central\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}} \right)^{\langle 2 \rangle} \right]$

Temperature Transients

Parameter Study: Plot_case = 1
Parameter_vector$_{Plot\_case}$ = "Base Case"

Base Case Description:
RT_name = "Clay"
WF_name = "UOX-40"
WP_cap = 21
WP_spacing = 20 m
Drift_spacing = 30 m
r_{DW} = 2.25 m r_{CP2} = 5.25 m
t_{store} = 50·yr t_{vent} = 120·yr

Temperature (°C)

Time out of Reactor (yr)

—— Waste Package Surface Temperature
······ EBS3 Temperature
---- EBS2 Temperature
-·-·- EBS1 Temperature
—— Drift Wall Temperature
········· Compliance point 2 Temperature

Contributions to the Wall Temperature

Parameter Study: Plot_case = 1
Parameter_vector$_{Plot\_case}$ = "Base Case"

Temperature (°C)

Time out of Reactor (yr)

—— Rock Wall Temperature (total)
······ Adjacent Waste Packages
---- Adjacent Drifts / Boreholes
-·-·- Central Line Source

$$T_{EBS}\left(r, t, Wall\_T, k_1, k_2, k_3, k_4\right) := Wall\_T \cdot K + \frac{Q_{L\_wp}\left(t, t_{store}, t_{operate}, WP\_cap\right)}{2 \cdot \pi \cdot r_{DW}} \cdot R_{continuous}\left(t, r, k_1, k_2, k_3, k_4\right)$$

$$Q_{L\_wp}\left(110 \cdot yr, t_{store}, t_{operate}, WP\_cap\right) = 167.803 \cdot \frac{W}{m}$$

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$$\text{tt\_rw} := \left[(\text{Peak\_values})^{\langle \text{Plot\_case} \cdot 2 \rangle} \right]_2 = 385$$

$$\text{Wall\_T\_at\_tt\_rw} := \left[(\text{Peak\_values})^{\langle \text{Plot\_case} \cdot 2 - 1 \rangle} \right]_2 = 100.744$$

$$\text{WP\_T\_at\_tt\_wp} := \left[(\text{Peak\_values})^{\langle \text{Plot\_case} \cdot 2 - 1 \rangle} \right]_6 = 157.563$$

$$\text{tt\_wp} := \left[(\text{Peak\_values})^{\langle \text{Plot\_case} \cdot 2 \rangle} \right]_6 = 195$$

$$\text{Wall\_T\_at\_tt\_wp} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 6 \rangle} \right]_{\frac{\left(\text{tt\_wp} - \frac{t_{\text{store}}}{\text{yr}}\right)}{\text{Step}}} = 87.705$$

$$\text{WP\_T\_at\_tt\_rw} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 10 \rangle} \right]_{\frac{\left(\text{tt\_rw} - \frac{t_{\text{store}}}{\text{yr}}\right)}{\text{Step}}} = 145.774$$

Temperature Gradient in the EBS

Parameter Study: Plot_case = 1
Parameter_vector$_{\text{Plot\_case}}$ = "Base Case"

Base Case Description:
RT_name = "Clay"
WP_spacing = 20 m
Drift_spacing = 30 m
WP_cap = 21
t_{store} = 50·yr

Rock wall ------>

<-- Waste Package Surface

Temperature (°C)

Radial Location in the EBS (m)

——— Gradient at the time of the Waste Package Peak T
······ Gradient at the time of the Rock Wall Peak T

OVERRIDE COUNTER AND STEP SIZE TO GET FINER CONVERGENCE ON THE ANSWER

$t_{vent} = 120 \cdot yr$ <mark>OPTIONALLY OVERRIDE VENTILATION TIME TO SHORTEN ITERATION CONVERGENCE</mark>

<mark>ITERATE_OK</mark> $:= $ "YES" $t_{convergence} = 1 \cdot yr$

$$t_{required\_storage}\left(t_{operate}, T_{criteria}, t_{convergence}\right) := \begin{vmatrix} time_{OK} \leftarrow t_{operate} - t_{convergence} \\ Peak\_Wall\_T_{check} \leftarrow (Peak\_Wall\_T + 273.15) \cdot K \\ time_{OK} \leftarrow t_{operate} \quad \text{if } Peak\_Wall\_T_{check} \leq T_{criteria} \\ \text{while } Peak\_Wall\_T_{check} > T_{criteria} \\ \qquad \begin{vmatrix} time_{OK} \leftarrow time_{OK} + t_{convergence} \\ calc_{array} \leftarrow outdata\left(r_{DW}, r_{CP2}, t_{store}, time_{OK}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha, k_1, k_2, k_3, k_4\right) \\ Peak\_Wall\_T_{check} \leftarrow \left(max\left(calc_{array}^{\langle 6 \rangle}\right) + 273.15\right) \cdot K \end{vmatrix} \\ return \begin{pmatrix} \dfrac{time_{OK}}{yr} \\ \dfrac{Peak\_Wall\_T_{check} - 273.15K}{K} \\ outdata\left(r_{DW}, r_{CP2}, t_{store}, time_{OK}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha, k_1, k_2, k_3, k_4\right) \end{pmatrix} \end{vmatrix}$$

$$Final\_array := \begin{vmatrix} t_{required\_storage}\left(t_{operate}, T_{criteria}, t_{convergence}\right) \quad \text{if } ITERATE\_OK = \text{"YES"} \\ \text{"No Iteration Performed"} \quad \text{otherwise} \end{vmatrix}$$

$t_{operate\_required} := Final\_array_1 \, yr = 177 \cdot yr$

$t_{vent\_required} := t_{operate\_required} - t_{store} = 127 \cdot yr$ <mark>REQUIRED VENTILATION TIME NEEDED TO MEET $T_{criteria} = 100 \cdot °C$</mark>

$Peak\_Wall\_T_{check} := \left(Final\_array_2 + 273.15\right) \cdot K = 99.931 \cdot °C$

Mathcad DSEF 3.0 parametric and iterative model - example for User's Manual.xmcd

$\text{Result} := \text{stack}\left(\text{Title\_array}_1, \text{Final\_array}_3\right)$ ==NOTE THAT THIS SECTION WILL BE BLANK IF NO ITERATIVE ANALYSIS IS PERFORMED (Iterate_OK = "No"==

Result =

	1	2	3	4	5	6	7
1	"Parameter value: Base Case"	""	""	""	""	""	""
2	"TooR (yr)"	"Wall ΔT Central Line Src"	"Wall ΔT Adj Drifts"	"Wall ΔT Adj Pkgs"	"Compliance Point 2, C"	"Rock Wall Temp, C"	"EBS 1 inner Temp, C"
3	50	0	0	0	27.5	27.5	27.513
4	55	23.349	0.269	1.181	38.116	52.299	52.311
5	60	22.931	1.341	2.422	40.833	54.195	54.206
6	65	21.989	2.532	3.206	42.678	55.227	55.238
7	70	20.933	3.643	3.728	43.983	55.804	55.814
8	75	19.895	4.644	4.085	44.978	56.124	56.133
9	80	18.909	5.536	4.332	45.748	56.278	56.287
10	85	17.992	6.332	4.501	46.352	56.325	56.333
11	90	17.14	7.042	4.612	46.831	56.294	56.302
12	95	16.364	7.675	4.681	47.21	56.22	56.227
13	100	15.639	8.245	4.719	47.518	56.103	56.111
14	105	14.98	8.756	4.735	47.767	55.972	55.979
15	110	14.372	9.214	4.728	47.957	55.814	55.82
16	115	13.82	9.628	4.71	48.116	55.658	...

$\text{Time\_array} := \left(\text{Final\_array}_3\right)^{\langle 1 \rangle}$

$\text{Peak\_Temp}(n) := \max\left[\left(\text{Final\_array}_3\right)^{\langle n \rangle}\right]$ $\text{Peak\_Temp}(6) = 99.931$

$\text{Peak\_t}(n) := \text{lookup}\left[\text{Peak\_Temp}(n), \left(\text{Final\_array}_3\right)^{\langle n \rangle}, \text{Time\_array}\right]$ $\text{Peak\_t}(6)_1 \cdot \text{yr} = 380 \cdot \text{yr}$

$nn := 5 .. 10$ $\text{Peak\_results}_{nn-4, 1} := \text{Peak\_Temp}(nn)$ $\text{Peak\_results}_{nn-4, 2} := \text{Peak\_t}(nn)_1$

$\text{Peak\_results} = \begin{pmatrix} 88.045 & 470 \\ 99.931 & 380 \\ 99.941 & 380 \\ 154.961 & 210 \\ 154.961 & 210 \\ 154.961 & 210 \end{pmatrix}$

CP2   , time of peak
Peak Wall T, time of peak
Peak EBS 1, time of peak
Peak EBS 2, time of peak
Peak EBS 3, time of peak
Waste Pkg T, time of peak

$\text{Array\_row\_at\_Wall\_T\_peak} := \text{match}\left[\text{Peak\_Temp}(6), \left(\text{Final\_array}_3\right)^{\langle 6 \rangle}\right]_1 = 67$

$\text{CP2\_at\_Wall\_T\_pk\_t} := \left[\left(\text{Final\_array}_3\right)^{\langle 5 \rangle}\right]_{\text{Array\_row\_at\_Wall\_T\_peak}} = 87.069$

$\text{Ceintral\_WP\_delta} := \left[\left(\text{Final\_array}_3\right)^{\langle 2 \rangle}\right]_{\text{Array\_row\_at\_Wall\_T\_peak}} = 23.638$

$\text{Adj\_Drift\_delta} := \left[\left(\text{Final\_array}_3\right)^{\langle 3 \rangle}\right]_{\text{Array\_row\_at\_Wall\_T\_peak}} = 38.538$

Mathcad DSEF 3.0 parametric and iterative model - example for User's Manual.xmcd

$$Adj\_WP\_delta := \left[\left(Final\_array_3\right)^{\langle 4 \rangle}\right]_{Array\_row\_at\_Wall\_T\_peak} = 10.254$$

$$Result\_Vector := \left(\frac{WP\_spacing}{m} \quad TC \quad \frac{Drift\_spacing}{m} \quad Peak\_results_{6,1} \quad Peak\_results_{6,2} \quad Peak\_results_{2,1} \quad Peak\_results_{2,2} \quad CP2\_at\_Wall\_T\_pk\_t \quad \frac{t_{vent\_required}}{yr} \quad Ceintral\_WP\_delta \quad Adj\_Drift\_delta \quad Adj\_WP\_delta\right)$$

Result_headings := ("WP Spacing" "Temp Criteria" "Drift Spacing" "Peak WP T" "Time of WP Peak" "Peak Wall T" "Time of Wall Peak" "Peak CP2 T" "Ventilation time" "Central WP delta" "Adj Drift delta" "Adj WP delta")

Result_Vector = (20 100 30 154.961 210 99.931 380 87.069 127 23.638 38.538 10.254)   ==This is the result vector for transcription to the Excel case results tracking fil==e

$$RV := augment\left(Result\_headings^T, Result\_Vector^T\right)$$ $T_{ambient} = 27.5 \cdot °C$ ==Contribution percentages at time of peak wall temperature==

$$RV = \begin{pmatrix} \text{"WP Spacing"} & 20 \\ \text{"Temp Criteria"} & 100 \\ \text{"Drift Spacing"} & 30 \\ \text{"Peak WP T"} & 154.961 \\ \text{"Time of WP Peak"} & 210 \\ \text{"Peak Wall T"} & 99.931 \\ \text{"Time of Wall Peak"} & 380 \\ \text{"Peak CP2 T"} & 87.069 \\ \text{"Ventilation time"} & 127 \\ \text{"Central WP delta"} & 23.638 \\ \text{"Adj Drift delta"} & 38.538 \\ \text{"Adj WP delta"} & 10.254 \end{pmatrix}$$

$$Percent\_central\_WP\_delta := \frac{Ceintral\_WP\_delta}{Peak\_Temp(6) - \frac{\left(T_{ambient} - 273.15 \cdot K\right)}{K}} \cdot 100 = 32.636$$

$$Percent\_adj\_Drift\_delta := \frac{Adj\_Drift\_delta}{Peak\_Temp(6) - \frac{\left(T_{ambient} - 273.15 \cdot K\right)}{K}} \cdot 100 = 53.207$$

$$Percent\_adj\_WP\_delta := \frac{Adj\_WP\_delta}{Peak\_Temp(6) - \frac{\left(T_{ambient} - 273.15 \cdot K\right)}{K}} \cdot 100 = 14.157$$

$$Percent\_central\_WP\_delta + Percent\_adj\_WP\_delta + Percent\_adj\_Drift\_delta = 100$$

Plot temperature results as a function of parameter data

$ip := 1 .. Cases$

$Peak\_WP\_T_{ip} := \left(Peak\_values^{\langle ip \cdot 2 - 1 \rangle} \right)_6$ $Peak\_EBS3\_T_{ip} := \left(Peak\_values^{\langle ip \cdot 2 - 1 \rangle} \right)_5$ $Peak\_EBS2\_T_{ip} := \left(Pea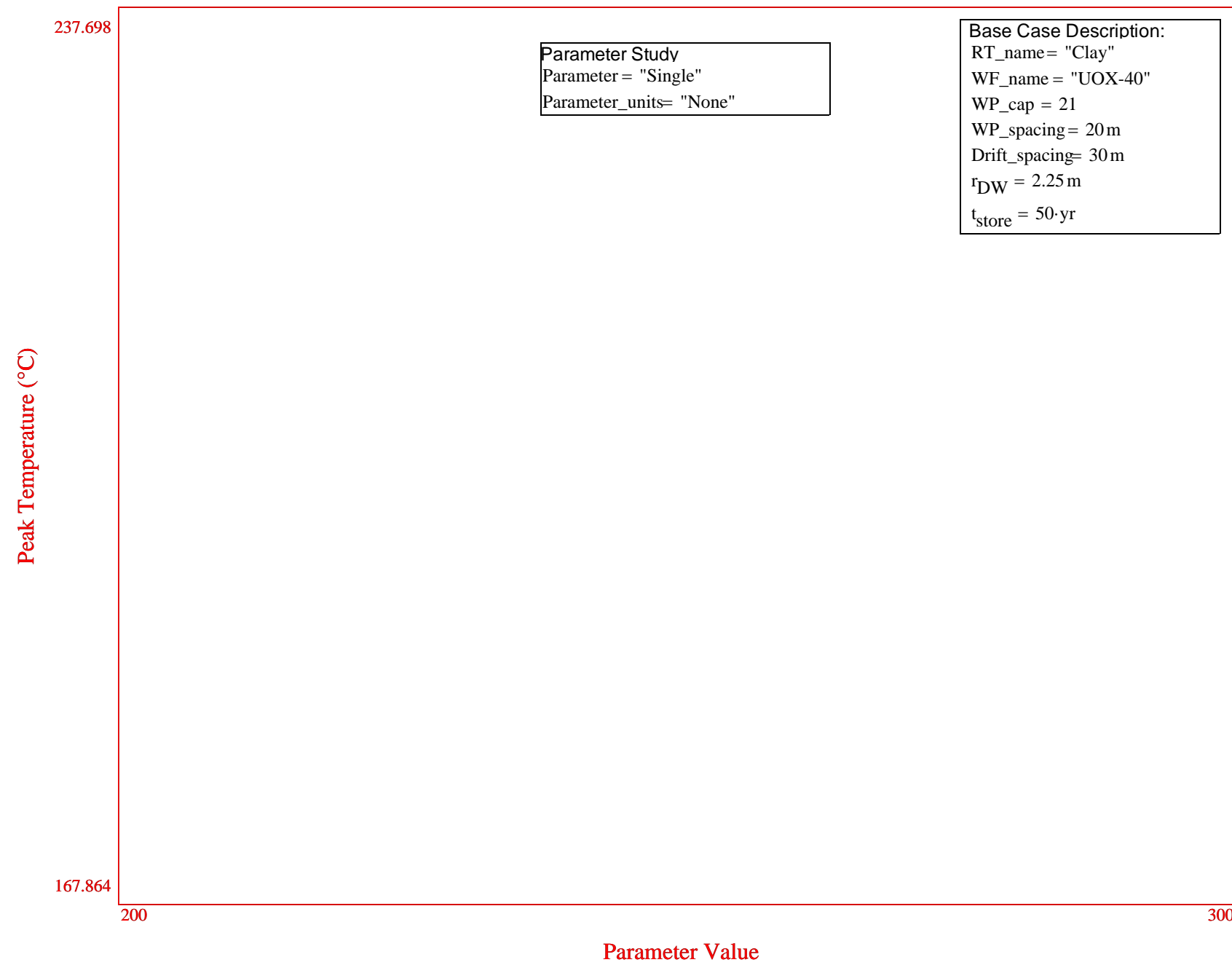k\_values^{\langle ip \cdot 2 - 1 \rangle} \right)_4$ $Peak\_EBS1\_T_{ip} := \left(Peak\_values^{\langle ip \cdot 2 - 1 \rangle} \right)_3$

$Peak\_WP\_T = (157.563)$ $Peak\_EBS3\_T = (157.563)$ $Peak\_EBS2\_T = (157.563)$ $Peak\_EBS1\_T = (100.755)$

$Peak\_Wall\_T_{ip} := \left(Peak\_values^{\langle ip \cdot 2 - 1 \rangle} \right)_2$ $Peak\_CP2\_T_{ip} := \left(Peak\_values^{\langle ip \cdot 2 - 1 \rangle} \right)_1$

$Peak\_Wall\_T = (100.744)$ $Peak\_CP2\_T = (88.663)$ $Parameter\_data = ("")$ $Parameter\_vector = ("Base Case")$

Peak Temperatures versus Parameter Study Data

Parameter Study
Parameter = "Single"
Parameter_units= "None"

Base Case Description:
RT_name = "Clay"
WF_name = "UOX-40"
WP_cap = 21
WP_spacing = 20 m
Drift_spacing= 30 m
r_{DW} = 2.25 m
t_{store} = 50·yr

237.698

167.864

200   300

Parameter Value

Peak Temperature (°C)

B.4 The Mathcad model with temperature and time dependent EBS thermal properties

This section documents a new DSEF Version 3.0 Mathcad model that allows temperature and time-dependent thermal properties within the EBS layers of the model. The PDF file and Mathcad document example shown applies these to salt for temperature-dependent thermal conductivity and time-dependent crushed salt porosity to model consolidation of the crushed salt layer with time and heat. The equations that implement these functions are shown on pages 2 and 3 of 24 in the PDF printout. The data for the time-dependent crushed salt consolidation comes from a finite element model in Hardin 2012b (Figure C-5). This model provides proof-of-principle that the thermal-analytical model can accommodate more complex thermal property modeling than the constant properties assumed in models and analysis using earlier versions of DSEF. The thermal results of this new model have a better fit to the FEM model results for the 12-PWR 40-GWd/MT burnup waste stream with 50 years of surface storage documented in Hardin 2012b than was possible with previous analyses using constant salt properties in the EBS (see Greenberg 2012b, Section G.6.2).

The EBS layer thermal conductivity values input by the DSEF Excel file have been replaced by the temperature and time-dependent functions at the beginning of the Mathcad document, and the programming loop shown on page 13 of 23 of the PDF file has been modified to use these new functions.

It should be noted that this model will work with all of the parametric study options except for parameter variations involving backfill thermal conductivity. The Mathcad model will convert any backfill thermal conductivity parameter study case into a "Single" analysis. The temperature and time-dependent EBS property functions will also work with the iterative convergence model.

With different temperature or time-dependence functions, this methodology could be used to model moisture-dependent properties covering dryout or re-wetting effects in other media. This would require other data or analysis to set the basic input functions, but then the benefits of the analytical-model approach could be applied to a broader class of problems.

DSEF R3.0 Single Model with collapsed areas - for rapid iteration cases

Allow output transients to be written back to DSEF FILE   Case_name := "229-61"

Variables for repository symmetry and extent: Write_OK := "No"

$N_{drifts} := 4$ $N_{adj} := 4$

NOTE - the Write_OK variable controls writing transient results back to Excel-DSEF, and Iterate_OK controls iterative convergence calculations for required ventilation times. This Mathcad model also allows temperature and time dependent thermal properties, and works with all DSEF parametric option cases except parametric cases involving backfill thermal conductivity..

REQUIRED REPOSITORY INPUT DATA (from DSEF):

file := "DSEF R3.0C_2013Jul29_HRG-Salt_UOX-40_Enclosed mode variable kth_Case-Kth-1.xlsm"

sheet := "Thermal-Analytical!"   DATA FOR ITERATION ON TEMPERATURE ACCEPTANCE CRITERIA:

READ DSEF INPUT FILE

TC := 100 $T_{criteria} := (TC + 273.15) \cdot K = 373.15\,K$ $T_{criteria} = 100 \cdot °C$

Input 1 = Operating Mode (enclosed or open)

$t_{convergence} := 1 \cdot yr$ CONVERGE CRITERIA FOR REQUIRED VENTILATION TIME IN YEARS

Input_1 := READEXCEL(file, concat(sheet, "A5:B5"))

Input_1 = ("MODE = Open or Enclosed:" "Enclosed") $Mode := Input_1_{1,2} = $ "Enclosed"

SET THE VARIABLE ITERATE_OK TO "NO" TO TURN OFF THE AUTOMATIC CONVERGENCE CALCULATION, AND MANUALLY RESET IT TO "YES" IF YOU WANT TO FINE TUNE YOUR ANSWER:

Input_2 := READEXCEL(file, concat(sheet, "A7:B16")) **Input 2 = Case Definitions**   ITERATE_OK := "NO"

Input 3 = Ventilation Parameters (for Open Modes)

Input_3 := READEXCEL(file, concat(sheet, "e7:f11"))

$$Input\_2 = \begin{pmatrix} \text{"Host Media"} & \text{"Salt"} \\ \text{"Rock thermal conductivity, W/m-K"} & 5.4 \\ \text{"Rock thermal diffusivity, m2/sec"} & 2.661 \times 10^{-6} \\ \text{"Repository Depth, m"} & 500 \\ \text{"Surface temperature, °C"} & 15 \\ \text{"Geothermal gradient, °C/km"} & 25 \\ \text{"Ambient temperature at depth, °C"} & 27.5 \\ \text{"Waste Package (axial) spacing, m"} & 20 \\ \text{"Drift / Borehole (lateral) spacing, m"} & 20 \\ \text{"Surface storage time, y"} & 50 \end{pmatrix}$$

$$Input\_3 = \begin{pmatrix} \text{"Ventilation Duration, yr"} & \text{"N/A"} \\ \text{"Unventilated Closure Duration (Backfill Installation), yr"} & \text{"N/A"} \\ \text{"Ventilation Thermal Efficiency, %"} & \text{"N/A"} \\ \text{"Rock Wall Emissivity"} & \text{"N/A"} \\ \text{"Waste Package Emissivity"} & \text{"N/A"} \end{pmatrix}$$

$RT_name := Input_2_{1,2} = $ "Salt"

$Kth := Input\_2_{2,2} \cdot \dfrac{W}{m \cdot K} = 5.4\,\dfrac{m \cdot kg}{K \cdot s^3}$

$\alpha := Input\_2_{3,2} \cdot \dfrac{m^2}{s} = 2.661 \times 10^{-6}\,\dfrac{m^2}{s}$

$WP\_depth := Input\_2_{4,2} \cdot m = 500\,m$

$T_{surface} := \left(Input\_2_{5,2} + 273.15\right) \cdot K = 288.15\,K$

$geothermal\_gradient := Input\_2_{6,2} \dfrac{K}{km} = 0.025\,\dfrac{K}{m}$

$t_{vent} := if\left[(Mode = \text{"Enclosed"}), 0, Input\_3_{1,2}\right] \cdot yr = 0 \cdot yr$

$t_{backfill} := if\left[(Mode = \text{"Enclosed"}), 0, Input\_3_{2,2}\right] \cdot yr = 0 \cdot yr$

$V_{eff} := if\left[(Mode = \text{"Enclosed"}), 0, Input\_3_{3,2}\right] = 0$

$\varepsilon_{wall} := if\left[(Mode = \text{"Enclosed"}), .9, Input\_3_{4,2}\right] = 0.9$

$\varepsilon_{WP} := if\left[(Mode = \text{"Enclosed"}), .6, Input\_3_{5,2}\right] = 0.6$

OVER-RIDE VENTILATION DURATION

$T_{ambient} := \left(Input\_2_{7,2} + 273.15\right) \cdot K = 300.65\ K$

$WP\_spacing := Input\_2_{8,2} \cdot m = 20\ m$

<mark>OVER-RIDE DRIFT SPACING</mark>

$Drift\_spacing := Input\_2_{9,2} \cdot m = 20\ m$

$t_{store} := Input\_2_{10,2} \cdot yr = 50 \cdot yr$

$\boxed{t_{operate} := \left(t_{store} + t_{vent}\right) = 50 \cdot yr}$ <mark>T_OPERATE = T_STORE + T_VENTILATE</mark>

$\boxed{t_{closure} := t_{operate} + t_{backfill} = 50 \cdot yr}$ <mark>TCLOSURE = TOPERATE + TIME TO BACKFILL</mark>

Input 4 = ENGINEERED BARRIER SYSTEM DATA: **Input 5 = COMPLIANCE POINT 2 INPUT DATA**

$Input\_4 := READEXCEL(file, concat(sheet, "A20:F27"))$ $Input\_5 := READEXCEL(file, concat(sheet, "C32"))$

$Input\_4 = \begin{pmatrix} \text{"Waste Form Outer Radius, m"} & 0.555 & \text{"N/A"} & 0.555 & \text{"UOX-40"} & \text{"N/A"} \\ \text{"Canister"} & 0 & 0.555 & 0.555 & \text{"Carbon Steel"} & \text{"N/A"} \\ \text{"Waste Package"} & 0.03 & 0.555 & 0.585 & \text{"Carbon Steel"} & \text{"N/A"} \\ \text{"Salt Layer 1"} & 0.821 & 0.585 & 1.406 & \text{"75\% Intact Salt at T4°C"} & 3.16 \\ \text{"Salt Layer 2"} & 0.821 & 1.406 & 2.227 & \text{"75\% Intact Salt at T3°C"} & 3.16 \\ \text{"Salt Layer 3"} & 0.821 & 2.227 & 3.048 & \text{"75\% Intact Salt at T2°C"} & 3.16 \\ \text{"Salt Layer 4"} & 0.952 & 3.048 & 4 & \text{"Intact Salt 100°C"} & 4.2 \\ \text{"Host Rock Inner Radius, m ----}{>}\text{"} & \text{NaN} & 4 & \text{NaN} & \text{NaN} & \text{NaN} \end{pmatrix}$

$Input\_5 = (5.25)$

$r_{CP2} := Input\_5_1 \cdot m = 5.25\ m$

<mark>DATA AND FORMULAS TO ALLOW TRANSIENT THERMAL CONDUCTIVITY WITHIN THE EBS</mark>

Thermal conductivity of intact and crushed salt, based on Reference:
3-D Thermal Analyses of High-Level Waste Emplaced in a Generic Salt Repository
AFCI-WAST-PMO-MI-DV-2009-000002; February, 2009. (D. J. Clayton, SNL, and C. W. Gable, Los Alamos).

<mark>SALT THERMAL CONDUCTIVITY AS A FUNCTION OF TEMPERATURE AND POROSITY</mark>

$k_{intact\_0} := 5.4 \dfrac{W}{m \cdot K}$ $k_{intact}(T) := k_{intact\_0} \cdot \left(\dfrac{300 \cdot K}{T}\right)^{1.14}$ Where T is in Kelvin $k_{intact}(372.15 \cdot K) = 4.224 \cdot \dfrac{W}{m \cdot K}$

$kcs(\varphi) := \left(-270\varphi^4 + 370\varphi^3 - 136\varphi^2 + 1.5\varphi + 5\right) \cdot 1.08 \cdot \dfrac{W}{m \cdot K}$ Where φ is porosity

$k_{crushed}(\varphi, T) := kcs(\varphi) \cdot \left(\dfrac{300 \cdot K}{T}\right)^{1.14}$ $k_{crushed}[0, (273.15 + 27.5) \cdot K] = 5.4 \cdot \dfrac{W}{m \cdot K}$ $k_{crushed}[0, (273.15 + 100) \cdot K] = 4.2 \cdot \dfrac{W}{m \cdot K}$

Crushed salt thermal k at 100°C vs porosity

$k_{crushed}(\varphi, 373.15 \cdot K)$
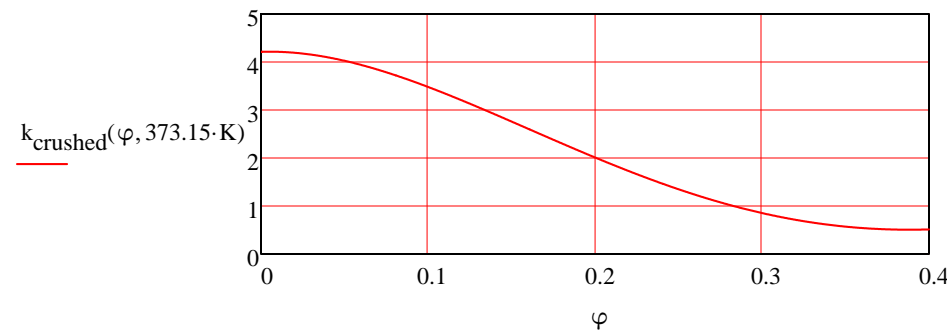
Intact salt thermal conductivity vs T (°C)

$\dfrac{k_{intact}[(x+273.15) \cdot K]}{\left(\dfrac{W}{m \cdot K}\right)}$
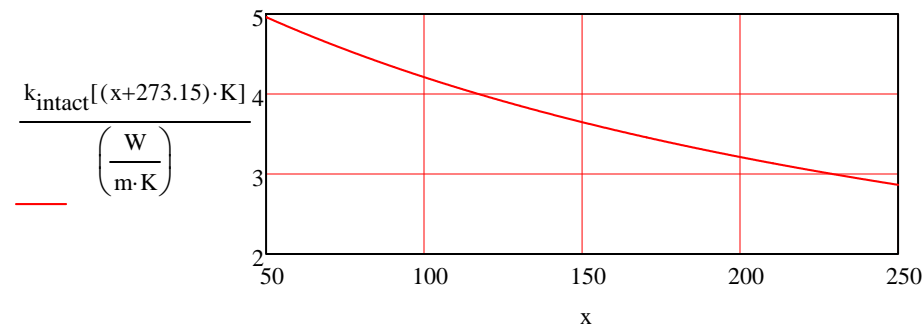
k.consolidate is based on an initial porosity of φ_0 and a final porosity of φ_1, and assumes a linear increase over time t.$_{consolidate}$: $\qquad \varphi_0 := 0.20 \qquad \varphi_1 := 0.02 \qquad t_{consolidate} := 10 \cdot yr$

For comparison with SNL caclulation (E**. Hardin, T. Hadgu, D. Clayton, R. Howard, H. Greenberg, J. Blink, M. Sharma, M. Sutton, J. Carter, M. Dupont, P. Rodwell.** *Repository Disposal Concepts and Thermal Load Management Analysis.* **FCRD-UFD-2012-00219 Rev. 2. November, 2012)** assume an initial crushed salt porosity $\varphi_0 = 0.20$, and use a piece-wise linear function to fit an set of data representing the time-dependent consolidation of crushed salt (from FCRD-UFD-2012-00219 figure C-5), where the first column is time in years, and the second column is porosity fraction.

$$\text{Consolidation\_data\_array} := \begin{pmatrix} 0 + \dfrac{t_{store}}{yr} & 0.20 \\[2mm] 20 + \dfrac{t_{store}}{yr} & 0.09 \\[2mm] 40 + \dfrac{t_{store}}{yr} & 0.06 \\[2mm] 60 + \dfrac{t_{store}}{yr} & 0.05 \\[2mm] 95 + \dfrac{t_{store}}{yr} & 0.04 \\[2mm] 200 + \dfrac{t_{store}}{yr} & 0.02 \\[2mm] 1000 + \dfrac{t_{store}}{yr} & 0.02 \end{pmatrix}$$

$$SS := lspline\left(\text{Consolidation\_data\_array}^{\langle 1 \rangle}, \text{Consolidation\_data\_array}^{\langle 2 \rangle}\right)$$

$$Porosity(t) := interp\left(SS, \text{Consolidation\_data\_array}^{\langle 1 \rangle}, \text{Consolidation\_data\_array}^{\langle 2 \rangle}, t\right)$$

$$Porosity(50) = 0.2 \qquad Porosity(80) = 0.068$$

$$k_{consolidate}(t, T) := \begin{vmatrix} k_{crushed}(Porosity(t), T) & \text{if } \left[t \le \left(\text{Consolidation\_data\_array}^{\langle 1 \rangle}\right)_6 \right] \\[2mm] k_{crushed}\left[\left(\text{Consolidation\_data\_array}^{\langle 2 \rangle}\right)_6, T\right] & \text{otherwise} \end{vmatrix}$$

$$k_{consolidate}\left(\dfrac{t_{store}}{yr}, 373.15 \cdot K\right) = 2.011 \cdot \dfrac{W}{m \cdot K}$$

Crushed salt consolidation as a function of time

Crushed salt thermal conductivity at 100°C (with consolidation)
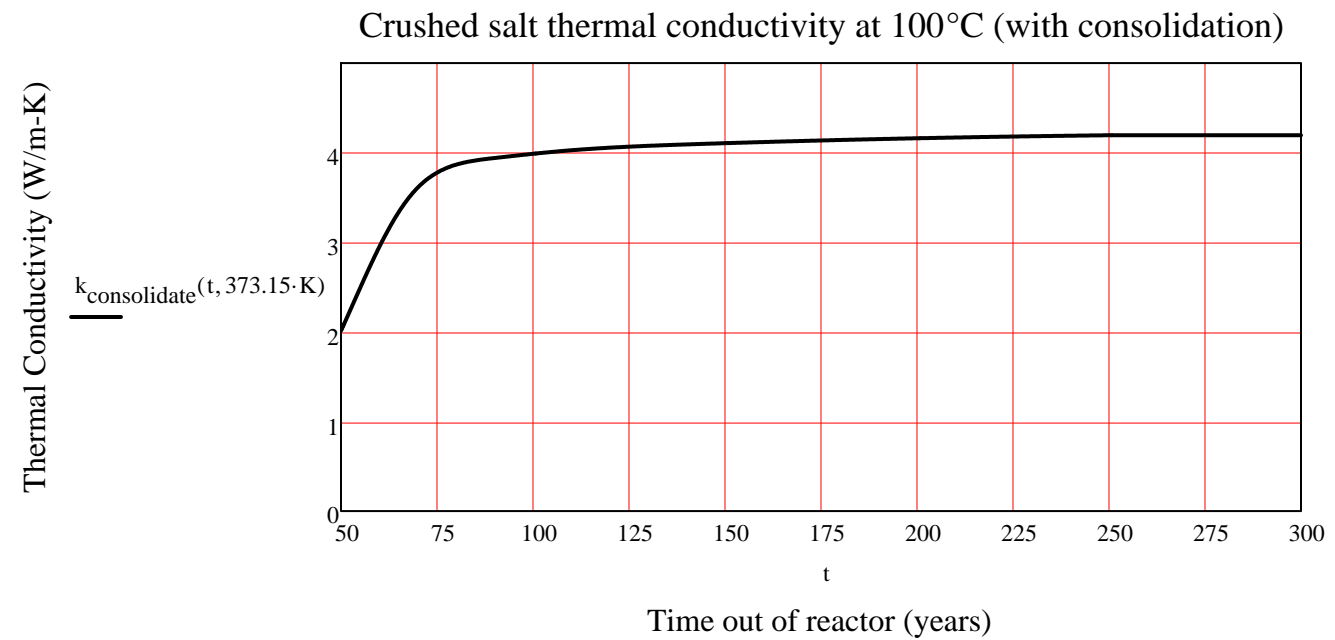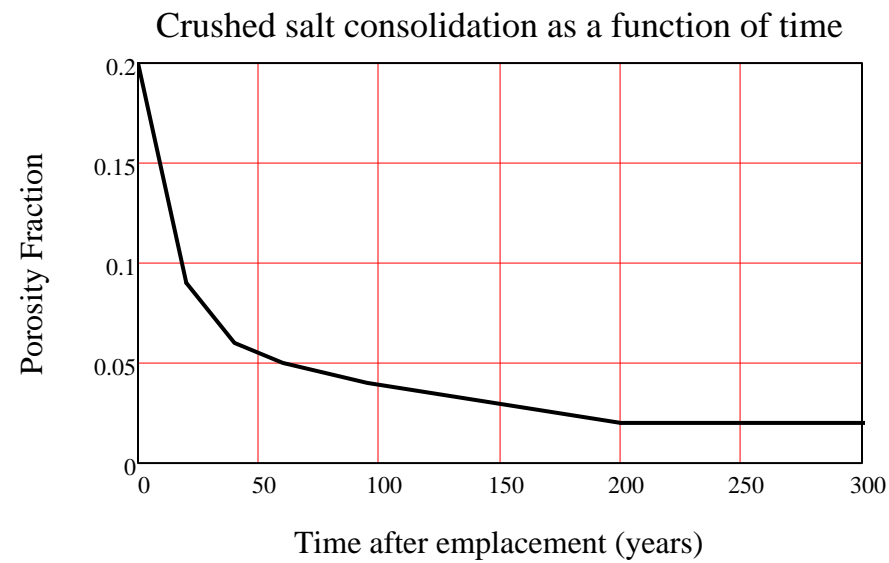
$r_{DW} := Input\_4_{8,3} \cdot m = 4\,m$

$r_{WP} := Input\_4_{3,4} \cdot m = 0.585\,m$

$EBS\_name_1 := Input\_4_{7,1} = \text{"Salt Layer 4"}$ $EBS\_material_1 := Input\_4_{7,5} = \text{"Intact Salt 100°C"}$

$thickness_1 := Input\_4_{7,2} \cdot m = 0.952\,m$ $r_1 := Input\_4_{7,4} \cdot m = 4\,m$

$k1 := Input\_4_{7,6} = 4.2$ $k_1 := if[(k1 = \text{"N/A"}),0,k1] \cdot \dfrac{W}{m \cdot K} = 4.2 \cdot \dfrac{W}{m \cdot K}$ $k_1(T) := if\left[(k1 = \text{"N/A"}),0,k_{intact}(T)\right]$

$EBS\_name_2 := Input\_4_{6,1} = \text{"Salt Layer 3"}$ $EBS\_material_2 := Input\_4_{6,5} = \text{"75% Intact Salt at T2°C"}$

$thickness_2 := Input\_4_{6,2} \cdot m = 0.821\,m$ $r_2 := Input\_4_{6,4} \cdot m = 3.048\,m$ THE FOLLOWING FORMULAS ASSUME 75% CONTACT WITH INTACT SALT AND 25% CONTACT WITH CRUSHED SALT.

$k2 := Input\_4_{6,6} = 3.16$ $k_2 := if[(k2 = \text{"N/A"}),0,k2] \cdot \dfrac{W}{m \cdot K} = 3.16 \cdot \dfrac{W}{m \cdot K}$ $k_2(t,T2) := if\left[(k2 = \text{"N/A"}),0,0.75 \cdot k_{intact}(T2) + 0.25 \cdot k_{consolidate}\left(\dfrac{t}{yr},T2\right)\right]$

$k_{radiation}(t,T2) := if\left[(Mode = \text{"Enclosed"}),k_2(t,T2),0\right]$

$EBS\_name_3 := Input\_4_{5,1} = \text{"Salt Layer 2"}$ $EBS\_material_3 := Input\_4_{5,5} = \text{"75% Intact Salt at T3°C"}$

$thickness_3 := Input\_4_{5,2} \cdot m = 0.821\,m$ $r_3 := Input\_4_{5,4} \cdot m = 2.227\,m$

$k3 := Input\_4_{5,6} = 3.16$ $k_3 := if[(k3 = \text{"N/A"}),0,k3] \cdot \dfrac{W}{m \cdot K} = 3.16 \cdot \dfrac{W}{m \cdot K}$ $k_3(t,T3) := if\left[(k2 = \text{"N/A"}),0,0.75 \cdot k_{intact}(T3) + 0.25 \cdot k_{consolidate}\left(\dfrac{t}{yr},T3\right)\right]$

$EBS\_name_4 := Input\_4_{4,1} = \text{"Salt Layer 1"}$ $EBS\_material_4 := Input\_4_{4,5} = \text{"75% Intact Salt at T4°C"}$

$thickness_4 := Input\_4_{4,2} \cdot m = 0.821\,m$ $r_4 := Input\_4_{4,4} \cdot m = 1.406\,m$

$k4 := Input\_4_{4,6} = 3.16$ $k_4 := if[(k4 = \text{"N/A"}),0,k4] \cdot \dfrac{W}{m \cdot K} = 3.16 \cdot \dfrac{W}{m \cdot K}$ $k_4(t,T4) := if\left[(k2 = \text{"N/A"}),0,0.75 \cdot k_{intact}(T4) + 0.25 \cdot k_{consolidate}\left(\dfrac{t}{yr},T4\right)\right]$

$k_4[0 \cdot yr,(100 + 273.15) \cdot K] = 3.619 \cdot \dfrac{W}{m \cdot K}$ $k_4[1 \cdot yr,(100 + 273.15) \cdot K] = 3.578 \cdot \dfrac{W}{m \cdot K}$

$k_4[2 \cdot yr,(100 + 273.15) \cdot K] = 3.542 \cdot \dfrac{W}{m \cdot K}$ $k_4[10 \cdot yr,(100 + 273.15) \cdot K] = 3.372 \cdot \dfrac{W}{m \cdot K}$

Define the total thermal resistance between the rock wall and the waste package surface based on a heat flux per unit area, it is then applied to a heat flux is per unit length adjusting to area per unit length and q_L (W/m):

$r_{WP} = 0.585 \ m$ $\qquad r_4 = 1.406 \ m$ $\qquad r_3 = 2.227 \ m$ $\qquad r_2 = 3.048 \ m$ $\qquad r_1 = 4 \ m$ $\qquad r_{DW} = 4 \ m$

$$R_1(T) := if\left[thickness_1 = 0 \lor (k1 = "N/A"), 0, \frac{r_{DW}}{k_1(T)} \cdot ln\left(\frac{r_1}{r_2}\right)\right]$$

$R_1[(100 + 273.15)\cdot K] = 0.258 \cdot \dfrac{m^2 \cdot K}{W}$ **Thermal resistance**

$EBS\_name_1 = "Salt \ Layer \ 4"$ $\quad EBS\_material_1 = "Intact \ Salt \ 100°C"$

$$R_2(t, t_{operate}, t_{backfill}, T2) := \left| \begin{array}{l} kk \leftarrow k_{radiation}(t, T2) \cdot \left[t < (t_{operate} + t_{backfill})\right] + k_2(t, T2) \cdot \left[t \geq (t_{operate} + t_{backfill})\right] \\[2mm] return \ if\left[\left[(thickness_2 = 0) \lor (kk = 0)\right], 0, \frac{r_{DW}}{kk} \cdot ln\left(\frac{r_2}{r_3}\right)\right] \end{array} \right.$$

$$\frac{r_{DW}}{k_2[0\cdot yr, (100 + 273.15)\cdot K]} \cdot ln\left(\frac{r_2}{r_3}\right) = 0.347 \cdot \frac{m^2 \cdot K}{W}$$

$EBS\_name_2 = "Salt \ Layer \ 3$ $\quad EBS\_material_2 = "75\% \ Intact \ Salt \ at \ T2°C"$

$$R_2(5\cdot yr, 300\cdot yr, 10\cdot yr, 373.15\cdot K) = 0.363 \cdot \frac{m^2 \cdot K}{W}$$

$$R_3(t, T3) := if\left[thickness_3 = 0 \lor (k3 = "N/A"), 0, \frac{r_{DW}}{k_3(t, T3)} \cdot ln\left(\frac{r_3}{r_4}\right)\right]$$

$R_3(0\cdot yr, 373.15\cdot K) = 0.508 \cdot \dfrac{m^2 \cdot K}{W}$

$EBS\_name_3 = "Salt \ Layer \ 2"$ $\qquad EBS\_material_3 = "75\% \ Intact \ Salt \ at \ T3°C"$

$$R_4(t, T4) := if\left[thickness_4 = 0 \lor (k4 = "N/A"), 0, \frac{r_{DW}}{k_4(t, T4)} \cdot ln\left(\frac{r_4}{r_{WP}}\right)\right]$$

$R_4(0\cdot yr, 373.15\cdot K) = 0.969 \cdot \dfrac{m^2 \cdot K}{W}$

$EBS\_name_4 = "Salt \ Layer \ 1"$ $\qquad EBS\_material_4 = "75\% \ Intact \ Salt \ at \ T4°C"$

$$R_{Total}(t, T1, T2, T3, T4) := R_1(T1) + R_2(t, t_{operate}, t_{backfill}, T2) + R_3(t, T3) + R_4(t, \ldots$$ Total thermal resistance between wall and waste package

$t_{backfill} = 0\cdot yr$ $\qquad t_{operate} = 50\cdot yr$

$R_{continuous}(t, r, T1, T2, T3, T4) :=$

$kk_2 \leftarrow k_{radiation}(t, T2) \cdot [t < (t_{operate} + t_{backfill})] + k_2(t, T2) \cdot [t \geq (t_{operate} + t_{backfill})]$

$R \leftarrow R_1(T1) + R_2(t, t_{operate}, t_{backfill}, T2) + R_3(t, T3) + if\left[\left[(thickness_4 = 0) \vee (k4 = "N/A")\right], 0, \dfrac{r_{DW}}{k_4(t, T4)} \cdot \ln\left(\dfrac{r_4}{r}\right)\right]$ if $r \leq r_4 \wedge r \geq r_{WP}$

$R \leftarrow R_1(T1) + R_2(t, t_{operate}, t_{backfill}, T2) + if\left[\left[(thickness_3 = 0) \vee (k3 = "N/A")\right], 0, \dfrac{r_{DW}}{k_3(t, T3)} \cdot \ln\left(\dfrac{r_3}{r}\right)\right]$ if $r \leq r_3 \wedge r > r_4$

$R \leftarrow R_1(T1) + if\left[\left[(thickness_2 = 0) \vee kk_2 = 0\right], 0, \dfrac{r_{DW}}{kk_2} \cdot \ln\left(\dfrac{r_2}{r}\right)\right]$ if $r \leq r_2 \wedge r \geq r_3$

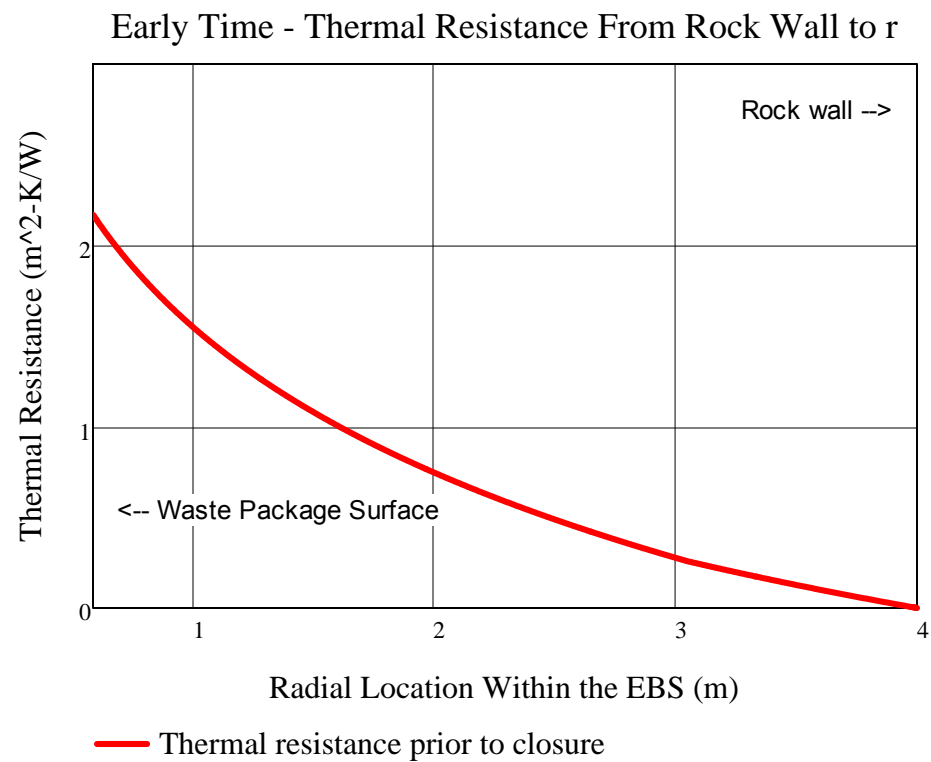$R \leftarrow if\left[\left[(thickness_1 = 0) \vee (k1 = "N/A")\right], 0, \dfrac{r_{DW}}{k_1(T1)} \cdot \ln\left(\dfrac{r_1}{r}\right)\right]$ if $r \leq r_{DW} \wedge r \geq r_2$

$R \leftarrow$ "Invalid Radius" otherwise

return R

$R_{continuous}(5 \cdot yr, r_{WP}, 373.15 \cdot K, 373.15 \cdot K, 373.15 \cdot K, 373.15 \cdot K) = 2.169 \cdot \dfrac{m^2 \cdot K}{W}$ $\qquad$ $R_{continuous}(5 \cdot yr, r_{WP}, 473.15 \cdot K, 373.15 \cdot K, 373.15 \cdot K, 373.15 \cdot K) = 2.249 \cdot \dfrac{m^2 \cdot K}{W}$

Early Time - Thermal Resistance From Rock Wall to r

Rock wall -->

<-- Waste Package Surface

Thermal Resistance (m^2-K/W)

Radial Location Within the EBS (m)

—— Thermal resistance prior to closure

$r_{DW} = 4\ m$

$r_1 = 4\ m$ $\qquad$ EBS_name$_1$ = "Salt Layer 4" EBS_material$_1$ = "Intact Salt 100°C"

$r_2 = 3.048\ m$ $\qquad$ Note that for "open modes", the backfill hasn't been emplaced at early time, and EBS-2 is only radiation.

$r_3 = 2.227\ m$ $\qquad$ EBS_name$_3$ = "Salt Layer 2" EBS_material$_3$ = "75% Intact Salt at T3°C"

$r_4 = 1.406\ m$ $\qquad$ EBS_name$_4$ = "Salt Layer EBS_material$_4$ = "75% Intact Salt at T4°C"

$r_{WP} = 0.585\ m$

$R_1(373.15 \cdot K) = 0.258 \cdot \dfrac{m^2 \cdot K}{W}$ $\qquad$ $R_2(5 \cdot yr, t_{operate}, t_{backfill}, 373.15 \cdot K) = 0.363 \cdot \dfrac{m^2 \cdot K}{W}$

$R_3(5 \cdot yr, 373.15 \cdot K) = 0.532 \cdot \dfrac{m^2 \cdot K}{W}$ $\qquad$ $R_4(5 \cdot yr, 373.15 \cdot K) = 1.015 \cdot \dfrac{m^2 \cdot K}{W}$

$R_{Total}(5yr, 373.15 \cdot K, 373.15 \cdot K, 373.15 \cdot K, 373.15 \cdot K) = 2.169 \cdot \dfrac{m^2 \cdot K}{W}$

Late Time - Thermal Resistance From Rock Wall to r

Thermal resistance prior to closure
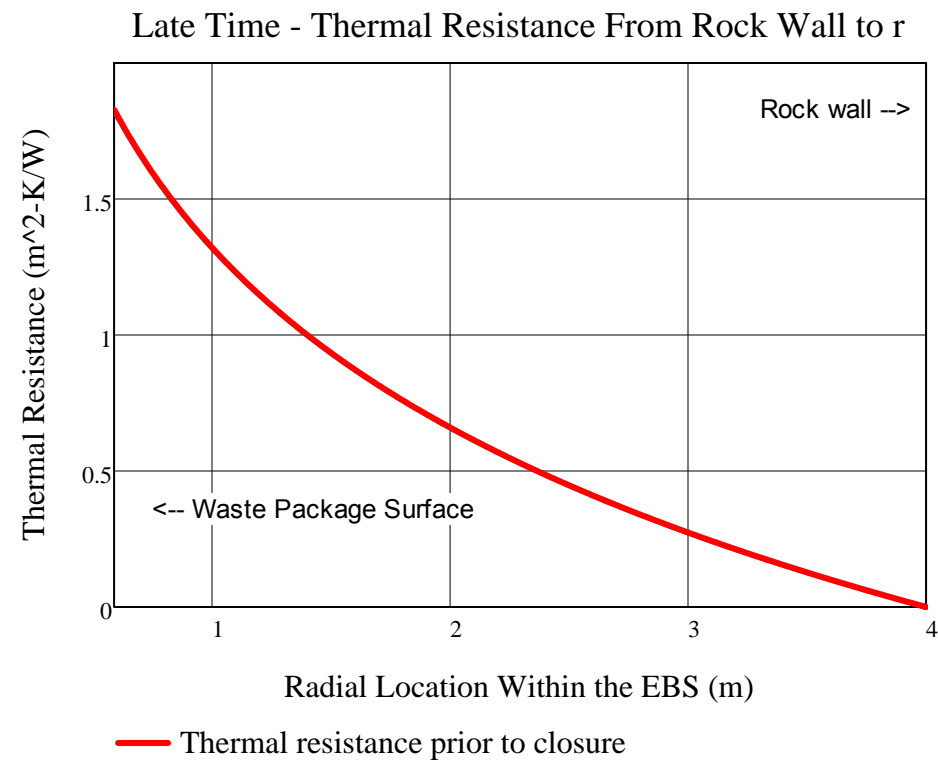
$r_{DW} = 4\,m$

$r_1 = 4\,m$ $EBS_name_1 = $ "Salt Layer 4" $EBS_material_1 = $ "Intact Salt 100°C"

$r_2 = 3.048\,m$ $EBS_name_2 = $ "Salt Layer 3" $EBS_material_2 = $ "75% Intact Salt at T2°C"

$r_3 = 2.227\,m$ $EBS_name_3 = $ "Salt Layer 2" $EBS_material_3 = $ "75% Intact Salt at T3°C"

$r_4 = 1.406\,m$ $EBS_name_4 = $ "Salt Layer $EBS_material_4 = $ "75% Intact Salt at T4°C"

$r_{WP} = 0.585\,m$

$R_1(373.15 \cdot K) = 0.258 \cdot \dfrac{m^2 \cdot K}{W}$ $R_2(1000 \cdot yr, t_{operate}, t_{backfill}, 373.15 \cdot K) = 0.298 \cdot \dfrac{m^2 \cdot K}{W}$

$R_3(1000 \cdot yr, 373.15 \cdot K) = 0.437 \cdot \dfrac{m^2 \cdot K}{W}$ $R_4(1000 \cdot yr, 373.15 \cdot K) = 0.834 \cdot \dfrac{m^2 \cdot K}{W}$

$R_{Total}(1000yr, 373.15 \cdot K, 373.15 \cdot K, 373.15 \cdot K, 373.15 \cdot K) = 1.828 \cdot \dfrac{m^2 \cdot K}{W}$

INPUT 6 = WASTE FORM DATA

$Input\_6 := READEXCEL(file, concat(sheet, "A35:B38"))$

$Input\_6 = \begin{pmatrix} \text{"Waste form short name"} & \text{"UOX-40"} \\ \text{"Waste form type"} & \text{"Assembly"} \\ \text{"Waste package capacity"} & 12 \\ \text{"Waste package length, m"} & 5 \end{pmatrix}$

$WF_name := Input_6_{1,2} = $ "UOX-40"

$WF_type := Input_6_{2,2} = $ "Assembly"

$WP\_cap := Input\_6_{3,2} = 12$

$WP\_length := Input\_6_{4,2} \cdot m = 5\,m$

Outside of the liner

$A_1 := 2 \cdot \pi \cdot r_1 \cdot WP\_length = 125.66\,m^2$

$A_{DW} := 2 \cdot \pi \cdot r_{DW} \cdot WP\_length = 125.664\,m^2$

Outside of the backfill

$A_2 := 2 \cdot \pi \cdot r_2 \cdot WP\_length = 95.76\,m^2$

Outside of the envelope

$A_3 := 2 \cdot \pi \cdot r_3 \cdot WP\_length = 69.96\,m^2$

Outside of the buffer

$A_4 := 2 \cdot \pi \cdot r_4 \cdot WP\_length = 44.17\,m^2$

$A_{WP} := 2 \cdot \pi \cdot r_{WP} \cdot WP\_length = 18.378\,m^2$

DSEF R3.0_Mathcad with temperature and time depndent EBS thermal conductivity.xmcd

Stefan Boltzmann constant $\qquad \sigma := 5.670 \cdot 10^{-8} \cdot \dfrac{W}{m^2 \cdot K^4}$

The basis for the rock and waste package emissivity assumed is F. P. Incropera and D.P. DeWitt, *Fundamentals of Heat and Mass Transfer*, 4th Edition, 1996, Table A-11, which shows a range of 0.88 to 0.93 is adapted from hemispherical emissivity of rock at around 300 K. This range is corroborated by the "Heat Transmission" section of Perry's Chemical Engineers Handbook, 6th Edition, 1984 (Table 10-17, pages 10-51 to 10-52) for normal emissivity of rough silica and rough fused quartz, ranging from 0.8 to 0.93. The waste package surface is assumed to be covered with dust and dirt. The emissivity values to the left were specified in DSEF, and should be changed there if necessary.

Waste Package emissivity $\qquad \varepsilon_{WP} = 0.6$

Rock wall or cementitious liner emissivity $\qquad \varepsilon_{wall} = 0.9$

Reference for radiation heat transfer coefficient, h_{rad}, is from Incropera and DeWitt, Table 13.3 for concentric infinite cylinders (based on the inner surface as the heat source), and is also referenced in the YMP *Ventilation Model and Analysis Report*, ANL-EBS-MD-000030 REV 04, Oct. 2004, page 6-8.

$$h_{rad\_infinite}(r_i, r_o, \varepsilon_i, \varepsilon_o) := \dfrac{\sigma}{\dfrac{1}{\varepsilon_i} + \left(\dfrac{1-\varepsilon_o}{\varepsilon_o}\right) \cdot \dfrac{r_i}{r_o}}$$

$h_{rad\_infinite}(r_{WP}, r_{DW}, \varepsilon_{WP}, \varepsilon_{wall}) = 3.369 \times 10^{-8} \cdot \dfrac{W}{m^2 K^4}$

For radiation between the liner and the envelope (both metal surfaces) use r_2 and r_3, and assume the same emissivity for both surfaces.

Usage is Q in watts = $h^*A_i{}^*(T_i{}^\wedge 4 - T_o{}^\wedge 4)$

$Q_{rad\_infinite}(r_i, r_o, \varepsilon_i, \varepsilon_o, L, T_{cold}, T_{hot}) := h_{rad\_infinite}(r_i, r_o, \varepsilon_i, \varepsilon_o) \cdot (2 \cdot \pi \cdot r_i \cdot L)\left(T_{hot}{}^4 - T_{cold}{}^4\right)$

$Q_{rad\_infinite}(r_3, r_2, \varepsilon_{WP}, \varepsilon_{wall}, WP\_length, 300 \cdot K, 600 \cdot K) = 2.758 \times 10^5 \, W$

$Q_{L\_rad\_infinite}(r_i, r_o, \varepsilon_i, \varepsilon_o, T_{cold}, T_{hot}) := h_{rad\_infinite}(r_i, r_o, \varepsilon_i, \varepsilon_o) \cdot (2 \cdot \pi \cdot r_i)\left(T_{hot}{}^4 - T_{cold}{}^4\right)$

$Q_{L\_rad\_infinite}(r_3, r_2, \varepsilon_{WP}, \varepsilon_{wall}, 300 \cdot K, 600 \cdot K) = 5.515 \times 10^4 \cdot \dfrac{W}{m}$

Heat transfer by radiation from NIRAS/ONDRAF December 2005 Report: Eef Weetjens and Xavier Sillen; *Thermal analysis of the Supercontainer concept 2D axisymmetric heat transport calculations,* Section 6.4.3. Pg 34, equation 29.

$$Q_{L\_infinite}(r_i, r_o, \varepsilon_i, \varepsilon_o, T_{cold}, T_{hot}) := \dfrac{2\pi\,\sigma \cdot \left(T_{hot}{}^4 - T_{cold}{}^4\right)}{\dfrac{1-\varepsilon_i}{\varepsilon_i \cdot r_i} + \dfrac{1}{r_i} + \dfrac{1-\varepsilon_o}{\varepsilon_o \cdot r_o}}$$

$Q_{L\_infinite}(r_3, r_2, \varepsilon_{WP}, \varepsilon_{wall}, 300 \cdot K, 600 \cdot K) = 5.515 \times 10^4 \cdot \dfrac{W}{m}$

This is the same as the Incropera and DeWitt result, $Q_{L\_rad\_infinite}$

INPUT 7 = PARAMETRIC STUDY VARIABLE INPUT DATA

$\text{Input\_7} := \text{READEXCEL}(\text{file}, \text{concat}(\text{sheet}, \text{"F29:F41"}))$

	1
1	1
2	"Single"
3	"None"
4	""
5	""
6	""
7	""
8	""
9	""
10	""
11	""
12	""
13	""

$\text{Input\_7} =$ (shown in table above)

$\blacksquare \neq \blacksquare$

PARAMETRIC STUDIES OF "BACKFILL THERMAL CONDUCTIVITY" NOT ALLOWED
FOR TEMPERATURE AND TIME-DEPENDENT THERMAL PROPERTY ANALYSES.
THEREFORE, PARAMETER TYPE IS RESET TO "SINGLE",

$\text{Cases} := \begin{vmatrix} \text{Input\_7}_1 & \text{if Input\_7}_2 \neq \text{"Backfill Thermal Conductivity"} \\ 1 & \text{otherwise} \end{vmatrix}$

$\text{Parameter} := \begin{vmatrix} \text{"Single"} & \text{if Input\_7}_2 = \text{"Backfill Thermal Conductivity"} \\ \text{Input\_7}_2 & \text{otherwise} \end{vmatrix}$

$\text{Parameter\_units} := \text{Input\_7}_3 = \text{"None"}$

$ij := 1 .. \text{Cases}$

$\text{Parameter\_data}_{ij} := \text{Input\_7}_{ij+3}$

$\text{Parameter\_description}_{ij} := \begin{vmatrix} \text{"Single Base Case"} & \text{if Cases} = 1 \\ \text{concat}\left[\text{num2str}\left[\text{Input\_7}_{(ij+3)}\right], \text{", "}, \text{Input\_7}_3\right] & \text{otherwise} \end{vmatrix}$

$\text{Parameter\_data} = (\text{""})$ $\text{Parameter\_description} = (\text{"Single Base Case"})$

INPUT 8 = DECAY HEAT INPUT DATA PER UNIT SOURCE (ASSEMBLY OR CANISTER):

$\text{Input\_8\_size} := \text{READEXCEL}(\text{file}, \text{concat}(\text{sheet}, \text{"C43"}))$ $\text{Input\_8\_size}_1 = 58$ $\text{Decay\_heat\_range} := \text{concat}\left[\text{"A43:B"}, \text{num2str}\left(\left(\text{Input\_8\_size}_1 + 42\right)\right)\right] = \text{"A43:B100"}$

$\text{Input\_8} := \text{READEXCEL}(\text{file}, \text{concat}(\text{sheet}, \text{Decay\_heat\_range}))$

$\text{Time\_out\_of\_Reactor} := \text{Input\_8}^{\langle 1 \rangle} \cdot \text{yr}$ $\text{Decay\_Heat\_per\_Cnt} := \text{Input\_8}^{\langle 2 \rangle} \cdot \text{W}$

$\text{Input\_8} =$

	1	2
1	5	$1.028 \cdot 10^3$
2	5.1	$1.011 \cdot 10^3$
3	5.5	949.125
4	5.75	916.671
5	6	887.984
6	8	742.948
7	10	670.028
8	11.5	634.239
9	15	576.929
10	20	...

$\text{Time\_out\_of\_Reactor} =$

	1
1	5
2	5.1
3	5.5
4	5.75
5	6
6	8
7	10
8	11.5
9	15
10	...

$\cdot \text{yr}$

$\text{Decay\_Heat\_per\_Cnt} =$

	1
1	$1.028 \cdot 10^3$
2	$1.011 \cdot 10^3$
3	949.125
4	916.671
5	887.984
6	742.948
7	670.028
8	634.239
9	576.929
10	...

$\cdot \text{W}$

$Q(t) := interp\left(cspline\left(Time\_out\_of\_Reactor, Decay\_Heat\_per\_Cnt\right), Time\_out\_of\_Reactor, Decay\_Heat\_per\_Cnt, t\right)$

Ventilation efficiency for open systems is $\boxed{V_{eff} = 0}$ between t_{store} and $t_{operate}$
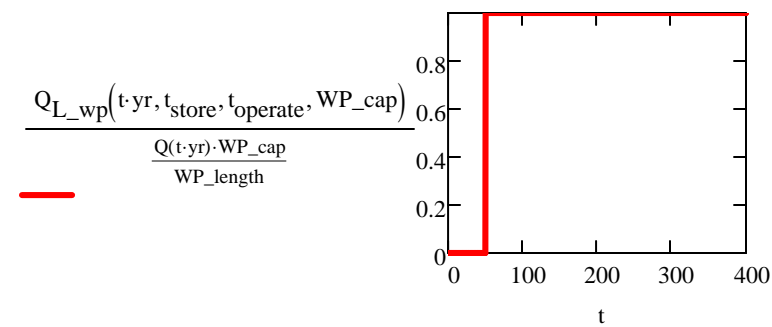
<mark>FUNCTION DEFINITION FOR ONE OUTPUT FILE</mark>

<mark>FORMULAS FOR CALCULATING THE TRANSIENT DRIFT WALL TEMPERATURE:</mark>

<mark>Central waste package:</mark>

$$Q_{L\_wp}\left(t, t_{store}, t_{operate}, WP\_cap\right) := \frac{Q(t) \cdot WP\_cap}{WP\_length} \cdot \left[1 - 1 \cdot \left(t \leq t_{store}\right)\right] \cdot \left[1 - V_{eff} \cdot \left(t \leq t_{operate}\right)\right]$$

$$Q_{L\_wp}\left(55 \cdot yr, t_{store}, t_{operate}, 12\right) = 709.459 \cdot \frac{W}{m}$$

$\dfrac{Q_{L\_wp}\left(t \cdot yr, t_{store}, t_{operate}, WP\_cap\right)}{\dfrac{Q(t \cdot yr) \cdot WP\_cap}{WP\_length}}$

<mark>Note - added r_{DW} as a function parameter to allow calculations at additional compliance points inside the rock, where r_{DW} would be replaced with new radius value.</mark>

$$DW\_T\_finite\_line\left(t, r_{DW}, y, t_{store}, t_{operate}, WP\_cap, Kth, \alpha\right) := \left[\int_0^t \frac{Q_{L\_wp}\left(\tau, t_{store}, t_{operate}, WP\_cap\right)}{8 \cdot (\pi \cdot Kth) \cdot (t - \tau)} \cdot e^{\frac{-\left(r_{DW}^2\right)}{4 \cdot \alpha \cdot (t - \tau)}} \cdot \left[erf\left[\frac{1}{2} \cdot \frac{\left(y + \frac{WP\_length}{2}\right)}{\sqrt{\alpha \cdot (t - \tau)}}\right] - erf\left[\frac{1}{2} \cdot \frac{\left(y - \frac{WP\_length}{2}\right)}{\sqrt{\alpha \cdot (t - \tau)}}\right]\right] d\tau\right]$$

Adjacent drifts:

$$Q_{L\_avg}\left(t, t_{store}, t_{operate}, WP\_cap, WP\_spacing\right) := \frac{Q(t) \cdot WP\_cap}{WP\_spacing} \cdot \left[1 - 1 \cdot \left(t \le t_{store}\right)\right] \cdot \left[1 - V_{eff} \cdot \left(t \le t_{operate}\right)\right]$$

Note - added r_{DW} as a function parameter to allow calculations at additional compliance points inside the rock, where r_{DW} would be replaced with new radius value.

$$DW\_T\_drifts\left(t, r_{DW}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha\right) := 2 \sum_{id=1}^{N_{drifts}} \int_0^t \frac{Q_{L\_avg}\left(\tau, t_{store}, t_{operate}, WP\_cap, WP\_spacing\right)}{4 \cdot (\pi \cdot Kth) \cdot (t - \tau)} \cdot e^{\frac{-\left[\left(r_{DW}\right)^2 + \left(id \cdot Drift\_spacing\right)^2\right]}{4 \cdot \alpha \cdot (t - \tau)}} d\tau$$

Adjacent waste packages:

$$Q_{wp}\left(t, t_{store}, t_{operate}, WP\_cap\right) := Q(t) \, WP\_cap \cdot \left[1 - 1 \cdot \left(t \le t_{store}\right)\right] \cdot \left[1 - V_{eff} \cdot \left(t \le t_{operate}\right)\right]$$

Note - added r_{DW} as a function parameter to allow calculations at additional compliance points inside the rock, where r_{DW} would be replaced with new radius value.

$$DW\_T\_adjacent\_pkgs\left(t, r_{DW}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Kth, \alpha\right) := 2 \sum_{ip=1}^{N_{adj}} \int_0^t \frac{Q_{wp}\left(\tau, t_{store}, t_{operate}, WP\_cap\right)}{8 \cdot Kth \cdot \sqrt{\alpha} \cdot \pi^{1.5} \cdot (t - \tau)^{1.5}} \cdot e^{\frac{-\left[r_{DW}^2 + \left(ip \cdot WP\_spacing\right)^2\right]}{4\alpha \cdot (t - \tau)}} d\tau$$

This command specifies two rows of column headings for output paramenter sensitivity runs

OutfileName := file = "DSEF R3.0C_2013Jul29_HRG-Salt_UOX-40_Enclosed mode variable kth_Case-Kth-1.xlsm"

Out_sheet := "Thermal-Analytical Output!"

This section specifies the column headings for output sensitivity studies

Cases = 1   Read in from Thermal-Analytical sheet in DSEF (Inputs_7)

$i := 1 .. Cases$

$$Parameter\_vector_i := \begin{cases} \text{"Base Case"} & \text{if } Cases = 1 \\ concat\left(Parameter, \text{" "}, Parameter\_description_i\right) & \text{otherwise} \end{cases}$$

$$\text{Parameter\_vector} = (\,\text{"Base Case"}\,)$$

$$\text{heading1}_i := \begin{pmatrix} \text{concat}(\text{"Parameter value: "}, \text{Parameter\_vector}_i) \\ \text{""} \\ \text{""} \\ \text{""} \\ \text{""} \\ \text{""} \\ \text{""} \\ \text{""} \\ \text{""} \\ \text{""} \end{pmatrix}$$

$$\text{heading2} := \begin{pmatrix} \text{"TooR (yr)"} \\ \text{"Wall } \Delta T \text{ Central Line Src"} \\ \text{"Wall } \Delta T \text{ Adj Drifts"} \\ \text{"Wall } \Delta T \text{ Adj Pkgs"} \\ \text{"Compliance Point 2, C"} \\ \text{"Rock Wall Temp, C"} \\ \text{"EBS 1 inner Temp, C"} \\ \text{"EBS 2 inner Temp, C"} \\ \text{"EBS 3 inner Temp, C"} \\ \text{"Waste Pkg Temp, C"} \end{pmatrix}$$

$$\text{heading1}_i := \text{heading1}_i^{\,T} \qquad \text{heading2} := \text{heading2}^{\,T}$$

$$\text{Title\_array}_i := \text{stack}\left(\text{heading1}_i, \text{heading2}\right)$$

$$\text{Title\_array}_2 = \blacksquare$$

==For-Loop analysis returning the output time, three temperature contribution terms, and six temperatures==

$\text{length}(\text{Parameter\_data}) = 1$ $\qquad r_{DW} = 4\,\text{m}$ $\qquad t_{store} = 50 \cdot \text{yr}$

$\qquad r_{CP2} = 5.25\,\text{m}$ $\qquad t_{operate} = 50 \cdot \text{yr}$ $\qquad t_{vent} = 0 \cdot \text{yr}$

$\qquad t_{closure} = 50 \cdot \text{yr}$

==Changed j vector to Parameter_data, Inserted row 2
in row 5 changed to $k_{radiation}$ and k_2 from k_2 and $k_{backfill}$
row 8 changed WP_spacej to WP_spacing.==

==Removed loop on "j", added r_{DW} into DW_T functions.==

==Note for enclosed modes $k_{radiation}$ = k_2==

| DEFINE STEP SIZE FOR OUTDATA | $\text{Counter} := 200$ | $\text{Step} := 5$ | $\text{time\_after\_emplacement\_analzyed} := (\text{Counter} \cdot \text{Step} \cdot \text{yr}) + t_{store} = 1050 \cdot \text{yr}$ |

==ADDED CORRECTION FOR PARAMETRIC $t_{closure}$
replaced $t_{closure}$ with $(t_{operate} + t_{backfill})$==

DSEF R3.0_Mathcad with temperature and time depndent EBS thermal conductivity.xmcd

$$\text{outdata}\left(r_{DW}, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha\right) :=$$

$\text{for } i \in 1 \mathbin{..} \text{Counter} + 1$

$\quad tt_i \leftarrow Step \cdot i \cdot yr + t_{store} - Step \cdot 1yr$

$\quad kk_2 \leftarrow k_{radiation}\left(tt_i, 373.15 \cdot K\right) \cdot \left[tt_i < \left(t_{operate} + t_{backfill}\right)\right] + k_2\left(tt_i, 373.15 \cdot K\right) \cdot \left[tt_i \geq \left(t_{operate} + t_{backfill}\right)\right] \quad \text{if } i = 1$

$\quad Wall\_deltaT\_finite\_line_i \leftarrow DW\_T\_finite\_line\left(tt_i, r_{DW}, 0, t_{store}, t_{operate}, WP\_cap, Kth, \alpha\right)$

$\quad Wall\_deltaT\_drifts_i \leftarrow DW\_T\_drifts\left(tt_i, r_{DW}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha\right)$

$\quad Wall\_deltaT\_adj\_pkgs_i \leftarrow DW\_T\_adjacent\_pkgs\left(tt_i, r_{DW}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Kth, \alpha\right)$

$\quad Wall\_T_i \leftarrow T_{ambient} + Wall\_deltaT\_finite\_line_i + Wall\_deltaT\_drifts_i + Wall\_deltaT\_adj\_pkgs_i$

$\quad CP2\_deltaT\_finite\_line_i \leftarrow DW\_T\_finite\_line\left(tt_i, r_{CP2}, 0, t_{store}, t_{operate}, WP\_cap, Kth, \alpha\right)$

$\quad CP2\_deltaT\_drifts_i \leftarrow DW\_T\_drifts\left(tt_i, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha\right)$

$\quad CP2\_deltaT\_adj\_pkgs_i \leftarrow DW\_T\_adjacent\_pkgs\left(tt_i, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Kth, \alpha\right)$

$\quad CP2\_T_i \leftarrow T_{ambient} + CP2\_deltaT\_finite\_line_i + CP2\_deltaT\_drifts_i + CP2\_deltaT\_adj\_pkgs_i$

$\quad Q_i \leftarrow Q_{L\_wp}\left(tt_i, t_{store}, t_{operate}, WP\_cap\right)$

$\quad EBS\_1_i \leftarrow Wall\_T_i + \dfrac{Q_i}{2 \cdot \pi \cdot r_{DW}} \cdot R_1\left(Wall\_T_i\right)$

$\quad EBS\_2_i \leftarrow \left| \begin{array}{l} EBS\_1_i + \dfrac{Q_i}{2 \cdot \pi \cdot r_{DW}} \cdot R_2\left(tt_i, t_{operate}, t_{backfill}, EBS\_1_i\right) \quad \text{if } kk_2 \neq 0 \cdot \dfrac{W}{m \cdot K} \\[2em] \left[\left[\dfrac{Q_i}{h_{rad\_infinite}\left(r_3, r_2, \varepsilon_{WP}, \varepsilon_{wall}\right) \cdot 2 \cdot \pi \cdot r_3} + \left(EBS\_1_i\right)^4\right]^{\frac{1}{4}}\right] \quad \text{otherwise} \end{array} \right.$

$\quad kk_2 \leftarrow k_{radiation}\left(tt_i, EBS\_2_i\right) \cdot \left[tt_i < \left(t_{operate} + t_{backfill}\right)\right] + k_2\left(tt_i, EBS\_2_i\right) \cdot \left[tt_i \geq \left(t_{operate} + t_{backfill}\right)\right]$

$\quad EBS\_3_i \leftarrow EBS\_2_i + \dfrac{Q_i}{2 \cdot \pi \cdot r_{DW}} \cdot R_3\left(tt_i, EBS\_2_i\right)$

$\quad WP\_T_i \leftarrow EBS\_3_i + \dfrac{Q_i}{2 \cdot \pi \cdot r_{DW}} \cdot R_4\left(tt_i, EBS\_3_i\right)$

$\quad T1_i \leftarrow CP2\_T_i - 273.15K$

$\quad T2_i \leftarrow Wall\_T_i - 273.15K$

$\quad T3_i \leftarrow EBS\_1_i - 273.15K$

$\quad T4_i \leftarrow EBS\_2_i - 273.15K$

$\quad T5_i \leftarrow EBS\_3_i - 273.15K$

$\quad T6_i \leftarrow WP\_T_i - 273.15K$

$Data\_array \leftarrow augment\left(tt \cdot \dfrac{1}{yr}, Wall\_deltaT\_finite\_line \cdot \dfrac{1}{K}, Wall\_deltaT\_drifts \cdot \dfrac{1}{K}, Wall\_deltaT\_adj\_pkgs \cdot \dfrac{1}{K}, T1 \cdot \dfrac{1}{K}, T2 \cdot \dfrac{1}{K}, T3 \cdot \dfrac{1}{K}, T4 \cdot \dfrac{1}{K}, T5 \cdot \dfrac{1}{K}, T6 \cdot \dfrac{1}{K}\right)$

DSEF R3.0_Mathcad with temperature and time depndent EBS thermal conductivity.xmcd

$$\text{outdata}\left(r_{DW}, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha\right)$$

$jjj := 1 .. Cases \qquad Cases = 1$

$X_{jjj} := Parameter\_data_{jjj} \qquad Parameter = "Single"$

PARAMETRIC STUDIES OF "BACKFILL THERMAL CONDUCTIVITY" NOT ALLOWED FOR TEMPERATURE AND TIME-DEPENDENT THERMAL PROPERTY ANALYSES. THEREFORE, PARAMETER TYPE IS RESET TO "SINGLE",

$$Temp\_array_{jjj} := \begin{vmatrix} \text{outdata}\left(r_{DW}, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha\right) & \text{if } Parameter = "Single" \\ \text{outdata}\left(r_{DW}, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, X_{jjj} \cdot m, Kth, \alpha\right) & \text{if } Parameter = "Drift Spacing" \\ \text{outdata}\left(r_{DW}, r_{CP2}, t_{store}, t_{operate}, WP\_cap, X_{jjj} \cdot m, Drift\_spacing, Kth, \alpha\right) & \text{if } Parameter = "WP Spacing" \\ \text{outdata}\left(r_{DW}, r_{CP2}, X_{jjj} \cdot yr, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha\right) & \text{if } Parameter = "Storage Time" \\ \text{outdata}\left(r_{DW}, r_{CP2}, t_{store}, t_{store} + X_{jjj} \cdot yr, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha\right) & \text{if } Parameter = "Ventilation Duration" \\ \text{outdata}\left(r_{DW}, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, X_{jjj} \cdot \frac{W}{m \cdot K}, \alpha\right) & \text{if } Parameter = "Rock Conductivity" \\ "Undefined" & \text{otherwise} \end{vmatrix}$$

$$Temp\_array_1 := \text{outdata}\left(r_{DW}, r_{CP2}, t_{store}, t_{operate}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha\right)$$

$$File\_array_{jjj} := \text{stack}\left(Title\_array_{jjj}, Temp\_array_{jjj}\right)$$

$File\_array_1 =$

	1	2	3	4	5	6
1	"Parameter value: Base Case"	""	""	""	""	""
2	"TooR (yr)"	"Wall ΔT Central Line Src"	"Wall ΔT Adj Drifts"	"Wall ΔT Adj Pkgs"	"Compliance Point 2, C"	"Rock Wall Temp, C"
3	50	0	0	0	27.5	27.5
4	55	10.991	7.223	3.07	45.86	48.785
5	60	10.687	12.867	4.27	52.544	55.323
6	65	10.188	16.843	4.835	56.761	59.367
7	70	9.666	19.727	5.112	59.55	62.005
8	75	9.166	21.846	5.232	61.43	63.745
9	80	8.695	23.415	5.259	62.685	64.868
10	85	8.263	24.576	5.229	63.499	65.568
11	90	7.871	25.432	5.163	63.997	65.966
12	95	7.505	26.048	5.082	64.261	66.134
13	100	7.171	26.493	4.977	64.355	66.141
14	105	6.864	26.797	4.872	64.327	66.033
15	110	6.584	26.984	4.759	64.193	65.827
16	115	6.328	27.091	4.652	64.021	...

$iii := 1 .. 10$

$Peak\_array_{jjj, iii} := \max\left[\left[\left(Temp\_array_{jjj}\right)^{\langle iii \rangle}\right]\right]$

	1
1	27.5
2	48.785
3	55.323
4	59.367
5	62.005
6	63.745
7	64.868
8	65.568
9	65.966
10	66.134
11	66.141
12	66.033
13	65.827
14	65.571
15	65.271
16	...

$\left(Temp\_array_1\right)^{\langle 6 \rangle} =$ (the table above)

$Peak\_array_{1, 2} = 10.991$

$Time\_array := \left(Temp\_array_1\right)^{\langle 1 \rangle}$

$Peak\_T(m, n) := \max\left[\left(Temp\_array_m\right)^{\langle n \rangle}\right]$

$Peak\_T(1, 5) = 64.355$

$Peak\_time(m, n) := lookup\left[Peak\_T(m, n), \left(Temp\_array_m\right)^{\langle n \rangle}, Time\_array\right]$

$Peak\_time(1, 5) = (100)$

$Time\_array =$

	1
1	50
2	55
3	60
4	65
5	70
6	75
7	80
8	85
9	90
10	95
11	100
12	105
13	110
14	115
15	120
16	...

Initialize the peak value data array:

$i := 1 .. 6 \qquad j := 1 .. 20$

$Peak\_values_{i, j} := ""$

$$Peak\_values = \begin{pmatrix} "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \end{pmatrix}$$

Fill in the peak temperatures and times:

$mj := 1 .. Cases \qquad nn := 1 .. 6$

$Peak\_values_{nn, mj \cdot 2 - 1} := Peak\_T(mj, nn + 4)$

$Peak\_values_{nn, mj \cdot 2} := Peak\_time(mj, nn + 4)_1$

$Parameter\_vector^T = ("Base Case")$

$t_{vent} = 0 \cdot yr$

$$Peak\_values = \begin{pmatrix} 64.355 & 100 & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ 66.141 & 100 & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ 70.231 & 90 & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ 75.418 & 85 & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ 83.791 & 75 & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \\ 102.771 & 65 & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" & "" \end{pmatrix}$$

$$Peak\_Wall\_T := \left(Peak\_values^{\langle 1 \rangle}\right)_2 = 66.141$$

outsheet := "Thermal-Analytical Output!"

$rows\left(Temp\_array_1\right) = 201$ $rows\left(File\_array_1\right) = 203$ Transient output starting row in DSEF on the Thermal-= 60

start_row := 100   end_row := $start\_row + rows\left(Temp\_array_1\right) - 1 = 300$ NOTE - USE File_array to write to stand-alone Excel files, and Temp_array to write back to the DSEF Excel file.

$$transient\_case\_cols := \begin{pmatrix} "A" & "J" \\ "L" & "U" \\ "W" & "AF" \\ "AH" & "AQ" \\ "AS" & "BB" \\ "BD" & "BM" \\ "BO" & "BX" \\ "BZ" & "CI" \\ "CK" & "CT" \\ "CV" & "DE" \end{pmatrix}$$

To write the transients for each case horizontally instead of vertically, the following location array includes 10 columns for each case with one column separating the cases.

iw := 1 .. Cases

start_row = 100   end_row = 300

$transient\_write\_range_{iw} := concat\left[outsheet, \left(transient\_case\_cols^{\langle 1 \rangle}\right)_{iw}, num2str(start\_row), ":", \left(transient\_case\_cols^{\langle 2 \rangle}\right)_{iw}, num2str(end\_row)\right]$

$transient\_write\_range_2 = \blacksquare$

peaks_write_range := concat(outsheet, "C6:V11") = "Thermal-Analytical Output!C6:V11"

transient_write_range = ("Thermal-Analytical Output!A100:J300")

Transient_size := (Counter Step)   Transient_size = (200 5)   Transient_size_range := concat(outsheet, "B92:C92") = "Thermal-Analytical Output!B92:C92"

Make writing an output file optional $t_{vent} = 0 \cdot yr$

DSEF R3.0_Mathcad with temperature and time depndent EBS thermal conductivity.xmcd

OutfileName = "DSEF R3.0C_2013Jul29_HRG-Salt_UOX-40_Enclosed mode variable kth_Case-Kth-1.xlsm"

Write_file := Write_OK = "No"

$$\text{write\_the\_peaks(Write\_file)} := \begin{vmatrix} \text{write\_it} \leftarrow \begin{vmatrix} \text{WRITEEXCEL}(\text{Peak\_values}, \text{OutfileName}, \text{peaks\_write\_range}) & \text{if } (\text{Write\_file} = \text{"Yes"}) \vee (\text{Write\_file} = \text{"YES"}) \\ \text{"File written"} \end{vmatrix} \\ \text{write\_it} \leftarrow \text{"No file written"} \quad \text{otherwise} \end{vmatrix}$$

write_the_peaks(Write_file) = "No file written"

$$\text{write\_the\_transient\_size(Write\_file)} := \begin{vmatrix} \text{write\_it} \leftarrow \begin{vmatrix} \text{WRITEEXCEL}(\text{Transient\_size}, \text{OutfileName}, \text{Transient\_size\_range}) & \text{if } (\text{Write\_file} = \text{"Yes"}) \vee (\text{Write\_file} = \text{"YES"}) \\ \text{"File written"} \end{vmatrix} \\ \text{write\_it} \leftarrow \text{"No file written"} \quad \text{otherwise} \end{vmatrix}$$

write_the_transient_size(Write_file) = "No file written"

Write_file = "No"   Cases = 1

iww := 1 .. Cases   NOTE - USE File_array to write to stand-alone Excel files, and Temp_array to write back to the DSEF Excel file.

$$\text{write\_the\_transients(jj)} := \begin{vmatrix} \text{write\_array} \leftarrow \text{Temp\_array}_{jj} \\ \text{write\_it} \leftarrow \begin{vmatrix} \text{WRITEEXCEL}\left(\text{write\_array}, \text{OutfileName}, \text{transient\_write\_range}_{jj}\right) & \text{if } (\text{Write\_file} = \text{"Yes"}) \vee (\text{Write\_file} = \text{"YES"}) \\ \text{"File written"} \end{vmatrix} \\ \text{write\_it} \leftarrow \text{"No file written"} \quad \text{otherwise} \end{vmatrix}$$
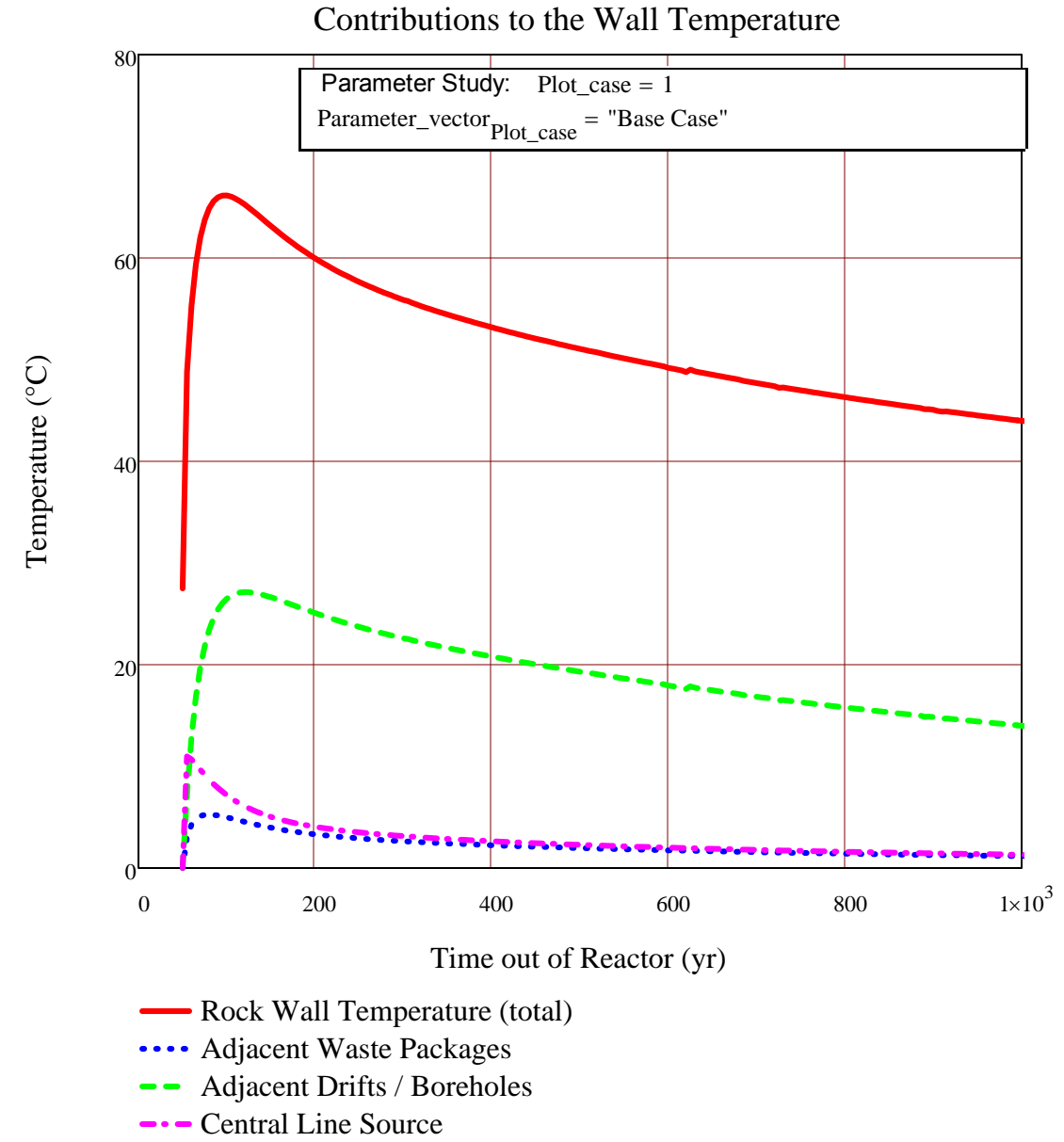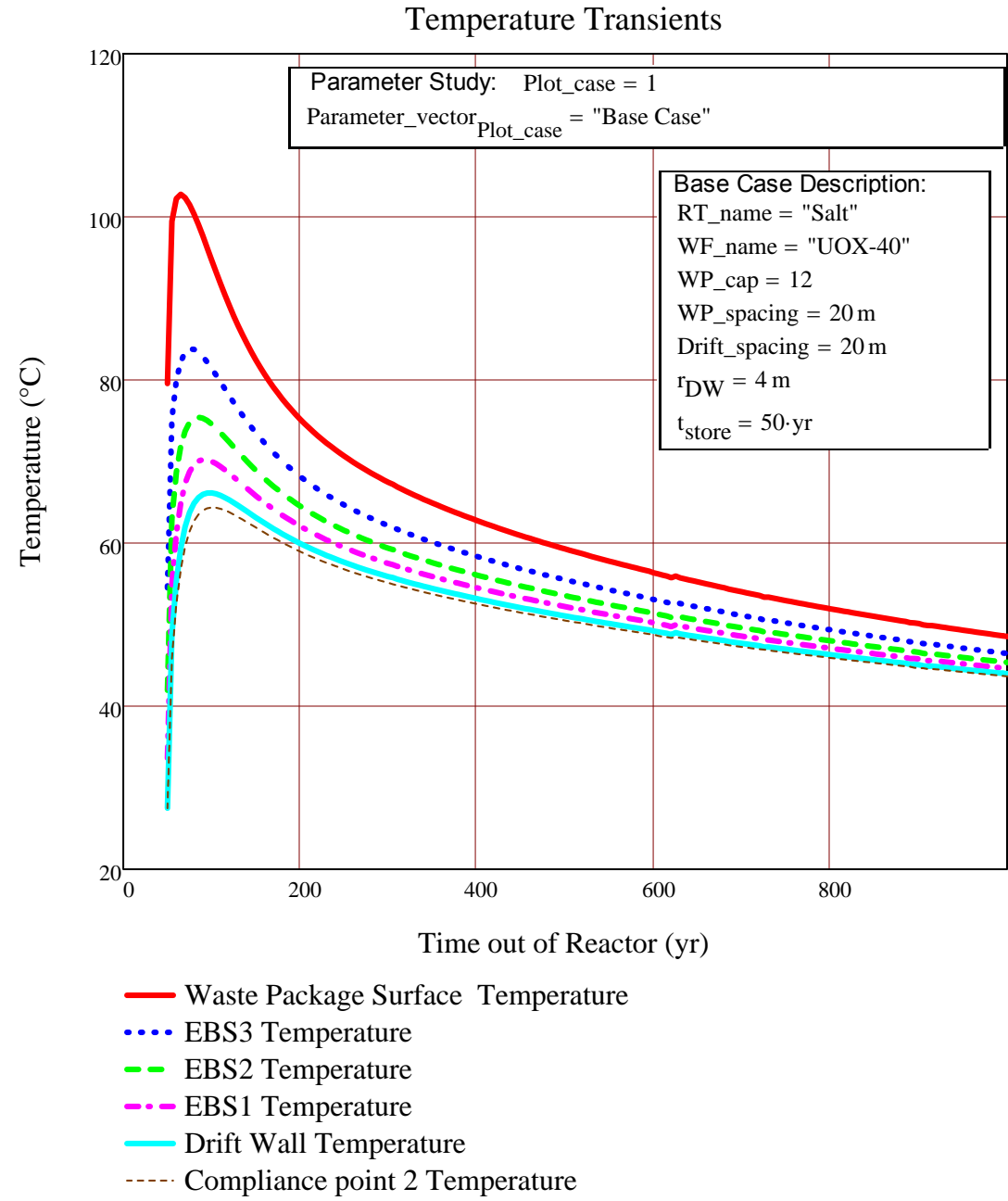
write_the_transients(iww) = ("No file written")

Plot_case := 1   Select parametric study case to plot (default plot is for case 1)

$$\text{WP\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 10 \rangle}\right] \quad \text{EBS3\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 9 \rangle}\right] \quad \text{EBS2\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 8 \rangle}\right] \quad \text{EBS1\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 7 \rangle}\right] \quad \text{Wall\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 6 \rangle}\right]$$

$$\text{CP2\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 5 \rangle}\right] \quad \text{Delta\_WPs\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 4 \rangle}\right] \quad \text{Delta\_drifts\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 3 \rangle}\right] \quad \text{Delta\_central\_T\_plot} := \left[\left(\text{Temp\_array}_{\text{Plot\_case}}\right)^{\langle 2 \rangle}\right]$$

Temperature Transients

Parameter Study: Plot_case = 1

Parameter_vector$_{Plot\_case}$ = "Base Case"

Base Case Description:
RT_name = "Salt"
WF_name = "UOX-40"
WP_cap = 12
WP_spacing = 20 m
Drift_spacing = 20 m
r_{DW} = 4 m
t_{store} = 50·yr

Time out of Reactor (yr)

— Waste Package Surface Temperature
···· EBS3 Temperature
- - - EBS2 Temperature
-·-·- EBS1 Temperature
— Drift Wall Temperature
----- Compliance point 2 Temperature

Contributions to the Wall Temperature

Parameter Study: Plot_case = 1

Parameter_vector$_{Plot\_case}$ = "Base Case"

Time out of Reactor (yr)

— Rock Wall Temperature (total)
···· Adjacent Waste Packages
- - - Adjacent Drifts / Boreholes
-·-·- Central Line Source

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$$tt\_rw := \left[(Peak\_values)^{\langle Plot\_case \cdot 2 \rangle} \right]_2 = 100$$

$$tt\_wp := \left[(Peak\_values)^{\langle Plot\_case \cdot 2 \rangle} \right]_6 = 65$$

$$CP2\_T\_at\_tt\_rw := \left[\left(Temp\_array_{Plot\_case} \right)^{\langle 5 \rangle} \right]_{\frac{\left(tt\_rw - \frac{t_{store}}{yr} \right)}{Step} + 1} = 64.355$$

$$CP2\_T\_at\_tt\_wp := \left[\left(Temp\_array_{Plot\_case} \right)^{\langle 5 \rangle} \right]_{\frac{\left(tt\_wp - \frac{t_{store}}{yr} \right)}{Step} + 1} = 56.761$$

$$Wall\_T\_at\_tt\_rw := \left[(Peak\_values)^{\langle Plot\_case \cdot 2 - 1 \rangle} \right]_2 = 66.141$$

$$Wall\_T\_at\_tt\_wp := \left[\left(Temp\_array_{Plot\_case} \right)^{\langle 6 \rangle} \right]_{\frac{\left(tt\_wp - \frac{t_{store}}{yr} \right)}{Step} + 1} = 59.367$$

$$EBS1\_T\_at\_tt\_rw := \left[\left(Temp\_array_{Plot\_case} \right)^{\langle 7 \rangle} \right]_{\frac{\left(tt\_rw - \frac{t_{store}}{yr} \right)}{Step} + 1} = 70.007$$

$$EBS1\_T\_at\_tt\_wp := \left[\left(Temp\_array_{Plot\_case} \right)^{\langle 7 \rangle} \right]_{\frac{\left(tt\_wp - \frac{t_{store}}{yr} \right)}{Step} + 1} = 64.949$$

$$EBS2\_T\_at\_tt\_rw := \left[\left(Temp\_array_{Plot\_case} \right)^{\langle 8 \rangle} \right]_{\frac{\left(tt\_rw - \frac{t_{store}}{yr} \right)}{Step} + 1} = 74.59$$

$$EBS2\_T\_at\_tt\_wp := \left[\left(Temp\_array_{Plot\_case} \right)^{\langle 8 \rangle} \right]_{\frac{\left(tt\_wp - \frac{t_{store}}{yr} \right)}{Step} + 1} = 71.879$$

$$EBS3\_T\_at\_tt\_rw := \left[\left(Temp\_array_{Plot\_case} \right)^{\langle 9 \rangle} \right]_{\frac{\left(tt\_rw - \frac{t_{store}}{yr} \right)}{Step} + 1} = 81.408$$

$$EBS3\_T\_at\_tt\_wp := \left[\left(Temp\_array_{Plot\_case} \right)^{\langle 9 \rangle} \right]_{\frac{\left(tt\_wp - \frac{t_{store}}{yr} \right)}{Step} + 1} = 82.272$$

$$WP\_T\_at\_tt\_rw := \left[\left(Temp\_array_{Plot\_case} \right)^{\langle 10 \rangle} \right]_{\frac{\left(tt\_rw - \frac{t_{store}}{yr} \right)}{Step} + 1} = 94.699$$

$$WP\_T\_at\_tt\_wp := \left[(Peak\_values)^{\langle Plot\_case \cdot 2 - 1 \rangle} \right]_6 = 102.771$$

$$r\_array := \begin{pmatrix} r_{WP} \\ r_4 \\ r_3 \\ r_2 \\ r_1 \\ r_{CP2} \end{pmatrix} = \begin{pmatrix} 0.585 \\ 1.406 \\ 2.227 \\ 3.048 \\ 4 \\ 5.25 \end{pmatrix} m$$

$$T\_at\_tt\_rw := \begin{pmatrix} WP\_T\_at\_tt\_rw \\ EBS3\_T\_at\_tt\_rw \\ EBS2\_T\_at\_tt\_rw \\ EBS1\_T\_at\_tt\_rw \\ Wall\_T\_at\_tt\_rw \\ CP2\_T\_at\_tt\_rw \end{pmatrix} = \begin{pmatrix} 94.699 \\ 81.408 \\ 74.59 \\ 70.007 \\ 66.141 \\ 64.355 \end{pmatrix}$$

$$T\_at\_tt\_wp := \begin{pmatrix} WP\_T\_at\_tt\_wp \\ EBS3\_T\_at\_tt\_wp \\ EBS2\_T\_at\_tt\_wp \\ EBS1\_T\_at\_tt\_wp \\ Wall\_T\_at\_tt\_wp \\ CP2\_T\_at\_tt\_wp \end{pmatrix} = \begin{pmatrix} 102.771 \\ 82.272 \\ 71.879 \\ 64.949 \\ 59.367 \\ 56.761 \end{pmatrix}$$

$$k\_at\_tt\_wp := \begin{bmatrix} k_4[tt\_wp \cdot yr, (WP\_T\_at\_tt\_wp + 273.15) \cdot K] \\ k_3[tt\_wp \cdot yr, (EBS3\_T\_at\_tt\_wp + 273.15) \cdot K] \\ k_2[tt\_wp \cdot yr, (EBS2\_T\_at\_tt\_wp + 273.15) \cdot K] \\ k_2[tt\_wp \cdot yr, (EBS1\_T\_at\_tt\_wp + 273.15) \cdot K] \\ k_1[(Wall\_T\_at\_tt\_wp + 273.15) \cdot K] \\ k_1[(CP2\_T\_at\_tt\_wp + 273.15) \cdot K] \end{bmatrix} = \begin{pmatrix} 3.958 \\ 4.219 \\ 4.364 \\ 4.466 \\ 4.802 \\ 4.846 \end{pmatrix} \cdot \frac{W}{m \cdot K}$$

$$k\_at\_tt\_rw := \begin{bmatrix} k_4[tt\_rw \cdot yr, (WP\_T\_at\_tt\_wp + 273.15) \cdot K] \\ k_3[tt\_rw \cdot yr, (EBS3\_T\_at\_tt\_rw + 273.15) \cdot K] \\ k_2[tt\_rw \cdot yr, (EBS2\_T\_at\_tt\_rw + 273.15) \cdot K] \\ k_2[tt\_rw \cdot yr, (EBS1\_T\_at\_tt\_rw + 273.15) \cdot K] \\ k_1[(Wall\_T\_at\_tt\_rw + 273.15) \cdot K] \\ k_1[(CP2\_T\_at\_tt\_rw + 273.15) \cdot K] \end{bmatrix} = \begin{pmatrix} 4.12 \\ 4.404 \\ 4.502 \\ 4.571 \\ 4.693 \\ 4.721 \end{pmatrix} \cdot \frac{W}{m \cdot K}$$
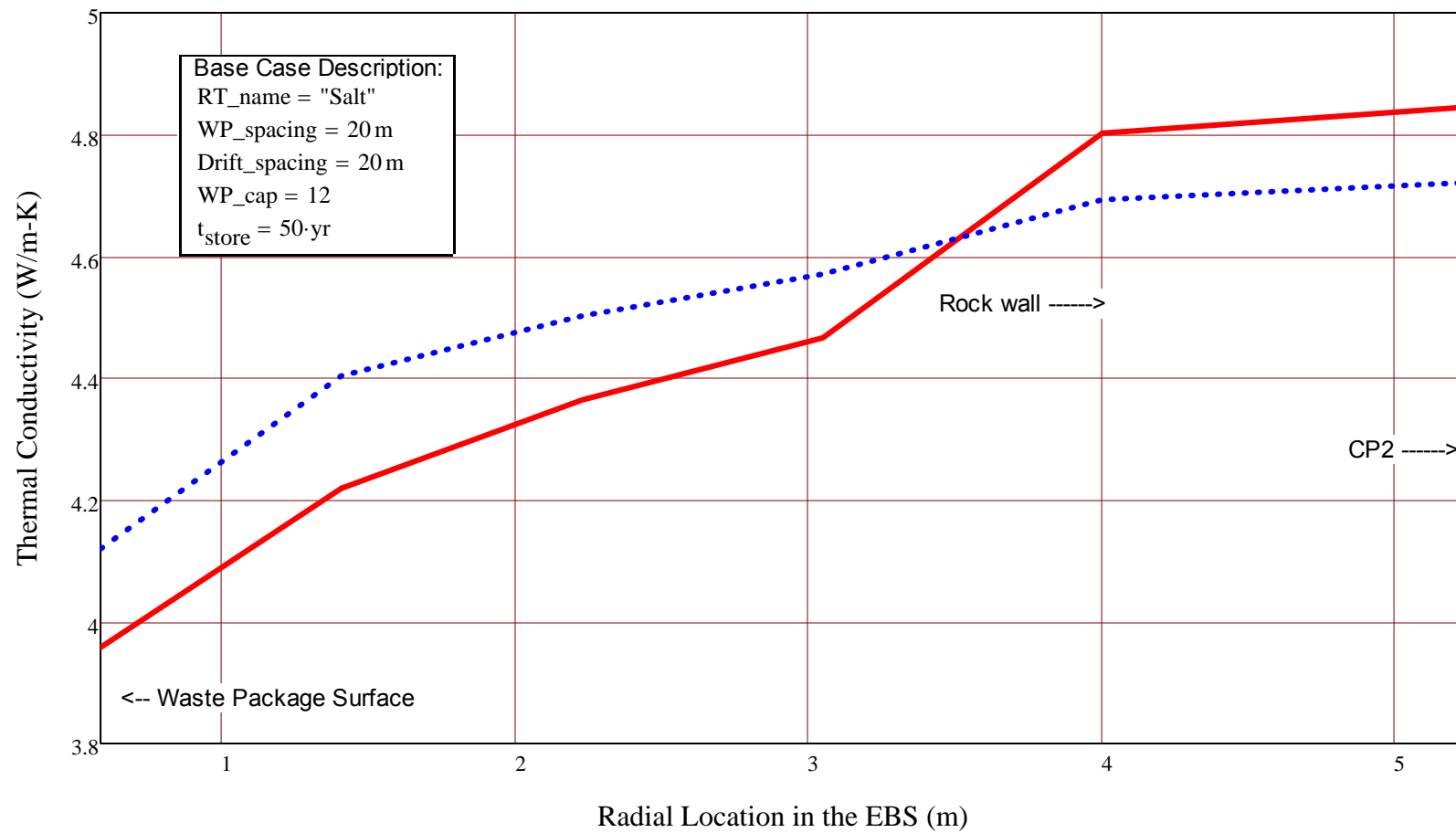
Temperature Gradient in the EBS

Base Case Description:
RT_name = "Salt"
WP_spacing = 20 m
Drift_spacing = 20 m
WP_cap = 12
$t_{store} = 50 \cdot yr$

Rock wall ----->

CP2 ----->

<-- Waste Package Surface

Temperature (°C)

Radial Location in the EBS (m)

——— Gradient at the time of the Waste Package Peak T
········ Gradient at the time of the Rock Wall Peak T

$$k\_at\_tt\_wp := \begin{bmatrix} k_4[tt\_wp \cdot yr, (WP\_T\_at\_tt\_wp + 273.15) \cdot K] \\ k_3[tt\_wp \cdot yr, (EBS3\_T\_at\_tt\_wp + 273.15) \cdot K] \\ k_2[tt\_wp \cdot yr, (EBS2\_T\_at\_tt\_wp + 273.15) \cdot K] \\ k_2[tt\_wp \cdot yr, (EBS1\_T\_at\_tt\_wp + 273.15) \cdot K] \\ k_1[(Wall\_T\_at\_tt\_wp + 273.15) \cdot K] \\ k_1[(CP2\_T\_at\_tt\_wp + 273.15) \cdot K] \end{bmatrix} = \begin{pmatrix} 3.958 \\ 4.219 \\ 4.364 \\ 4.466 \\ 4.802 \\ 4.846 \end{pmatrix} \cdot \frac{W}{m \cdot K}$$

$$k\_at\_tt\_rw := \begin{bmatrix} k_4[tt\_rw \cdot yr, (WP\_T\_at\_tt\_wp + 273.15) \cdot K] \\ k_3[tt\_rw \cdot yr, (EBS3\_T\_at\_tt\_rw + 273.15) \cdot K] \\ k_2[tt\_rw \cdot yr, (EBS2\_T\_at\_tt\_rw + 273.15) \cdot K] \\ k_2[tt\_rw \cdot yr, (EBS1\_T\_at\_tt\_rw + 273.15) \cdot K] \\ k_1[(Wall\_T\_at\_tt\_rw + 273.15) \cdot K] \\ k_1[(CP2\_T\_at\_tt\_rw + 273.15) \cdot K] \end{bmatrix} = \begin{pmatrix} 4.12 \\ 4.404 \\ 4.502 \\ 4.571 \\ 4.693 \\ 4.721 \end{pmatrix} \cdot \frac{W}{m \cdot K}$$

$$0.75 \cdot k_{intact}[(WP\_T\_at\_tt\_wp + 273.15) \cdot K] + 0.25 \cdot k_{crushed}[Porosity(tt\_wp), (WP\_T\_at\_tt\_wp + 273.15) \cdot K] = 3.958 \cdot \frac{W}{m \cdot K}$$

$$0.75 \cdot k_{intact}[(WP\_T\_at\_tt\_wp + 273.15) \cdot K] = 3.132 \cdot \frac{W}{m \cdot K}$$

$$Porosity(tt\_wp) = 0.111$$

$$0.25 \cdot k_{crushed}[Porosity(tt\_wp), (WP\_T\_at\_tt\_wp + 273.15) \cdot K] = 0.826 \cdot \frac{W}{m \cdot K}$$

$$0.25 \cdot k_{consolidate}[tt\_wp, (WP\_T\_at\_tt\_wp + 273.15) \cdot K] = 0.826 \cdot \frac{W}{m \cdot K}$$

Previous analysis with constant salt thermal properties in the EBS assumed 75% surface contact with intact salt, and took no credit for conduction through the crushed salt.

$$0.75 \, k_{intact}[(100 + 273.15) \cdot K] = 3.158 \cdot \frac{W}{m \cdot K}$$

$$0.75 \, k_{intact}[(200 + 273.15) \cdot K] = 2.409 \cdot \frac{W}{m \cdot K}$$

$$k_{crushed}[Porosity(tt\_wp), (WP\_T\_at\_tt\_wp + 273.15) \cdot K] = 3.305 \cdot \frac{W}{m \cdot K}$$

$$k_{consolidate}[Porosity(tt\_wp), (WP\_T\_at\_tt\_wp + 273.15) \cdot K] = 1.809 \cdot \frac{W}{m \cdot K}$$

Thermal Conductivity Variation in the EBS

Base Case Description:
RT_name = "Salt"
WP_spacing = 20 m
Drift_spacing = 20 m
WP_cap = 12
t_{store} = 50·yr

Rock wall ------>

CP2 ------>

<-- Waste Package Surface

Thermal Conductivity (W/m-K)

Radial Location in the EBS (m)

——— At the time of the Waste Package Peak T
····· At the time of the Rock Wall Peak T

OVERRIDE COUNTER AND STEP SIZE TO GET FINER CONVERGENCE ON THE ANSWER

$t_{vent} = 0 \cdot yr$ OPTIONALLY OVERRIDE VENTILATION TIME TO SHORTEN ITERATION CONVERGENCE

ITERATE_OK = "NO"" $\qquad t_{convergence} = 1 \cdot yr$

$$t_{required\_storage}\left(t_{operate}, T_{criteria}, t_{convergence}\right) := \begin{array}{|l} time_{OK} \leftarrow t_{operate} - t_{convergence} \\ Peak\_Wall\_T_{check} \leftarrow (Peak\_Wall\_T + 273.15) \cdot K \\ time_{OK} \leftarrow t_{operate} \quad if \;\; Peak\_Wall\_T_{check} \leq T_{criteria} \\ while \;\; Peak\_Wall\_T_{check} > T_{criteria} \\ \quad \begin{array}{|l} time_{OK} \leftarrow time_{OK} + t_{convergence} \\ calc_{array} \leftarrow outdata\left(r_{DW}, r_{CP2}, t_{store}, time_{OK}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha\right) \\ Peak\_Wall\_T_{check} \leftarrow \left(max\left(calc_{array}^{\langle 6 \rangle}\right) + 273.15\right) \cdot K \end{array} \\ return \left[\begin{array}{c} \dfrac{time_{OK}}{yr} \\ \dfrac{Peak\_Wall\_T_{check} - 273.15K}{K} \\ outdata\left(r_{DW}, r_{CP2}, t_{store}, time_{OK}, WP\_cap, WP\_spacing, Drift\_spacing, Kth, \alpha\right) \end{array}\right] \end{array}$$

$$Final\_array := \begin{array}{|l} t_{required\_storage}\left(t_{operate}, T_{criteria}, t_{convergence}\right) \quad if \;\; ITERATE\_OK = "YES" \\ "No \; Iteration \; Performed" \quad otherwise \end{array}$$

$t_{operate\_required} := Final\_array_1 \; yr = \blacksquare \cdot yr$

$t_{vent\_required} := t_{operate\_required} - t_{store} = \blacksquare \cdot yr$ REQUIRED VENTILATION TIME NEEDED TO MEET $T_{criteria} = 100 \cdot °C$

$Peak\_Wall\_T_{check} := \left(Final\_array_2 + 273.15\right) \cdot K = \blacksquare \cdot °C$

$Result := stack\left(Title\_array_1, Final\_array_3\right)$

Result = ▪

$$\text{Time\_array} := \left(\text{Final\_array}_3\right)^{\langle 1 \rangle}$$

$$\text{Peak\_Temp(n)} := \max\left[\left(\text{Final\_array}_3\right)^{\langle n \rangle}\right] \qquad \text{Peak\_Temp(6)} = ▪$$

$$\text{Peak\_t(n)} := \text{lookup}\left[\text{Peak\_Temp(n)}, \left(\text{Final\_array}_3\right)^{\langle n \rangle}, \text{Time\_array}\right] \qquad \text{Peak\_t(6)}_1 \cdot \text{yr} = ▪ \cdot \text{yr}$$

$$\text{nn} := 5 .. 10 \qquad \text{Peak\_results}_{nn-4, 1} := \text{Peak\_Temp(nn)} \qquad \text{Peak\_results}_{nn-4, 2} := \text{Peak\_t(nn)}_1$$

	CP2 , time of peak
	Peak Wall T, time of peak
Peak_results = ▪	Peak EBS 1, time of peak
	Peak EBS 2, time of peak
	Peak EBS 3, time of peak
	Waste Pkg T, time of peak

$$\text{Array\_row\_at\_Wall\_T\_peak} := \text{match}\left[\text{Peak\_Temp(6)}, \left(\text{Final\_array}_3\right)^{\langle 6 \rangle}\right]_1 = ▪$$

$$\text{CP2\_at\_Wall\_T\_pk\_t} := \left[\left(\text{Final\_array}_3\right)^{\langle 5 \rangle}\right]_{\text{Array\_row\_at\_Wall\_T\_peak}} = ▪$$

$$\text{Central\_WP\_delta} := \left[\left(\text{Final\_array}_3\right)^{\langle 2 \rangle}\right]_{\text{Array\_row\_at\_Wall\_T\_peak}} = ▪$$

$$\text{Adj\_Drift\_delta} := \left[\left(\text{Final\_array}_3\right)^{\langle 3 \rangle}\right]_{\text{Array\_row\_at\_Wall\_T\_peak}} = ▪$$

$$\text{Adj\_WP\_delta} := \left[\left(\text{Final\_array}_3\right)^{\langle 4 \rangle}\right]_{\text{Array\_row\_at\_Wall\_T\_peak}} = ▪$$

$$\text{Result\_Vector} := \left(\frac{\text{WP\_spacing}}{m} \quad \text{TC} \quad \frac{\text{Drift\_spacing}}{m} \quad \text{Peak\_results}_{6,1} \quad \text{Peak\_results}_{6,2} \quad \text{Peak\_results}_{2,1} \quad \text{Peak\_results}_{2,2} \quad \text{CP2\_at\_Wall\_T\_pk\_t} \quad \frac{t_{\text{vent\_required}}}{yr} \quad \text{Central\_WP\_delta} \quad \text{Adj\_Drift\_delta} \quad \text{Adj\_WP\_delta}\right)$$

Result_headings := ("WP Spacing" "Temp Criteria" "Drift Spacing" "Peak WP T" "Time of WP Peak" "Peak Wall T" "Time of Wall Peak" "Peak CP2 T" "Ventilation time" "Central WP delta" "Adj Drift delta" "Adj WP delta")

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Result_Vector = ▮

$$RV := augment\left(Result\_headings^T, Result\_Vector^T\right)$$

$T_{ambient} = 27.5 \cdot °C$

Contribution percentages at time of peak wall temperature

$$Percent\_central\_WP\_delta := \frac{Central\_WP\_delta}{Peak\_Temp(6) - \frac{\left(T_{ambient} - 273.15 \cdot K\right)}{K}} \cdot 100 = ▮$$

$$Percent\_adj\_Drift\_delta := \frac{Adj\_Drift\_delta}{Peak\_Temp(6) - \frac{\left(T_{ambient} - 273.15 \cdot K\right)}{K}} \cdot 100 = ▮$$

NOTE THAT THESE RESULTS WILL BE MISSING IF Iterate_OK = "No"

RV = ▮

$$Percent\_adj\_WP\_delta := \frac{Adj\_WP\_delta}{Peak\_Temp(6) - \frac{\left(T_{ambient} - 273.15 \cdot K\right)}{K}} \cdot 100 = ▮$$

$$Percent\_central\_WP\_delta + Percent\_adj\_WP\_delta + Percent\_adj\_Drift\_delta = ▮$$