LAWRENCE LIVERMORE NATIONAL LABORATORY

LLNL-TR-629812

Disposal Systems Evaluation Framework DSEF Version 2.1 User's Manual

H. R. Greenberg, J. A. Blink, M. Sutton, T. J. Wolery

March 25, 2013

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

DISPOSAL SYSTEMS EVALUATION FRAMEWORK

DSEF VERSION 2.1 USER MANUAL

Used Fuel Disposition Campaign

Level 4 Milestone (M4): M4FT-12LL0806043

Generic Engineered Barrier System Evaluation

(Work Package FT-12LL080604)

Harris R. Greenberg, James A. Blink, Mark Sutton and Thomas J. Wolery

Lawrence Livermore National Laboratory

MARCH, 2013

LLNL-TR-629812

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Table of Contents

Table of Contents 3

List of Figures 4

List of Acronyms 6

1. Overview 7

2. Information Flow 9

3. Finding Your Way Around – the NAVIGATION, README, LISTS and REV HISTORY Worksheets 11

4. Getting Started – Working with the DSEF Workbook 13

5. The Starting Point to Define an Analysis Case - the INPUTS Worksheet 16

6. The INPUTS CHECKLIST Worksheet 23

7. Reviewing Previous Analyses – the CASE LIBRARY and the THERMAL-INTERPOLATE Worksheets 24

8. Getting a Quick Overview of the Latest Analysis – the RESULTS and the THERMAL-ANALYTICAL OUTPUT Worksheets 32

9. The COST Worksheets 34

10. The WASTE FORM Worksheet 37

11. Defining Thermal Data Inputs and Outputs -the THERMAL Worksheets 40

12. Finding and Comparing Material Properties - the MATERIALS Worksheets 43

13. Placeholder worksheets for future development 46

14. References 47

Appendix A – Setting up Excel to Allow the DSEF Macros to Work 48

Appendix B – The Mathcad Thermal-Analytical Component of DSEF 51

List of Figures

Figure 1- DSEF Input-Process-Output Diagram 9

Figure 2 – Example of the information flow in DSEF 10

Figure 3 – Using the Excel tab navigation bar 11

Figure 4 – The two lists of worksheets in the NAVIGATION worksheet 12

Figure 5 – A drop-down list to select the waste form 14

Figure 6 – A spinner control to select the number of assemblies in a waste package 14

Figure 7 - An example of some of the cross-checks and cautions displayed in the INPUTS worksheet 16

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 17

Figure 9 – Example of Repository Level Cost Input Data 20

Figure 10 – Example of Cost Contingency Input Data 21

Figure 11 – Example of comparison of thermal results against thermal constraints from the RESULTS worksheet 21

Figure 12 – Example of parametric study input data from Step 13 on the INPUTS worksheet 22

Figure 13 - Example from a section of the inputs checklist 23

Figure 14 - The data fields used in the CASE LIBRARY 25

Figure 15 - The enclosed mode analysis case catalog 26

Figure 16 - The open mode analysis base case catalog 27

Figure 17 - The open mode sensitivity studies case catalog 28

Figure 18 - Side-by-side case comparison table 30

Figure 19 - The template for variable interpolation between relevant cases 31

Figure 20 - Example of repository level calculation performed on the COST CALCULATIONS worksheet as shown on the RESULTS worksheet 36

Figure 21 – Example of excavation and backfill cost calculations as shown on the RESULTS worksheet 36

Figure 22 – Tables from the WASTE FORM worksheet 38

Figure 23 - WASTE FORM worksheet – calculated waste form outer radius lookup table 39
Figure 24- Example of parametric study plots on the THERMAL-ANALYTICAL OUTPUT worksheet 41
Figure 25 - Example transient output data plotted in the THERMAL-ANALYTICAL OUTPUT worksheet 41
Figure 26 – Decay heat data built-in to the THERMAL-SOURCE worksheet 42
Figure 27 - Examples of decay heat update caution and confirmation prompts 42
Figure 28 - The first step – selecting the materials data to plot 44
Figure 29 - Example output of the materials data plotting macro 44
Figure 30 - Example of data structure in the MATERIALS-THERMAL PROPERTIES worksheet 44
Figure 31 - Example of data structure in the MATERIALS-TRANSPORT PROPERTIES worksheet 45
Figure A-1– The FILE menu choices 48
Figure A-2 – The OPTIONS menu choices 49
Figure A-3 – Select Trust Center Settings 49
Figure A-4 – Trust Center Settings 49
Figure A-5 – Prompt before enabling all controls with minimal restrictions 50
Figure A-6 – Macro settings 50
Figure A-7 – Message bar settings 50

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**
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) is being 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 300 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 constructing and operating a repository concept that uses the design values from the DSEF INPUTS worksheet. LLNL will work with SRNL to abstract the detailed costing done for several design options; the data included in DSEF 2.1 are from a simple reading of SRNL high-level cost results. Hence, caution should be used when calculating costs in DSEF 2.1. The cost data included are for demonstration purposes only and should not currently be used for comparison of design options.

Interfaces with various repository analysis codes are planned for DSEF. Version 2.1 currently provides input to, and retrieves output data from, a Mathcad Version 15 thermal-analytical model developed at LLNL (see Appendix B).

This User's Guide describes the structure and use of the various types of worksheets contained in the DSEF Version 2.1 workbook. Many of the worksheets are fully operational. Some worksheets are placeholders pending further development in FY13 or later. 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 have 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's Guide delivered in September and August 2012 respectively met the requirements of Deliverable M4FT-12LL0806043.

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).

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

- **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

PROCESS

- **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

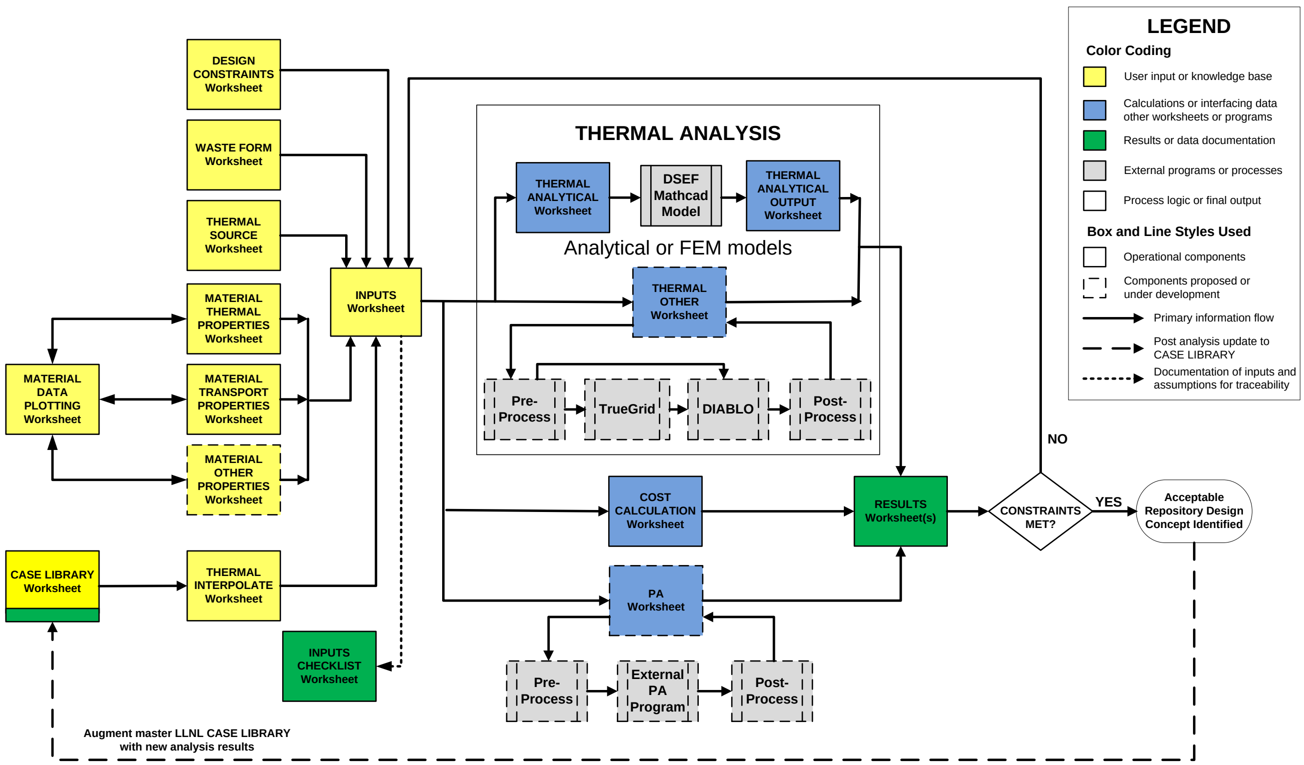
OUTPUT

- **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:
** DSEF Version 2.1 currently includes only subsurface development costs.*
***Not currently implemented in DSEF VERSION 2.1.*

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.

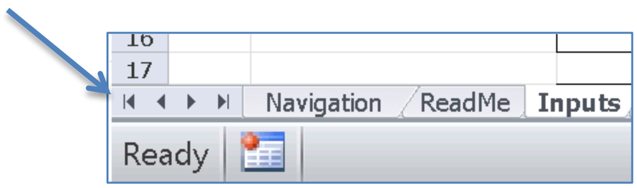
Figure 2 – Example of the information flow in DSEF



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's Guide, 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 sometimes used to distinguish different subsets of analysis cases in the CASE CATALOG or CASE LIBRARY and on other worksheets
- 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

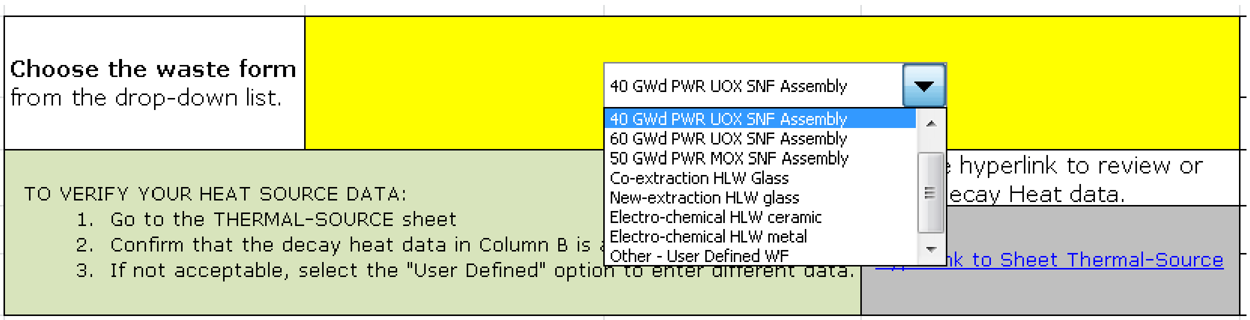
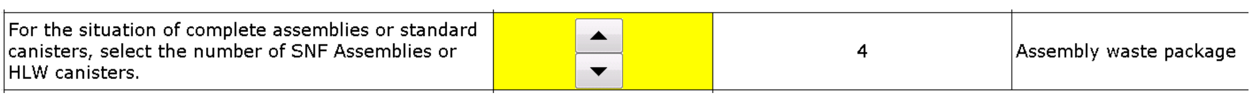


Figure 6 – A spinner control to select the number of assemblies in a waste package



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's Guide, 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 18 - 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. At this time, these costs are for testing purposes only, until LLNL and SRNL can jointly review this algorithm and compare it to the more detailed results SRNL has developed in another UFD work package. 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 the MTU for a single spent fuel assembly size. The user also enters the number of waste packages per drift, the number of drifts per panel, the access main radius, the extra spacing at the ends of the emplacement drifts, and the extra spacing at the ends of the access mains. 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. This limitation will be removed in Version 3 of DSEF.

- 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

MTU per Repository	70,000	<-- Repository_MTU
MTU per assembly	0.47	<-- Repository_avg_MTU_per_assembly
WP/ (Emplacement Drift)	15	<-- Repository_WP_per_drift
# Emplacement Drifts / panel	48	<-- Repository_drifts_per_panel
Radius (m) of Access Main (r_{AM})	2.75	<-- Repository_access_main_r
Extra Spacing (m) at ends of Emplacement Drift	5	<-- Repository_drift_extra_length
Extra Spacing (m) at ends of Access Main	5	<-- Repository_access_extra_length

Figure 10 – Example of Cost Contingency Input Data

See Table 5-3 on the COST REFERENCES sheet (from the Cost-1 reference) for guidance on selection of high and low contingencies for various processes. Note recommended values for mining = 5% and 30%		
Low Range Contingency (%)	5%	<-- Repository_low_contingency
High Range Contingency (%)	30%	<-- Repository_high_contingency
Nominal Contingency (Average of High & Low)	18%	<-- Repository_nominal_contingency

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

Single or parametric calculation		Select Mode ○ Single Parametric Options ○ WP Spacing ○ Drift Spacing ○ Storage Time ◉ Ventilation Duration ○ Rock Conductivity ○ Backfill Conductivity	Base value of Ventilation Duration = 250	Ventilation Duration	<-- Calculation_mode
Fill in up to 10 values, starting at the top (with no blank rows in the middle)	Value 1	200		<--- Cells reserved for user defined data	
	Value 2	250		<--- Cells reserved for user defined data	
	Value 3	300		<--- Cells reserved for user defined data	
	Value 4			<--- Cells reserved for user defined data	
	Value 5			<--- Cells reserved for user defined data	
	Value 6			<--- Cells reserved for user defined data	
	Value 7			<--- Cells reserved for user defined data	
	Value 8			<--- Cells reserved for user defined data	
	Value 9			<--- Cells reserved for user defined data	
	Value 10			<--- Cells reserved for user defined data	
	Number of Values Entered	3	<-- Parametric_data_count	<--- Cells reserved for user defined data	
Minimum	Maximum	Average	Single Case Value	Variable Units	
200	300	250	250	yr	
CROSS-CHECK: Average of the range equals the single case value					
The single case value is used in the cost estimate, and the parametric values are used in the thermal calculations.					

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.

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 about 300 records (rows) with 54 fields (columns) of data. Figure 14 shows the data fields.

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, Figure 16, and Figure 17 show the CASE CATALOG tables for enclosed mode cases, open mode cases, and open mode sensitivity cases, 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	
1	Case Number
2	Case Description
3	Design Mode
4	Date of Calc
5	Reference Document
6	Author / Org
7	Geologic Medium
8	Waste Form
9	WP Capacity (# SNFAs or Canisters)
10	WP Length, m
11	EBS Components
12	Waste Form Outer/ Canister Inner Radius, m
13	Canister Wall Thickness m
14	WP Wall Thickness m
15	Buffer Thickness m
16	Envelope Thickness m
17	Backfill Thickness m
18	Liner Thickness m
19	Calculated Rock Wall Radius, m
20	Canister Wall Material
21	WP Wall Material
22	Buffer Material
23	Envelope Material
24	Backfill Material
25	Liner Material
26	Canister Wall kth, W/m-K
27	WP Wall kth, W/m-K

Columns in Interp_Data_Table (continued)	
28	Buffer kth, W/m-K
29	Envelope Wall kth, W/m-K
30	Backfill kth, W/m-K
31	Liner kth, W/m-K
32	Rock k_th, W/m-K
33	Rock alpha, m2/s
34	Time Out of Reactor (Storage Time, yr)
35	Depth of Repository Horizon, m
36	Ambient T, °C
37	Center to Center Axial Spacing, m
38	Center to Center Lateral Spacing, m
39	Time of Peak T at Rock Wall, yr
40	Peak Rock Wall T, °C
41	% Contribution to Peak Rock Wall T from Central WP
42	% Contribution to Peak from Axial Neighbor WPs
43	% Contribution to Peak from Lateral Neighbor WP Lines
44	Time of Peak WP T, yr
45	Peak WP T, °C
46	Third T Location
47	Time of T at Third Location (Note 1)
48	Third Location T, °C (Note 1)
49	Ventilation thermal efficiency %
50	Ventilation Period (yr)
51	Backfill Duration
52	Time of Operation
53	Rock Wall Emissivity
54	Waste Package Emissivity

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

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 18. Following the color conventions introduced in Section 4, the yellow highlighted cells along the left column and in the top row of Figure 18 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 19, 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 18 (the first tool). Other parameters should also be checked using Figure 19 (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 19, 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.

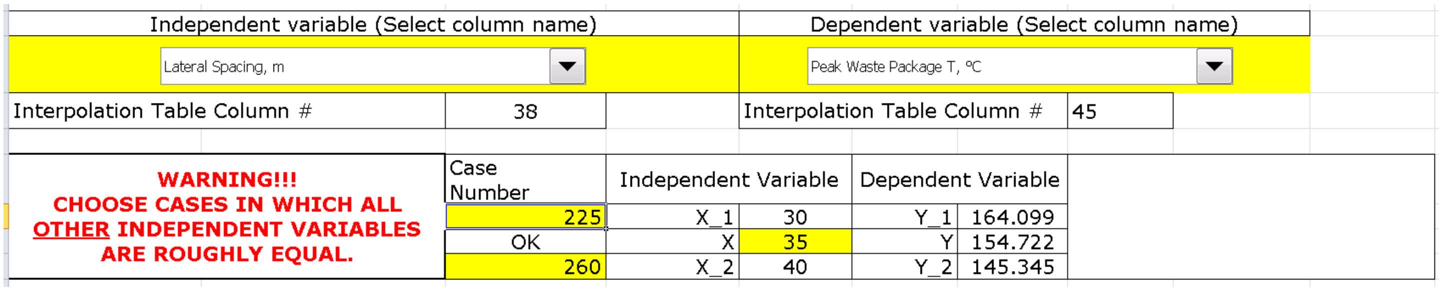
Figure 19, panel (b), shows the error message if the user inadvertently specifies the same point for each end of the interpolation. Figure 19, panel (c), shows an example of one of the drop-down lists and some of the choices for independent variables.

Figure 18 - Side-by-side case comparison table

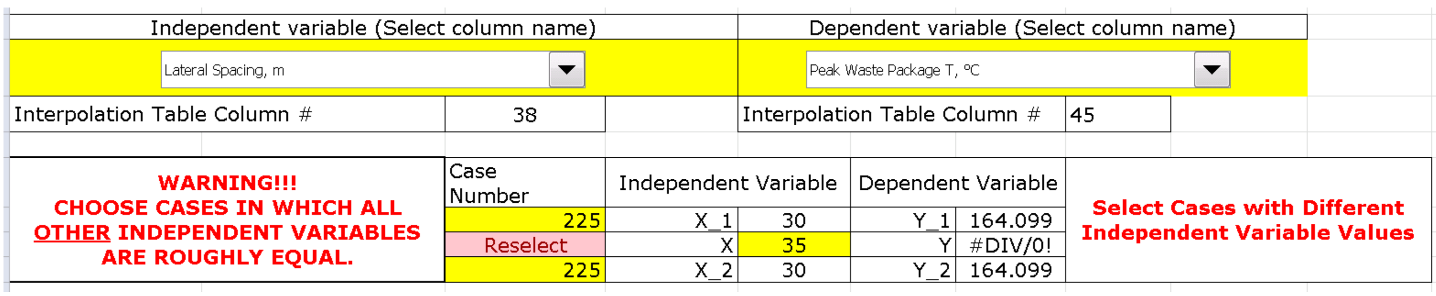
Side by side Case Comparison Section - see the CASE LIBRARY for additional description of the categories of cases in the library										
Column # -->	2	40	39	45	44	21	38	37	50	
Case Number	Case Description	Peak Rock Wall T, °C	Time of Peak T at Rock Wall, yr	Peak WP T, °C	Time of Peak WP T, yr	WP Wall 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 19 - The template for variable interpolation between relevant cases

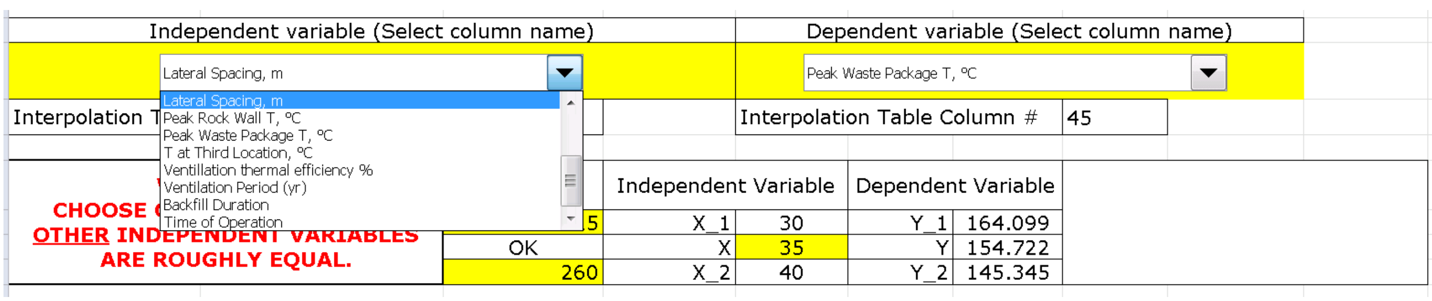
(a) – Good selection with no error messages.



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



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



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 24 and Figure 25).

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 - including intermediate calculation results for length and volume of excavated materials for emplacement drifts and access mains, as well as the backfill materials chosen and cost to backfill. See Figure 20 and Figure 21 for examples of the cost calculation results.

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.

POTENTIAL AREAS FOR DSEF VERSION 3.0 IMPROVEMENTS TO THE RESULTS SHEET:

- Addition of more comparison of results to design acceptance criteria, such as more thermal gradient results, and discussion of the thickness of sacrificial layers within the EBS and the host rock where thermal acceptance criteria are exceeded
- Cost trade-off analysis for surface storage costs versus extended repository footprint, repository operating times, and ventilation system flow rate and efficiency.

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. LLNL will work with SRNL to abstract the detailed costing done for several design options; the data included in DSEF 2.1 are from a simple reading of SRNL high-level cost results. Hence, caution should be used when calculating costs in DSEF 2.1. The cost data included are for demonstration purposes only and should not currently be used for comparison of design options.

Rough order-of-magnitude cost data were developed in Carter 2012, and presented in Hardin 2012a (and updated in Hardin 2012b).

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

- COST CALCULATIONS
- COST REFERENCES

(1) This COST CALCULATIONS sheet calculates part of the repository cost for the case defined in INPUTS, prior to setting up parametric thermal cases (which can vary one of the parameters used in the cost reference case to develop other thermal analysis results in Mathcad).

(2) In DSEF Version 3, this cost sheet will be modified to cost each of the parametric cases.

(3) This cost sheet calculates mining cost based on mining distance (and diameter) for the emplacement drifts and access mains.

(4) In Version 3, costs will be extended to include other items, such as waste packages.

(5) In Version 3, costs will be of the form "A + bB + cC" where A is a fixed cost (once per repository), B is a type cost (once per drift or once per WP, independent of WP capacity, e.g.), and C is a unit cost (per m of drift or per ton of steel in a WP, e.g.)

All of the required inputs that describe the repository level details of the number of emplacement drifts, waste packages per drift, number and diameter of access mains, number of drifts per panel, number of panels per repository, etc. are supplied by the user on the INPUTS worksheet.

The first part of the COST CALCULATIONS worksheet assembles the total emplacement drift length, total excavated volume, number of waste packages, and other results needed to estimate the cost of repository construction. An example is shown in Figure 20.

Figure 21 shows the COST CALCULATIONS section where the excavation and backfill costs are calculated for the emplacement drifts and access mains. Note that currently the cost calculations only include material costs based on the overall repository design concept defined in DSEF. Later versions of DSEF will account for construction, operations, monitoring, and closure costs, as well as the cost of waste packages, or other external costs (like transportation) other than the material costs above.

The COST-REFERENCES worksheet is included to provide source data for user. The backfill section of this worksheet includes a number of web pages for current data. However, this is neither an endorsement nor recommendation for using these particular web pages, which were chosen as examples for a ballpark estimate as a starting point for the user.

Figure 20 - Example of repository level calculation performed on the COST CALCULATIONS worksheet as shown on the RESULTS worksheet

Repository Configuration - for the COST calculations

MTU	MT/assembly	Number of Assemblies	WP Capacity (PWR)	WP Length (m)	WP Outer Radius (m)	Radius (m) of Emplacement Drift (r_{DW})	WP Spacing (m)	Emplacement Drift Spacing (m)
70,000	0.47	148,936	32	5	1	2.25	10	30

WP/ (Emplacement Drift)	# Emplacement Drifts / panel	Radius (m) of Access Main (r_{AM})	Extra Spacing (m) at ends of Emplacement Drift	Extra Spacing (m) at ends of Access Main
15	48	2.75	5	5

Figure 21 – Example of excavation and backfill cost calculations as shown on the RESULTS worksheet

Emplacement Drift Cross-section (m^2)	Access Main Cross-section (m^2)	Emplacement Drift Length (m)	Access Main Length (m)	Emplacement Drift Volume (m^3)	Access Main Volume (m^3)	# of WP	# of Drifts	# Panels	Backfill Volume per emplacement drift (m^3) (drift vol. - waste pkg vol.)
16	24	155	1,425	2,465	33,844	4,654	310	6	2,230

		Number of items	Length[2] (m)	Excavation Volume[3, 5] (m3)	Backfill Volume[4] (m3) (drift vol. - waste pkg vol.)
Emplacement Drift Calculations	Per Drift	1	155	2,465	2,230
	Per Panel	48	7,440	118,328	107,018
	Per Repository	310	48,094	764,902	691,793
Access Main Calculations	Per Main	1	1,425	33,844	0
	Per Panel[1]	1	1,425	33,844	0
	Per Repository	6	9,208	218,774	0

Notes:

1. Only one access main per panel, since the next panel is adjacent and shares the other main
2. For N waste packages, drift length = (N-1)*(axial spacing) + (waste package length) + 2*(extra spacing at ends of drift)
3. For M drifts per panel, access main length = (M-1)*(lateral spacing) + (drift diameter) + 2*(extra spacing at ends of access main)
4. The net backfill volume calculation conservatively ignores the volume of the invert, liner, support pedestals, and other components.
5. ignores shaft volume, access drifts other than those that connect emplacement drifts, and any backfill other than in emplacement drifts

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 22 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 23 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. A similar BWR waste form lookup table will be developed for DSEF 3.0 in FY13. 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.

Other potential developments of this worksheet in FY13 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 22 – 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

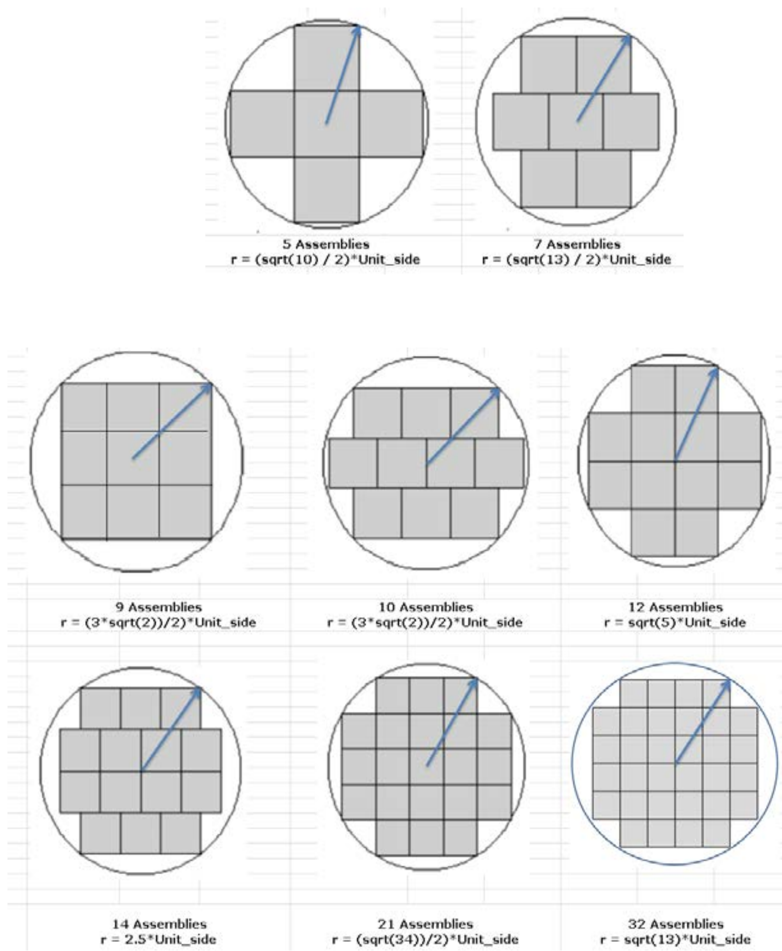
Enclosed Mode Cases	
Waste Form	Waste Package Length (m)
SNF (UOX and MOX)	5
HLW (Co-X, New-X, and EC-C)	4.572 (15 ft)
HWL (EC-M)	3.048 (10 ft)

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 23 - 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



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 Mahcad, 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 24. 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 25.

Figure 24- Example of parametric study plots on the THERMAL-ANALYTICAL OUTPUT worksheet

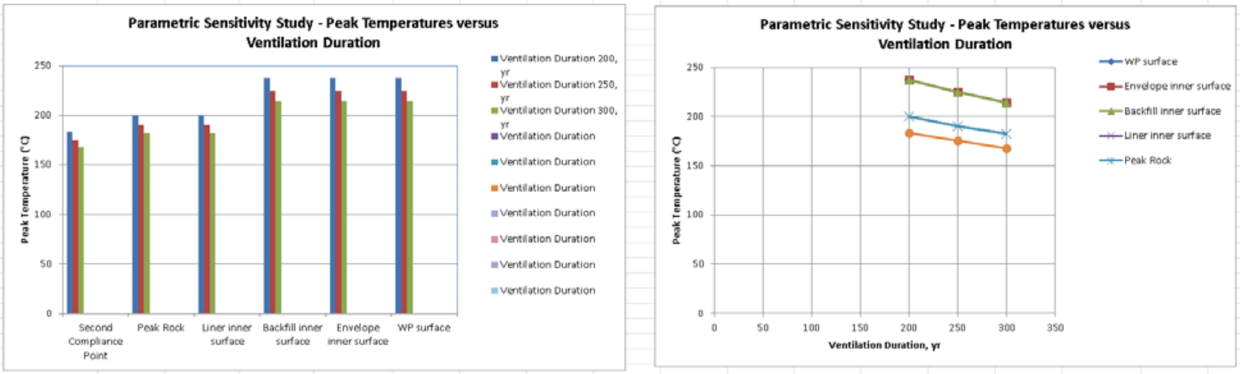
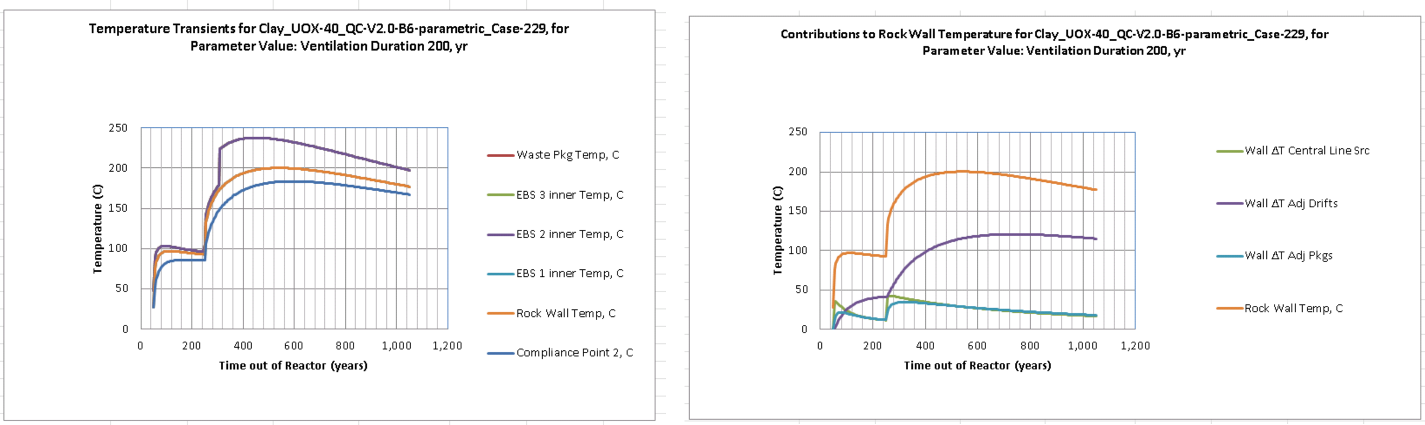


Figure 25 - Example transient output data plotted in the THERMAL-ANALYTICAL OUTPUT worksheet



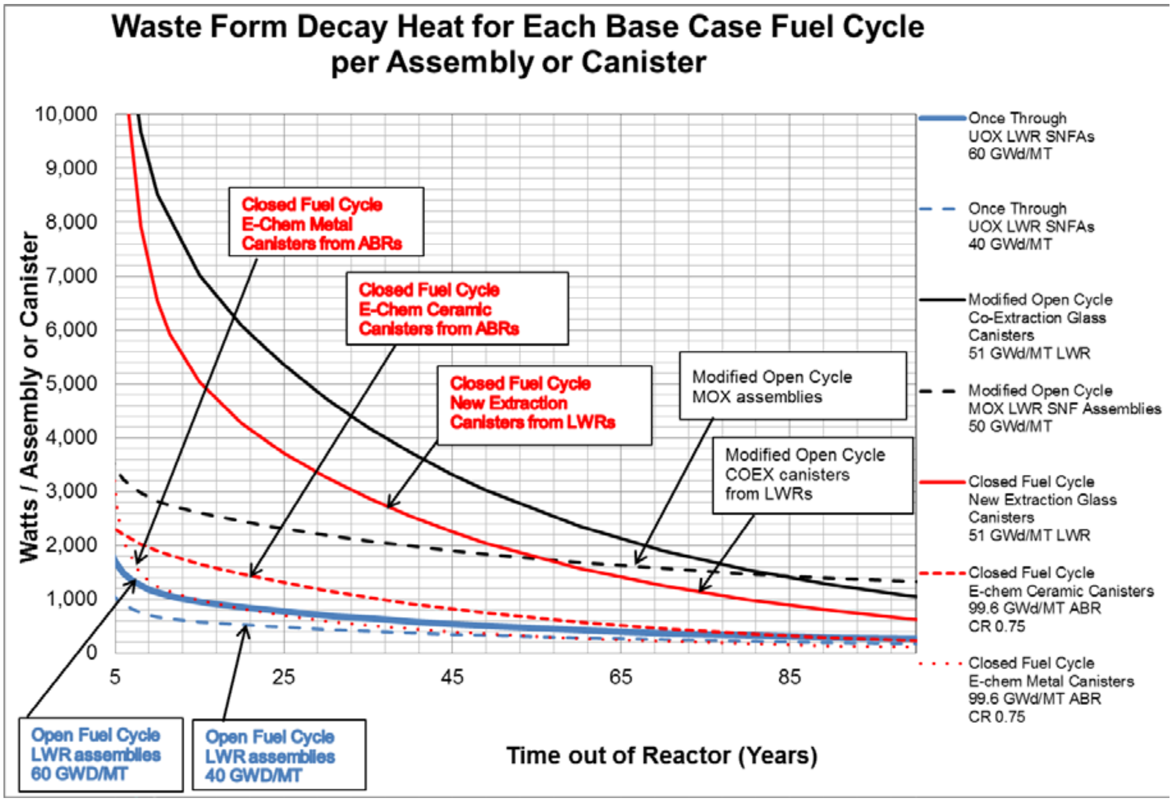
The THERMAL SOURCE Worksheet – Defining the Waste Form Decay Heat

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 26 shows a plot of the pre-defined waste form decay heat data available for selection on the THERMAL-SOURCE worksheet (Greenberg 2012).

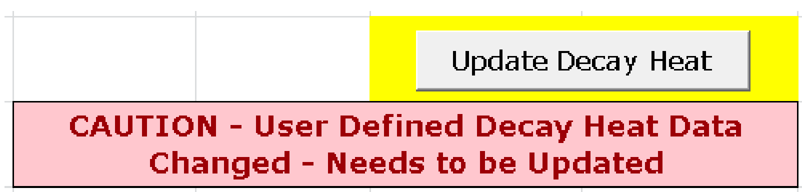
Figure 26 – Decay heat data built-in to the THERMAL-SOURCE worksheet



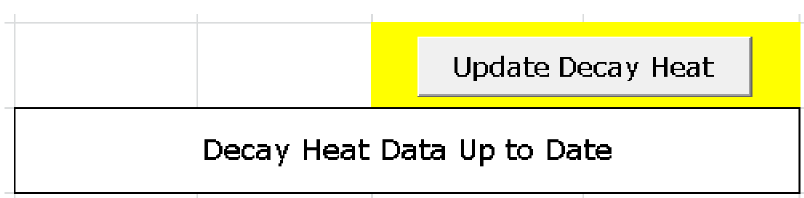
A drop-down list on the INPUTS worksheet allows the user to select one of these data sets, or choose to enter their own data. A prompt and a hyperlink are provided to go the THERMAL-SOURCE worksheet to examine the data, and to click on a macro button to update the decay heat input curve if necessary. Figure 27 shows an example of the "*Update Decay Heat"* macro button and the two types of prompts.

Figure 27 - 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

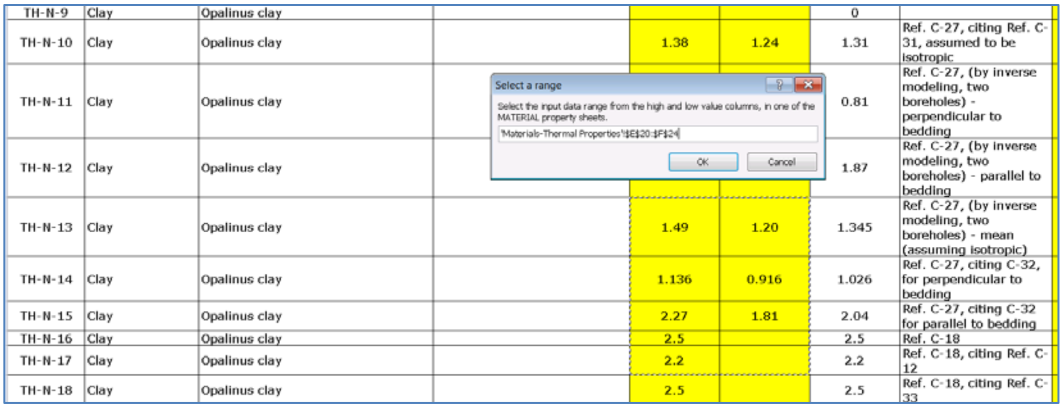
These worksheets are all linked together by the main MATERIALS worksheet, which includes hyperlinks to the other materials worksheets, and then back to the INPUTS worksheet where the derived material properties will be used.

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 28. 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.

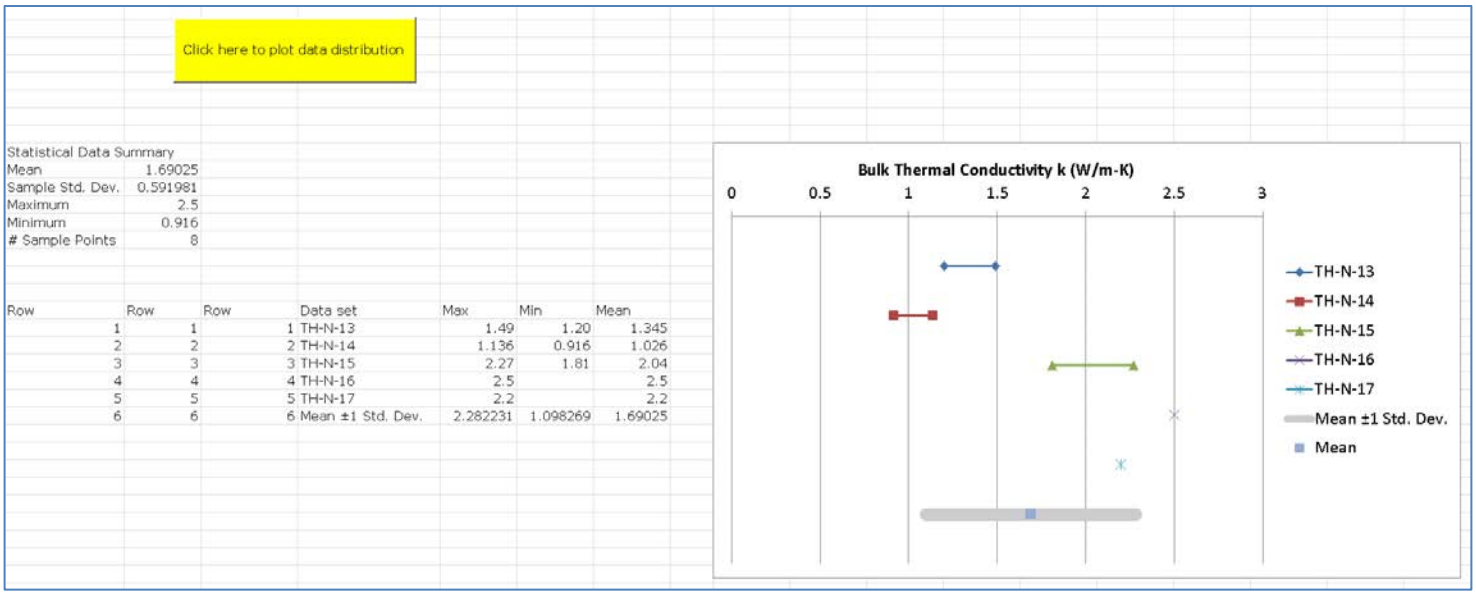
The range of data selected can be a continuous block of data values or a separate collection of different data sets (use the CTRL key with the mouse to select non-contiguous sets of data). Any blank rows in the middle of a range of data will be ignored. After clicking OK on the range selection box the 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 29 and Figure 29. 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 28 - 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 29 - 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 30.

Figure 30 - Example of data structure in the MATERIALS-THERMAL PROPERTIES worksheet

	Host Rock			Range		Mean	
Data Set Number	General Material Category	Specific Material Data Source	Source Organization / Reference	High Bulk Thermal Conductivity k (W/m-K)	Low Bulk Thermal Conductivity k (W/m-K)	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 31.

Figure 31 - Example of data structure in the MATERIALS-TRANSPORT PROPERTIES worksheet

	Host Rock			Range		Mean	
Data Set Number	General Material Category	Specific Material Subcategory	Source Organization / Reference	High Permeability (m^2)	Low Permeability (m^2)	Permeability (m^2)	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 2.1 has all of these hyperlinks removed.

13. Placeholder worksheets for future development

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 is currently entered in Step 11 of the INPUTS worksheet. However, future use of the DESIGN CONSTRAINTS worksheet is intended to document experimental results and other information currently being developed.

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. We could more fully define and structure the input extractions

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 will 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 will include some post-processing of data to write the results back to the THERMAL-ANALYTICAL OUTPUT worksheet

14. References

(Carter 2012). Joe T. Carter, Phillip O. Rodwell, Mark DuPont, *Generic Repository ROM Cost Study*, FCRD-UFD-2012-000211 Rev 0, July 31, 2012

(Greenberg 2012), 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

(Hardin 2011). Hardin, E., J. Blink, H. Greenberg, M. Sutton, M. Fratoni, J. Carter, M. DuPont and R. Howard 2011. *Generic Repository Design Concepts and Thermal Analysis (FY11)*. FCRD-USED-2011-000143 Rev. 2. December, 2011

(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

Figure A-2 – The OPTIONS menu choices

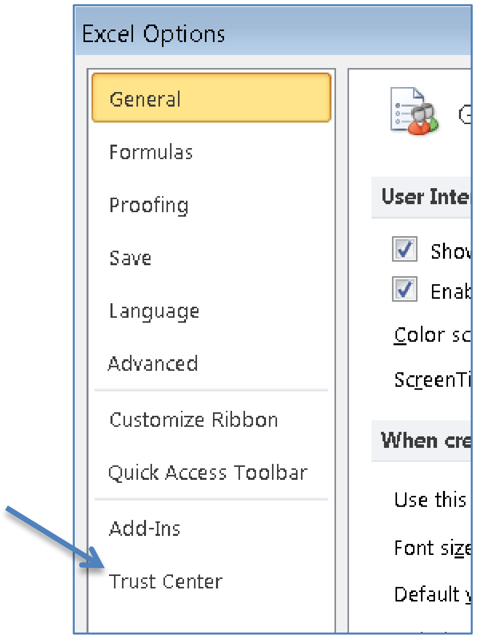


Figure A-3 – Select Trust Center Settings

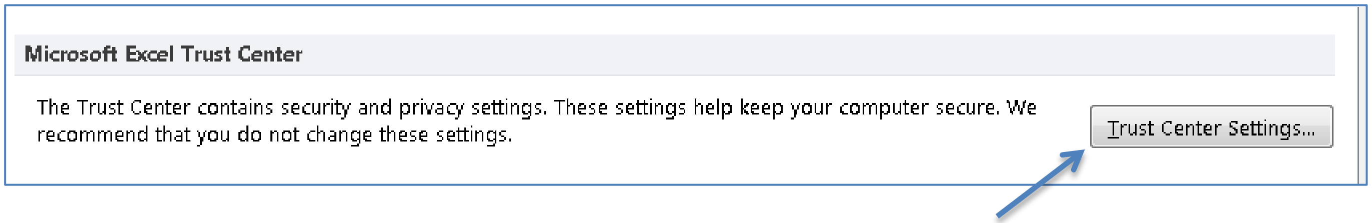


Figure A-4 – Trust Center Settings

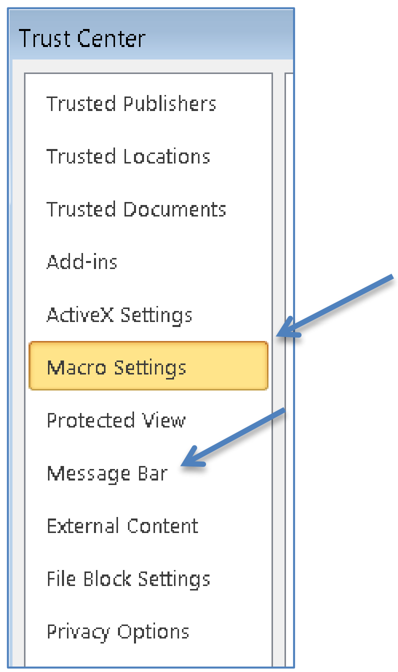


Figure A-5 – Prompt before enabling all controls with minimal restrictions

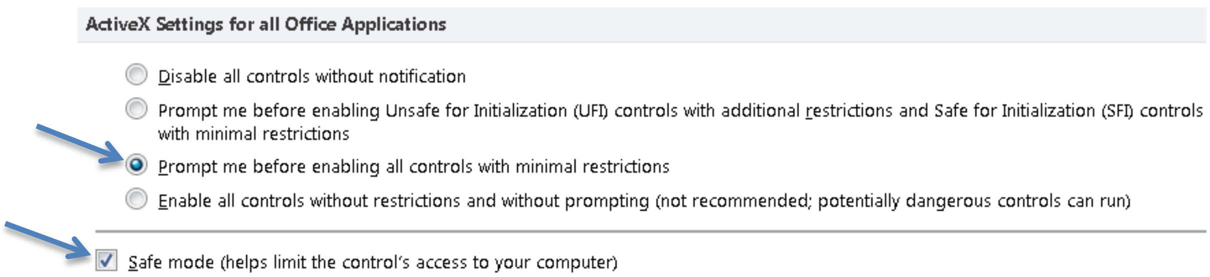


Figure A-6 – Macro settings

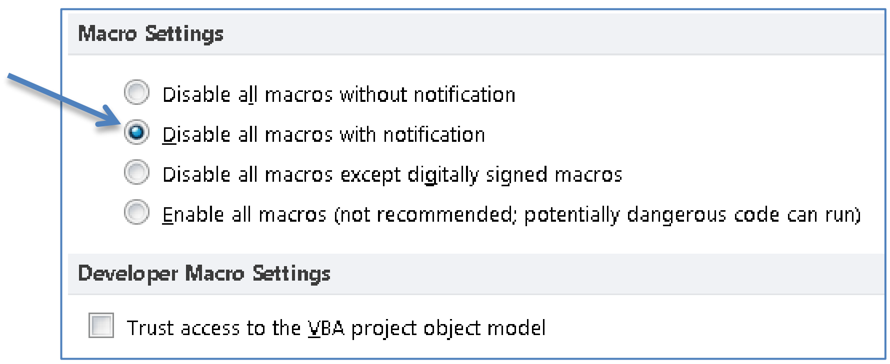
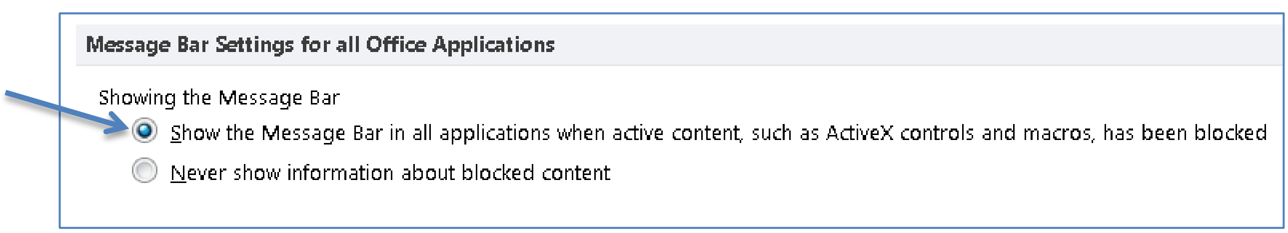


Figure A-7 – Message bar settings



Appendix B – The Mathcad Thermal-Analytical Component of DSEF

This appendix contains PDF pages of the DSEF Version 2.1 Mathcad thermal-analytical model that receives input from the THERMAL-ANALYTICAL worksheet, and returns transient and peak summary data to the THERMAL-ANALYTICAL OUTPUT worksheet in DSEF.

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 Mahcad, 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.

DSEF R2.1 Parametric Sensitivity Study Mathcad Model

Variables for repository symmetry and extent:

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

Allow output transients to be written back to DSEF FILE

Write_OK := "No"

NOTE THAT VERSION 3.0 OF DSEF AND ITS ASSOCIATED MATHCAD WILL USE THE Write OK variable to control writing back to Excel-DSEF, another Excel file, or not at all. Further, that DSEF will enable the user to start MATHCAD for a case, due multiple runs with overrides (and optional file-writes, and decide when to do the final run and write back to the Excel-DSEF file.

REQUIRED REPOSITORY INPUT DATA (from DSEF):

file := "DSEF R2.1_2013Mar4_HRG-Clay_UOX-40_QC-V2.1-parametric_Case-229p.xlsm"

sheet := "Thermal-Analytical!"

READ DSEF INPUT FILE

Input 1 = Operating Mode (enclosed or open)

Return to Table of Contents

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

Input_1 = ("MODE = Open or Enclosed:" "Open")

$Mode := Input_1_{1,2} = $ "Open"

Input 2 = Case Definitions

Input_2 := READEXCEL(file, concat(sheet, "A7:B16"))

Input_2 =

"Host Media"	"Clay"
"Rock thermal conductivity, W/m-K"	1.75
"Rock thermal diffusivity, m2/sec"	6.45×10^{-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"	10
"Drift / Borehole (lateral) spacing, m"	30
"Surface storage time, y"	50

Input 3 = Ventilation Parameters (for Open Modes)

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

Input_3 =

"Ventilation Duration, yr"	250
"Unventilated Closure Duration (Backfill Installation), yr"	10
"Ventilation Thermal Efficiency, %"	0.75
"Rock Wall Emissivity"	0.9
"Waste Package Emissivity"	0.6

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

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

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

$WP\_depth := Input\_2_{4,2} \cdot m = 500 m$

$T_{surface} := (Input\_2_{5,2} + 273.15) \cdot K = 288.15 K$

$geothermal\_gradient := Input\_2_{6,2} \frac{K}{km} = 0.025 \frac{K}{m}$

$T_{ambient} := (Input\_2_{7,2} + 273.15) \cdot K = 300.65 K$

$WP\_spacing := Input\_2_{8,2} \cdot m = 10 m$

$Drift\_spacing := Input\_2_{9,2} \cdot m = 30 m$

$t_{store} := Input\_2_{10,2} \cdot yr = 50 \cdot yr$

$t_{vent} := if[(Mode = "Enclosed"), 0, Input\_3_{1,2}] \cdot yr = 250 \cdot yr$

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

$V_{eff} := Input\_3_{3,2} = 0.75$

$\varepsilon_{wall} := Input\_3_{4,2} = 0.9$

$\varepsilon_{WP} := Input\_3_{5,2} = 0.6$

$t_{operate} := (t_{store} + t_{vent}) = 300 \cdot yr$ T_OPERATE = T_STORE + T_VENTILATE

$t_{closure} := t_{operate} + t_{backfill} = 310 \cdot yr$ TCLOSURE = TOPERATE + TIME TO BACKFILL

Input 4 = ENGINEERED BARRIER SYSTEM DATA:

Input_4 := READEXCEL(file, concat(sheet, "A20:F27"))

Input_4 =

"Waste Form Outer Radius, m"	0.89	"N/A"	0.89	"UOX-40"	"N/A"
"Canister"	0	0.89	0.89	"None"	"N/A"
"Waste Package"	0.11	0.89	1	"Carbon Steel"	"N/A"
"Buffer"	0	1	1	"None"	"N/A"
"Envelope"	0	1	1	"None"	"N/A"
"Backfill"	1.225	1	2.225	"70% Bentonite 30% Sand"	1.2
"Liner"	0.025	2.225	2.25	"Steel"	46
"Host Rock Inner Radius, m ---->"	NaN	2.25	NaN	NaN	NaN

$r_{DW} := Input\_4_{8,3} \cdot m = 2.25 m$

$r_{WP} := Input\_4_{3,4} \cdot m = 1 m$

Input 5 = COMPLIANCE POINT 2 INPUT DATA

Input_5 := READEXCEL(file, concat(sheet, "C32"))

$Input\_5 = (5.25)$

$r_{CP2} := Input\_5_1 \cdot m = 5.25 m$

$EBS\_name_1 := Input\_47_{,1} = \text{"Liner"}$

$EBS\_material_1 := Input\_47_{,5} = \text{"Steel"}$

$thickness_1 := Input\_47_{,2} \cdot m = 0.025\,m$

$r_1 := Input\_47_{,4} \cdot m = 2.25\,m$

$k1 := Input\_47_{,6} = 46$

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

$EBS\_name_2 := Input\_46_{,1} = \text{"Backfill"}$

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

$thickness_2 := Input\_46_{,2} \cdot m = 1.225\,m$

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

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

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

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

$EBS\_name_3 := Input\_45_{,1} = \text{"Envelope"}$

$EBS\_material_3 := Input\_45_{,5} = \text{"None"}$

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

$r_3 := Input\_45_{,4} \cdot m = 1\,m$

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

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

$EBS\_name_4 := Input\_44_{,1} = \text{"Buffer"}$

$EBS\_material_4 := Input\_44_{,5} = \text{"None"}$

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

$r_4 := Input\_44_{,4} \cdot m = 1\,m$

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

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

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):

$r_{WP} = 1\,m$ $r_4 = 1\,m$ $r_3 = 1\,m$ $r_2 = 2.225\,m$ $r_1 = 2.25\,m$ $r_{DW} = 2.25\,m$

$R_1(k_1) := if\left[\left[thickness_1 = 0 \vee (k1 = \text{"N/A"})\right], 0, \frac{r_{DW}}{k_1} \cdot \ln\left(\frac{r_1}{r_2}\right)\right]$

$R_1(k_1) = 5.465 \times 10^{-4} \cdot \frac{m^2 \cdot K}{W}$

Thermal resistance

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

$$R_2(k_2,t) := \left| \begin{array}{l} kk \leftarrow k_{radiation}\cdot(t < t_{closure}) + k_2\cdot(t \geq t_{closure}) \\ \text{return } \text{if}\left[\left[(thickness_2 = 0) \vee (kk = 0)\right], 0, \frac{r_{DW}}{kk}\cdot\ln\left(\frac{r_2}{r_3}\right)\right] \end{array} \right.$$

$$\frac{r_{DW}}{k_2}\cdot\ln\left(\frac{r_2}{r_3}\right) = 1.5\cdot\frac{m^2\cdot K}{W}$$

EBS_name$_2$ = "Backfill"   EBS_material$_2$ = "70% Bentonite 30% Sand"

$$R_2(k_2, 5\cdot yr) = 0\cdot\frac{m^2\cdot K}{W} \qquad R_2(k_2, 1000\cdot yr) = 1.499544\cdot\frac{m^2\cdot K}{W}$$

$$R_3(k_3) := \text{if}\left[\left[thickness_3 = 0 \vee (k3 = \text{"N/A"})\right], 0, \frac{r_{DW}}{k_3}\cdot\ln\left(\frac{r_3}{r_4}\right)\right] \qquad R_3(k_3) = 0\cdot\frac{m^2\cdot K}{W}$$

EBS_name$_3$ = "Envelope"   EBS_material$_3$ = "None"

$$R_4(k_4) := \text{if}\left[\left[thickness_4 = 0 \vee (k4 = \text{"N/A"})\right], 0, \frac{r_{DW}}{k_4}\cdot\ln\left(\frac{r_4}{r_{WP}}\right)\right] \qquad R_4(k_4) = 0\cdot\frac{m^2\cdot K}{W}$$

EBS_name$_4$ = "Buffer"   EBS_material$_4$ = "None"

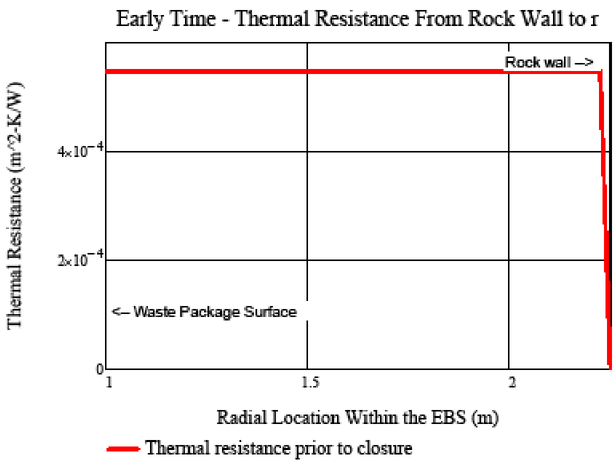
$$R_{Total}(t,k_1,k_2,k_3,k_4) := R_1(k_1) + R_2(k_2,t) + R_3(k_3) + R_4(k_4)$$

Total thermal resistance between wall and waste package

$$R_{continuous}(t,r,k_1,k_2,k_3,k_4) := \left| \begin{array}{l} kk_2 \leftarrow k_{radiation}\cdot(t < t_{closure}) + k_2\cdot(t \geq t_{closure}) \\ R \leftarrow R_1(k_1) + R_2(k_2,t) + R_3(k_3) + \text{if}\left[\left[(thickness_4 = 0) \vee (k4 = \text{"N/A"})\right], 0, \frac{r_{DW}}{k_4}\cdot\ln\left(\frac{r_4}{r}\right)\right] \text{ if } r \leq r_4 \wedge r \geq r_{WP} \\ R \leftarrow R_1(k_1) + R_2(k_2,t) + \text{if}\left[\left[(thickness_3 = 0) \vee (k3 = \text{"N/A"})\right], 0, \frac{r_{DW}}{k_3}\cdot\ln\left(\frac{r_3}{r}\right)\right] \text{ if } r \leq r_3 \wedge r > r_4 \\ R \leftarrow R_1(k_1) + \text{if}\left[\left[(thickness_2 = 0) \vee kk_2 = 0\right], 0, \frac{r_{DW}}{kk_2}\cdot\ln\left(\frac{r_2}{r}\right)\right] \text{ if } r \leq r_2 \wedge r \geq r_3 \\ R \leftarrow \text{if}\left[\left[(thickness_1 = 0) \vee (k1 = \text{"N/A"})\right], 0, \frac{r_{DW}}{k_1}\cdot\ln\left(\frac{r_1}{r}\right)\right] \text{ if } r \leq r_{DW} \wedge r \geq r_2 \\ R \leftarrow \text{"Invalid Radius" otherwise} \\ \text{return } R \end{array} \right.$$

Mathcad-DSEF Version 2.1 Parametric Sensitivty Model.xmcd

$R_{continuous}(5\cdot yr, r_{WP}, k_1, k_2, k_3, k_4) = 5.465\times10^{-4}\frac{K\cdot s^3}{kg}$ $R_{continuous}(1000\cdot yr, r_{WP}, k_1, k_2, k_3, k_4) = 1.500091\frac{K\cdot s^3}{kg}$



$r_{DW} = 2.25m$

$r_1 = 2.25m$ EBS_name$_1$ = "Liner" EBS_material$_1$ = "Steel"

$r_2 = 2.225m$ Note that for "open modes", the backfill hasn't been emplaced at early time, and EBS-2 is only radiation.

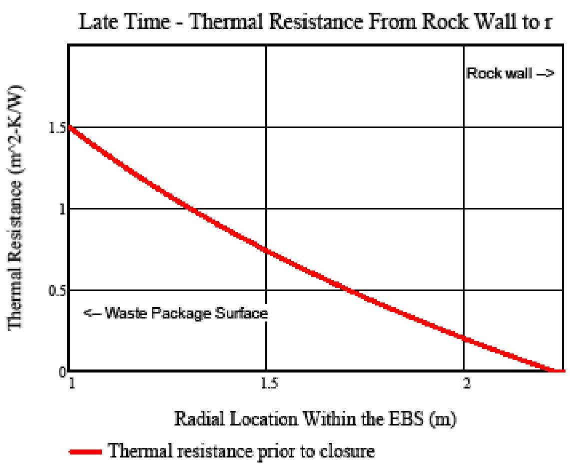
$r_3 = 1m$ EBS_name$_3$ = "Envelope" EBS_material$_3$ = "None"

$r_4 = 1m$ EBS_name$_4$ = "Buffer" EBS_material$_4$ = "None"

$r_{WP} = 1m$

$R_1(k_1) = 5.465\times10^{-4}\cdot\frac{m^2\cdot K}{W}$ $R_2(k_2, 5\cdot yr) = 0\cdot\frac{m^2\cdot K}{W}$ $R_3(k_3) = 0\cdot\frac{m^2\cdot K}{W}$ $R_4(k_4) = 0\cdot\frac{m^2\cdot K}{W}$

$R_{Total}(50yr, k_1, k_2, k_3, k_4) = 5.465\times10^{-4}\cdot\frac{m^2\cdot K}{W}$



$r_{DW} = 2.25m$

$r_1 = 2.25m$ EBS_name$_1$ = "Liner" EBS_material$_1$ = "Steel"

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

$r_3 = 1m$ EBS_name$_3$ = "Envelope" EBS_material$_3$ = "None"

$r_4 = 1m$ EBS_name$_4$ = "Buffer" EBS_material$_4$ = "None"

$r_{WP} = 1m$

$R_1(k_1) = 5.465 \times 10^{-4} \cdot \frac{m^2 \cdot K}{W}$ $R_2(k_2, t_{closure}) = 1.5 \cdot \frac{m^2 \cdot K}{W}$ $R_3(k_3) = 0 \cdot \frac{m^2 \cdot K}{W}$

$R_{Total}(1000yr, k_1, k_2, k_3, k_4) = 1.5 \cdot \frac{m^2 \cdot K}{W}$

INPUT 6 = WASTE FORM DATA

Input_6 := READEXCEL(file, concat(sheet, "A35:B38"))

"Waste form short name"	"UOX-40"
"Waste form type"	"Assembly"
"Waste package capacity"	32
"Waste package length, m"	5

WF_name := Input_6$_{1,2}$ = "UOX-40"

WF_type := Input_6$_{2,2}$ = "Assembly"

WP_cap := Input_6$_{3,2}$ = 32

WP_length := Input_6$_{4,2}$·m = 5m

Outside of the liner: $A_1 := 2 \cdot \pi \cdot r_1 \cdot WP\_length = 70.69m^2$

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

Outside of the backfill: $A_2 := 2 \cdot \pi \cdot r_2 \cdot WP\_length = 69.9m^2$

Outside of the envelope: $A_3 := 2 \cdot \pi \cdot r_3 \cdot WP\_length = 31.42m^2$

Outside of the buffer: $A_4 := 2 \cdot \pi \cdot r_4 \cdot WP\_length = 31.42m^2$

$A_{WP} := 2 \cdot \pi \cdot r_{WP} \cdot WP\_length = 31.416m^2$

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.

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

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

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

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

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.

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.

$$h_{rad\_infinite}(r_i, r_o, \epsilon_i, \epsilon_o) := \frac{\sigma}{\frac{1}{\epsilon_i} + \left(\frac{1-\epsilon_o}{\epsilon_o}\right) \cdot \frac{r_i}{r_o}}$$

$$h_{rad\_infinite}(r_{WP}, r_{DW}, \epsilon_{WP}, \epsilon_{wall}) = 3.304 \times 10^{-8} \cdot \frac{W}{m^2 K^4}$$

Usage is Q in watts = h*A$_i$*(T$_i$^4 - T$_o$^4)

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

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

$$Q_{rad\_infinite}(r_3, r_2, \epsilon_{WP}, \epsilon_{wall}, WP\_length, 300 \cdot K, 600 \cdot K) = 1.261 \times 10^5 W$$

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

$$Q_{L\_rad\_infinite}(r_3, r_2, \epsilon_{WP}, \epsilon_{wall}, 300 \cdot K, 600 \cdot K) = 2.522 \times 10^4 \cdot \frac{W}{m}$$

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.

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

$$Q_{L\_infinite}(r_3, r_2, \epsilon_{WP}, \epsilon_{wall}, 300 \cdot K, 600 \cdot K) = 2.522 \times 10^4 \cdot \frac{W}{m}$$

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.

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

$$Q_{L\_conduction\_comparison}(r_3, r_2, 300 \cdot K, 600 \cdot K) = 2.797 \times 10^3 \cdot \frac{W}{m}$$

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

$$Q_{ratio}(r_3, r_2, \epsilon_{WP}, \epsilon_{wall}, 300 \cdot K, 600 \cdot K) = 9.016$$

INPUT 7 = PARAMETRIC STUDY VARIABLE INPUT DATA

Input_7 := READEXCEL(file, concat(sheet, "F29:F41"))

Cases := $Input\_7_1$ = 3

Parameter := $Input\_7_2$ = "Ventilation Duration"

Parameter_units := $Input\_7_3$ = "yr"

ij := 1 .. Cases

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

Input_7 =

	1
1	3
2	"Ventilation Duration"
3	"yr"
4	200
5	250
6	300
7	""
8	""
9	""
10	""
11	""
12	""
13	""

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

Parameter_data = $\begin{pmatrix} 200 \\ 250 \\ 300 \end{pmatrix}$ Parameter_description = ("200, yr", "250, yr", "300, yr")

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

Input_8_size := READEXCEL(file, concat(sheet, "C43")) $Input\_8\_size_1$ = 58 Decay_heat_range := concat["A43:B", num2str(($Input\_8\_size_1$ + 42))] = "A43:B100"

Input_8 := READEXCEL(file, concat(sheet, Decay_heat_range))

Time_out_of_Reactor := $Input\_8^{\langle 1\rangle}\cdot yr$ Decay_Heat_per_Cnt := $Input\_8^{\langle 2\rangle}\cdot W$

Input_8 =

	1	2
1	5	$1.028\cdot10^3$
2	5.1	$1.011\cdot10^3$
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	...

Time_out_of_Reactor = (·yr)

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

Decay_Heat_per_Cnt = (W)

	1
1	$1.028\cdot10^3$
2	$1.011\cdot10^3$
3	949.125
4	916.671
5	887.984
6	742.948
7	670.028
8	634.239
9	576.929
10	...

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

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

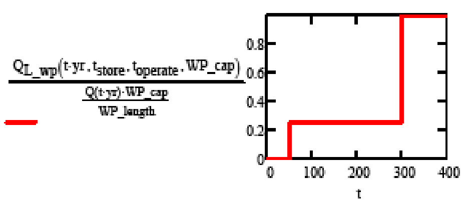
FUNCTION DEFINITION FOR ONE OUTPUT FILE

FORMULAS FOR CALCULATING THE TRANSIENT DRIFT WALL TEMPERATURE:

Central waste package:

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

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



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.

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

Adjacent drifts:

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

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.

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

Adjacent waste packages:

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

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.

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

This command specifies two rows of column headings for output paramenter sensitivity runs

OutfileName := file = "DSEF R2.1_2013Mar4_HRG-Clay_UOX-40_QC-V2.1-parametric_Case-229p.xlsm"

Out_sheet := "Thermal-Analytical Output!"

This section specifies the column headings for output sensitivity studies

Cases = 3 Read in from Thermal-Analytical sheet in DSEF (Inputs_7)

Mathcad-DSEF Version 2.1 Parametric Sensitivty Model.xmcd

$i := 1..Cases$

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

$Parameter\_vector = \begin{pmatrix} \text{"Ventilation Duration 200, yr"} \\ \text{"Ventilation Duration 250, yr"} \\ \text{"Ventilation Duration 300, yr"} \end{pmatrix}$

$heading1_i := \begin{pmatrix} concat(\text{"Parameter value: "}, Parameter\_vector_i) \\ \text{""} \\ \text{""} \\ \text{""} \\ \text{""} \\ \text{""} \\ \text{""} \\ \text{""} \\ \text{""} \\ \text{""} \end{pmatrix}$

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

$heading1_i := {heading1_i}^T \qquad heading2 := heading2^T$

$Title\_array_i := stack(heading1_i, heading2)$

$Title\_array_2 =$

	1	2	3	4	5	6	7
1	Ventilation Duration 250, yr"	""	""	""	""	""	""
2	"TooR (yr)"	"Wall ΔT Central Line Src"	"Wall ΔT Adj Drifts"	"Wall ΔT Adj Pkgs"	"Compliance Point 2, C"	"Rock Wall Temp, C"	...

For-Loop analysis returning the output time, three temperature contribution terms, and six temperatures

$length(Parameter\_data) = 3$

$r_{DW} = 2.25 m \qquad r_{CP2} = 5.25 m$

$t_{store} = 50 \cdot yr \qquad t_{operate} = 300 \cdot yr \qquad t_{closure} = 310 \cdot yr \qquad t_{vent} = 250 \cdot yr$

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_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

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

Mathcad Component of DSEF 2.1 Page 11 of 21

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

```
for i ∈ 1 .. Counter + 1
    tt_i ← Step·i·yr + t_store − Step·1yr
    kk_2 ← k_radiation·(tt_i < t_closure) + k_2·(tt_i ≥ t_closure)
    Wall_deltaT_finite_line_i ← DW_T_finite_line(tt_i, r_DW, 0, t_store, t_operate, WP_cap, Kth, α)
    Wall_deltaT_drifts_i ← DW_T_drifts(tt_i, r_DW, t_store, t_operate, WP_cap, WP_spacing, Drift_spacing, Kth, α)
    Wall_deltaT_adj_pkgs_i ← DW_T_adjacent_pkgs(tt_i, r_DW, t_store, t_operate, WP_cap, WP_spacing, Kth, α)
    Wall_T_i ← T_ambient + Wall_deltaT_finite_line_i + Wall_deltaT_drifts_i + Wall_deltaT_adj_pkgs_i
    CP2_deltaT_finite_line_i ← DW_T_finite_line(tt_i, r_CP2, 0, t_store, t_operate, WP_cap, Kth, α)
    CP2_deltaT_drifts_i ← DW_T_drifts(tt_i, r_CP2, t_store, t_operate, WP_cap, WP_spacing, Drift_spacing, Kth, α)
    CP2_deltaT_adj_pkgs_i ← DW_T_adjacent_pkgs(tt_i, r_CP2, t_store, t_operate, WP_cap, WP_spacing, Kth, α)
    CP2_T_i ← T_ambient + CP2_deltaT_finite_line_i + CP2_deltaT_drifts_i + CP2_deltaT_adj_pkgs_i
    Q_i ← Q_L_wp(tt_i, t_store, t_operate, WP_cap)
```

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

$$EBS\_2_i \leftarrow \begin{cases} EBS\_1_i + \dfrac{Q_i}{2\cdot\pi\cdot r_{DW}}\cdot R_2(kk_2, tt_i) & \text{if } kk_2 \neq 0\cdot\dfrac{W}{m\cdot K} \\ \left[\left[\dfrac{Q_i}{h_{rad\_infinite}(r_3, r_2, \epsilon_{WP}, \epsilon_{wall})\cdot 2\cdot\pi\cdot r_3} + (EBS\_1_i)^4\right]^{\frac{1}{4}}\right] & \text{otherwise} \end{cases}$$

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

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

```
    T1_i ← CP2_T_i − 273.15K
    T2_i ← Wall_T_i − 273.15K
    T3_i ← EBS_1_i − 273.15K
    T4_i ← EBS_2_i − 273.15K
    T5_i ← EBS_3_i − 273.15K
    T6_i ← WP_T_i − 273.15K
```

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

$jjj := 1..Cases$ $\quad Cases = 3$

$X_{jjj} := Parameter\_data_{jjj}$ $\quad Parameter = $ "Ventilation Duration"

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

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

File_array1 =

	1	2	3	4	5	6	7
1	Ventilation Duration 200, yr"	""	""	""	""	""	""
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	27.52
4	55	35.579	0.82	12.28	52.73	76.179	76.198
5	60	34.943	4.087	17.206	61.455	83.735	83.752
6	65	33.507	7.718	19.555	67.274	88.281	88.297
7	70	31.898	11.104	20.723	71.393	91.225	91.24
8	75	30.316	14.152	21.243	74.485	93.211	93.225
9	80	28.814	16.873	21.378	76.855	94.565	94.578
10	85	27.416	19.298	21.277	78.705	95.492	95.504
11	90	26.118	21.463	21.03	80.17	96.11	96.122
12	95	24.936	23.385	20.709	81.327	96.53	96.541
13	100	23.83	25.128	20.297	82.28	96.756	96.767
14	105	22.827	26.686	19.879	83.049	96.892	...

File_array2 =

	1	2	3	4	5	6	7
1	Ventilation Duration 250, yr"	""	""	""	""	""	""
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	27.52
4	55	35.579	0.82	12.28	52.73	76.179	76.198
5	60	34.943	4.087	17.206	61.455	83.735	83.752
6	65	33.507	7.718	19.555	67.274	88.281	88.297
7	70	31.898	11.104	20.723	71.393	91.225	91.24
8	75	30.316	14.152	21.243	74.485	93.211	93.225
9	80	28.814	16.873	21.378	76.855	94.565	94.578
10	85	27.416	19.298	21.277	78.705	95.492	95.504
11	90	26.118	21.463	21.03	80.17	96.11	96.122
12	95	24.936	23.385	20.709	81.327	96.53	96.541
13	100	23.83	25.128	20.297	82.28	96.756	96.767
14	105	22.827	26.686	19.879	83.049	96.892	...

File_array3 =

	1	2	3	4	5	6	7
1	Ventilation Duration 300, yr"	""	""	""	""	""	""
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	27.52
4	55	35.579	0.82	12.28	52.73	76.179	76.198
5	60	34.943	4.087	17.206	61.455	83.735	83.752
6	65	33.507	7.718	19.555	67.274	88.281	88.297
7	70	31.898	11.104	20.723	71.393	91.225	91.24
8	75	30.316	14.152	21.243	74.485	93.211	93.225
9	80	28.814	16.873	21.378	76.855	94.565	94.578
10	85	27.416	19.298	21.277	78.705	95.492	95.504
11	90	26.118	21.463	21.03	80.17	96.11	96.122
12	95	24.936	23.385	20.709	81.327	96.53	96.541
13	100	23.83	25.128	20.297	82.28	96.756	96.767
14	105	22.827	26.686	19.879	83.049	96.892	...

$iii := 1..10$

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

$Peak\_array_{1,2} = 42.504$

$\left(Temp\_array1\right)^{\langle 6 \rangle} =$

	1
1	27.5
2	76.179
3	83.735
4	88.281
5	91.225
6	93.211
7	94.565
8	95.492
9	96.11
10	96.53
11	96.756
12	96.892
13	96.906
14	...

$Time\_array := \left(Temp\_array1\right)^{\langle 1 \rangle}$

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

$Peak\_T(1,5) = 183.584$

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

$Peak\_time(1,5) = (600)$

$Time\_array =$

	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:

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

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

$Peak\_values =$

""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""
""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""
""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""
""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""
""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""
""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""	""

Fill in the peak temperatures and times:

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

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

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

$Parameter\_vector^{T} =$ ("Ventilation Duration 200, yr" "Ventilation Duration 250, yr" "Ventilation Duration 300, yr")

$Peak\_values =$

183.584	600	175.391	680	167.864	705	""	""	""	""	""	""	""	""	""	""	""	""	""	""
200.185	525	190.618	600	182.252	665	""	""	""	""	""	""	""	""	""	""	""	""	""	""
200.198	525	190.63	600	182.263	665	""	""	""	""	""	""	""	""	""	""	""	""	""	""
237.698	455	225.192	515	214.339	580	""	""	""	""	""	""	""	""	""	""	""	""	""	""
237.698	455	225.192	515	214.339	580	""	""	""	""	""	""	""	""	""	""	""	""	""	""
237.698	455	225.192	515	214.339	580	""	""	""	""	""	""	""	""	""	""	""	""	""	""

outsheet := "Thermal-Analytical Output!"

$rows(Temp\_array_1) = 201$ $rows(File\_array_1) = 203$ Transient output starting row in DSEF on the Thermal-= 60

start_row := 100 end_row := start_row + rows(Temp_array1) − 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 :=

"A"	"J"
"L"	"U"
"W"	"AF"
"AH"	"AQ"
"AS"	"BB"
"BD"	"BM"
"BO"	"BX"
"BZ"	"CI"
"CK"	"CT"
"CV"	"DE"

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

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

$transient\_write\_range_2$ = "Thermal-Analytical Output!L100:U300"

peaks_write_range := concat(outsheet, "C6:V11") = "Thermal-Analytical Output!C6:V11"

transient_write_range =

"Thermal-Analytical Output!A100:J300"
"Thermal-Analytical Output!L100:U300"
"Thermal-Analytical Output!W100:AF300"

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

$t_{vent} = 250 \cdot yr$

OutfileName = "DSEF R2.1_2013Mar4_HRG-Clay_UOX-40_QC-V2.1-parametric_Case-229p.xlsm"

Write_file := Write_OK = "No"

```
write_the_peaks(Write_file) := | write_it ← | WRITEEXCEL(Peak_values, OutfileName, peaks_write_range)   if (Write_file = "Yes") ∨ (Write_file = "YES")
                               |            | "File written"
                               | write_it ← "No file written"   otherwise
```

write_the_peaks(Write_file) = "No file written"

```
write_the_transient_size(Write_file) := | write_it ← | WRITEEXCEL(Transient_size, OutfileName, Transient_size_range)   if (Write_file = "Yes") ∨ (Write_file = "YES")
                                        |            | "File written"
                                        | write_it ← "No file written"   otherwise
```

write_the_transient_size(Write_file) = "No file written"

Write_file := Write_OK = "No" Cases = 3

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.

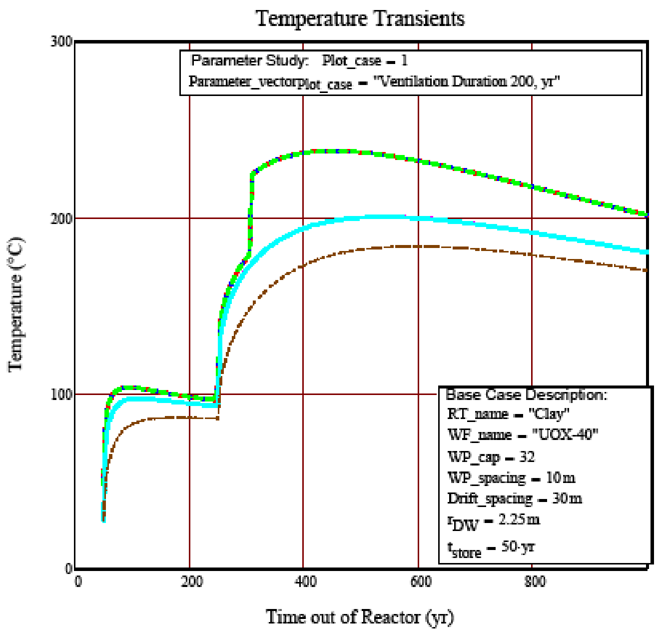
```
write_the_transients(jj) := | write_array ← Temp_array_jj
                            | write_it ← | WRITEEXCEL(write_array, OutfileName, transient_write_range_jj)   if (Write_file = "Yes") ∨ (Write_file = "YES")
                            |            | "File written"
                            | write_it ← "No file written"   otherwise
```

$$\text{write\_the\_transients(iww)} = \begin{pmatrix} \text{"No file written"} \\ \text{"No file written"} \\ \text{"No file written"} \end{pmatrix}$$

Plot_case := 1 Select parametric study case to plot (default plot is for case 1)

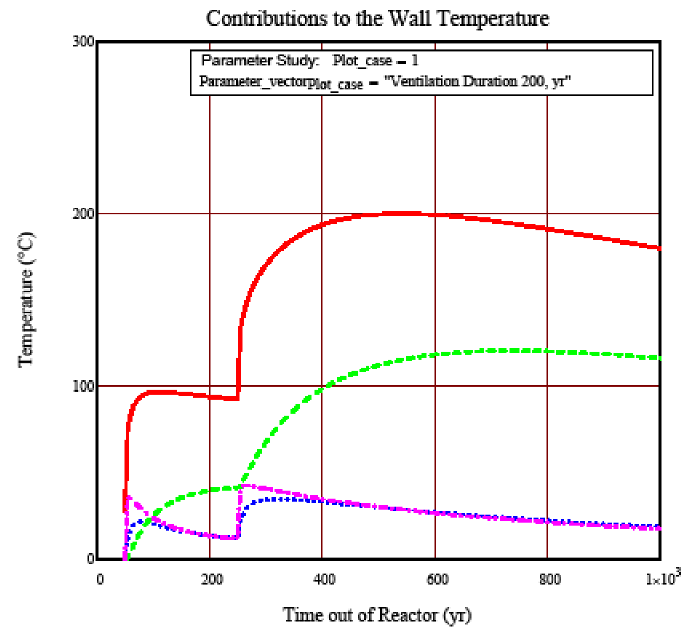
$WP\_plot := \left[\left(Temp\_array_{Plot\_case}\right)^{\langle 10\rangle}\right]$ $EBS3\_T\_plot := \left[\left(Temp\_array_{Plot\_case}\right)^{\langle 9\rangle}\right]$ $EBS2\_T\_plot := \left[\left(Temp\_array_{Plot\_case}\right)^{\langle 8\rangle}\right]$ $EBS1\_T\_plot := \left[\left(Temp\_array_{Plot\_case}\right)^{\langle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

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



Waste Package Surface Temperature
EBS3 Temperature
EBS2 Temperature
EBS1 Temperature
Drift Wall Temperature
Compliance point 2 Temperature

NOTE THAT THE BASE CASE DESCRIPTION BOX ON THE PLOT WILL BE REVISED IN VERSION 3.0 TO REFLECT A PARAMETRIC VALUE THAT MAY BE DIFFERENT THAN THE BASE CASE VALUE



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

Mathcad-DSEF Version 2.1 Parametric Sensitivty Model.xmcd

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

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

$$tt\_rw := \left[(Peak\_values)^{\langle Plot\_case\cdot 2\rangle}\right]_2 = 525$$

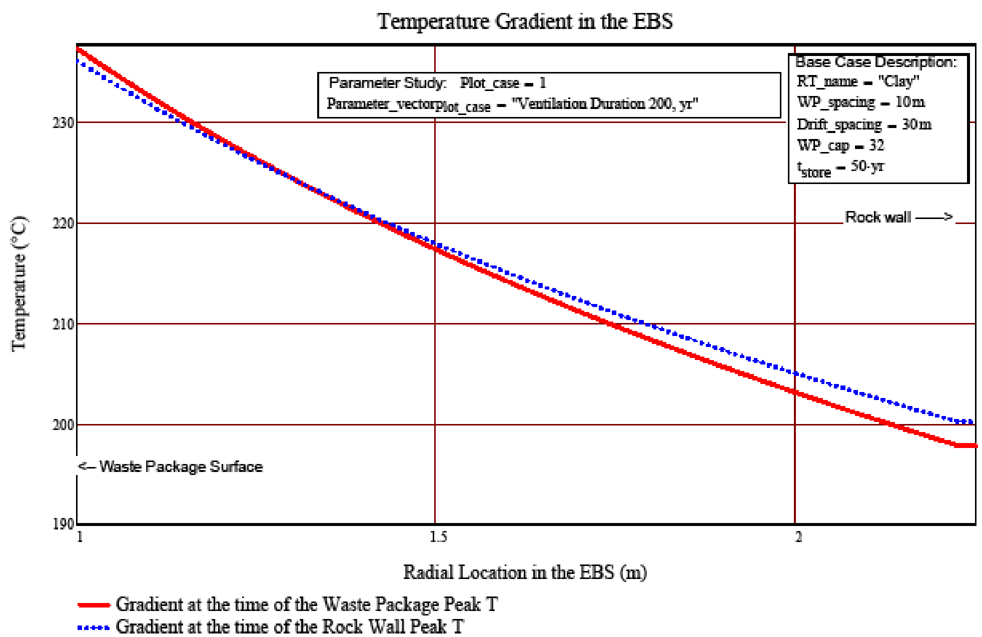
$$Wall\_T\_at\_tt\_rw := \left[(Peak\_values)^{\langle Plot\_case\cdot 2-1\rangle}\right]_2 = 200.185$$

$$WP\_T\_at\_tt\_wp := \left[(Peak\_values)^{\langle Plot\_case\cdot 2-1\rangle}\right]_6 = 237.698$$

$$tt\_wp := \left[(Peak\_values)^{\langle Plot\_case\cdot 2\rangle}\right]_6 = 455$$

$$Wall\_T\_at\_tt\_wp := \left[\left(Temp\_array_{Plot\_case}\right)^{\langle 6\rangle}\right]_{\frac{\left(tt\_wp-\frac{t_{store}}{yr}\right)}{Step}} = 197.802$$

$$WP\_T\_at\_tt\_rw := \left[\left(Temp\_array_{Plot\_case}\right)^{\langle 10\rangle}\right]_{\frac{\left(tt\_rw-\frac{t_{store}}{yr}\right)}{Step}} = 236.227$$



NOTE THAT IN VERSION 3.0 THE GRADIENT WILL BE EXTENDED TO INCLUDE COMPLIANCE POINT 2.

Mathcad Component of DSEF 2.1 Page 19 of 21

Plot temperature results as a function of parameter data

$ip := 1 .. Cases$

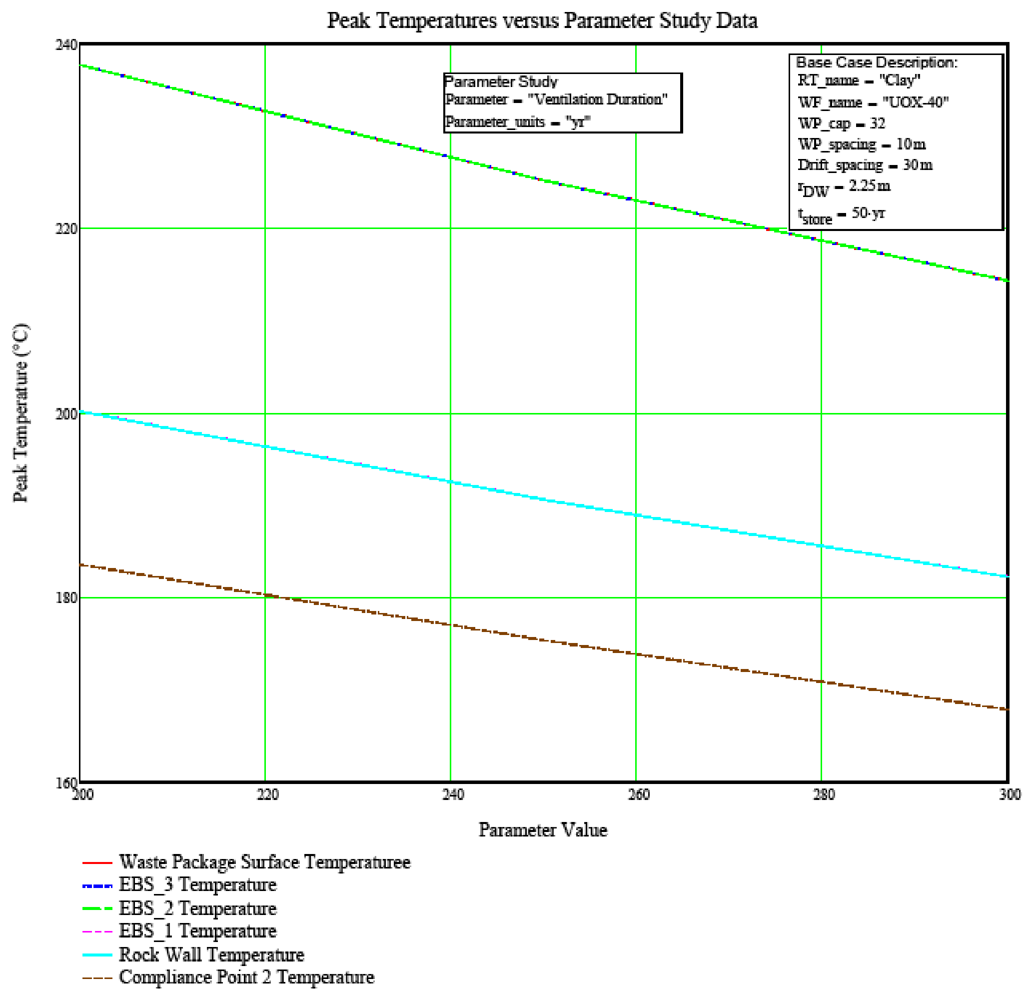
$Peak\_WP\_T_{ip} := \left(Peak\_values^{\langle ip\cdot 2-1\rangle}\right)_6$ $Peak\_EBS3\_T_{ip} := \left(Peak\_values^{\langle ip\cdot 2-1\rangle}\right)_5$ $Peak\_EBS2\_T_{ip} := \left(Peak\_values^{\langle ip\cdot 2-1\rangle}\right)_4$ $Peak\_EBS1\_T_{ip} := \left(Peak\_values^{\langle ip\cdot 2-1\rangle}\right)_3$

$Peak\_WP\_T = \begin{pmatrix} 237.698 \\ 225.192 \\ 214.339 \end{pmatrix}$ $Peak\_EBS3\_T = \begin{pmatrix} 237.698 \\ 225.192 \\ 214.339 \end{pmatrix}$ $Peak\_EBS2\_T = \begin{pmatrix} 237.698 \\ 225.192 \\ 214.339 \end{pmatrix}$ $Peak\_EBS1\_T = \begin{pmatrix} 200.198 \\ 190.63 \\ 182.263 \end{pmatrix}$

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

$Peak\_Wall\_T = \begin{pmatrix} 200.185 \\ 190.618 \\ 182.252 \end{pmatrix}$ $Peak\_CP2\_T = \begin{pmatrix} 183.584 \\ 175.391 \\ 167.864 \end{pmatrix}$ $Parameter\_data = \begin{pmatrix} 200 \\ 250 \\ 300 \end{pmatrix}$ $Parameter\_vector = \begin{pmatrix} \text{"Ventilation Duration 200, yr"} \\ \text{"Ventilation Duration 250, yr"} \\ \text{"Ventilation Duration 300, yr"} \end{pmatrix}$

Mathcad-DSEF Version 2.1 Parametric Sensitivty Model.xmcd



Mathcad Component of DSEF 2.1 Page 21 of 21