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LLNL-TR-484011

Disposal System Evaluation Framework (DSEF) Version 1.0 - Progress Report

M. Sutton, J. A. Blink, M. Fratoni, H. R. Greenberg, W. G. Halsey, T. J. Wolery

May 13, 2011

Disclaimer

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

Used Fuel Disposition Campaign

Generic Engineered Barrier System Evaluation
(Work Package FTLL11UF0330)

Level 4 Milestone (M4): M41UF033001
"FY11 LLNL Input to SNL L2 Milestone:
Evaluation of THMC Processes at EBS Interfaces"

DISPOSAL SYSTEMS EVALUATION FRAMEWORK VERSION 1.0
PROGRESS REPORT

Lawrence Livermore National Laboratory

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JUNE 3RD 2011

LLNL-TR-484011

EXECUTIVE SUMMARY

The Disposal Systems Evaluation Framework (DSEF) is being developed at Lawrence Livermore National Laboratory to formalize the development and documentation of repository conceptual design options for each waste form and environment combination. This report summarizes current status and plans for the remainder of FY11 and for FY12.

This progress report defines the architecture and interface parameters of the DSEF *Excel* workbook, which contains worksheets that link to each other to provide input and document output from external codes such that concise comparisons between fuel cycles, disposal environments, repository designs and engineered barrier system materials can be performed. Collaborations between other Used Fuel Disposition Campaign work packages and US Department of Energy / Nuclear Energy campaigns are clearly identified. File naming and configuration management is recommended to allow automated abstraction of data from multiple DSEF runs.

Waste forms are examined with respect to three fuel cycles: open, modified open and closed. The resulting six waste types from each cycle are identified as examples with dimensions, mass, reactor burnup and 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 pre-emplacement aging times (short, moderate and extended), 24 base case models are proposed. Additionally, evaluation of the DSEF using tuff (Yucca Mountain) and salt (WIPP) will be used as validation test cases.

The DSEF interfaces with more sophisticated models for thermal analysis, and is capable of efficient calculations using simplified conceptual models. The DSEF will document the thermal calculations, but will not duplicate development or calculation results done by other UFD work packages. LLNL (as part of other UFD work packages) is also developing an interface to its sophisticated finite element thermal code that was developed outside of the UFD campaign. Thermal models have been identified and initially tested within the DSEF – analytic and finite element. Finite element modeling employs *TOPAZ3D* (Wemhoff et al, 2007) together with *TrueGrid* (Rainsberger 2006) to generate geometric shapes that represent waste packages. The analytic models use *Mathcad* (*Mathcad* 15.0). This tool will be available to all the UFD participants, including the Generic Disposal System

Environments Performance Assessment development team, which currently does not incorporate a sophisticated thermal model.

In the performance assessment area, the DSEF documents the inputs going to, and the results coming from such GDSE performance assessment models, therefore documenting and integrating results rather than generating results directly. More importantly, DSEF is a knowledge management tool that creates a reference location for PA models to be documented and compared. Material properties to be used in the performance assessment portion of DSEF are identified and follow a *Features, Events and Processes* methodology for determination of relevance. Additionally, the impacts of DSEF on fuel cycle systems are explained. Cost analysis of each disposal environment is initially examined, with the goal of ultimately being able to derive rough estimated costs of repository construction quickly from linked *Thermal*, *Materials Longevity* and *PA* worksheets within the DSEF.

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The authors gratefully acknowledge the technical review, comments and discussion provided by Carlos Jove-Colon (SNL) and Bill Spezialetti (DOE NE-53).

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ACRONYMS

ANL	Argonne National Laboratory
BWR	Boiling Water Reactor
CFC	Closed Fuel Cycle
COEX	Co-Extraction
COTS	Commercially available Off-The-Shelf
CSNF	Commercial Spent Nuclear Fuel
DOE	U.S. Department of Energy
DSEF	Disposal Systems Evaluation Framework
DSNF	DOE Spent Nuclear Fuel
EBS	Engineered Barrier System
EC, Echem	Electro-Chemical
FCT	Fuel Cycle Technology
FEPs	Features, Events and Processes
GDSE	Generic Disposal System Environment
GTCC	Greater Than Class C
GWd	Gigawatt days
GWd/MT	Gigawatt (thermal) - days per Metric Ton
GWe	Gigawatts electric
GWt	Gigawatts thermal
HLW	High-Level nuclear Waste
HM	Heavy Metal
HTGR	High Temperature Gas Reactor
IED	Information Exchange Document
INL	Idaho National Laboratory
LANL	Los Alamos National Laboratory
LLNL	Lawrence Livermore National Laboratory
LLW	Low Level Waste
LTHLW	Lower Than High-Level nuclear Waste
LWR	Light Water Reactor
MWd	Megawatt days
MOC	Modified Open Cycle
MOX	Mixed Oxide fuel
MT	Metric Ton
MTHM	Metric Tons of Heavy Metal
MTIHM	Metric Tons of Initial Heavy Metal
MTU	Metric Tons of Uranium
NBS	Natural Barrier System
NE	DOE-Nuclear Energy
NUEX	New Extraction

PA	Performance Assessment
PNNL	Pacific Northwest National Laboratory
PWR	Pressurized Water Reactor
OC	Open Cycle
SFR	Sodium Fast Reactor
SNL	Sandia National Laboratories
SRNL	Savannah River National Laboratory
SZ	Saturated Zone
TALSPEAK	Trivalent Actinide Lanthanide Separation by Phosphorus-based Aqueous Komplexes [sic.]
TRISO	Tristructural-isotropic (fuel)
TRU	Transuranic
UDS	Undissolved Solids
UFD	Used Fuel Disposition
UNF	Used Nuclear Fuel
UOX	Uranium Oxide Fuel
UREX	Uranium Extraction
UZ	Unsaturated Zone

NOMENCLATURE AND SYMBOLS

α	thermal diffusivity, $m^2/s = k/(\rho \cdot C_p)$
ρ	density, kg/m^3
C_p	specific heat, J/kg°K
τ	dimensionless time (Fourier number) = $(\alpha \cdot t)/L^2$
ξ	dimensionless distance = x/L
k	thermal conductivity, J/m°K
L	characteristic length, m
L_{offset}	offset distance between multiple line sources, m
q(t)	continuous point heat source, W
$q_L(t)$	continuous line heat source, W/m
$q_p(t)$	continuous planar heat source, W/m^2
t	time, s
T	temperature, °C
W_P	width of a finite plane, m

1. INTRODUCTION TO THE DISPOSAL SYSTEMS EVALUATION FRAMEWORK (DSEF)

The Used Fuel Disposition (UFD) Campaign within the Department of Energy's Office of Nuclear Energy (DOE-NE) Fuel Cycle Technology (FCT) program has been tasked with investigating the disposal of the nation's high-level nuclear waste (HLW) for a range of potential waste forms and geologic environments.

For each waste form and geologic environment combination, there are multiple options for a repository conceptual design. The Disposal Systems Evaluation Framework (DSEF) is being developed to formalize the development and documentation of options for each waste form and environment combination.

The DSEF is being implemented in two parts. One part is a *Microsoft Excel* workbook with multiple worksheets. This workbook is designed to be user friendly, such that anyone within the UFD campaign can use it as a guide to develop repository conceptual designs that respect thermal, geometric, and other constraints. The other part is a *Microsoft Access* relational database file that will be centrally maintained to document the ensemble of conceptual designs developed with individual implementations of the *Excel* workbook. At the present time, only the *Excel* portion of DSEF is under development, with the *Access* portion scheduled for development later in FY11 and FY12.

The DSEF *Access* relational database file will collect the key inputs, results, and interface parameters from each *Excel* workbook implementation. The power of a relational database will then be available to sort and organize groups of designs, and to answer queries about what evaluations have been done in the UFD campaign.

The DSEF *Excel* workbook includes worksheets for aspects of the repository design process, including waste form, environment, geometric constraints, engineered barrier system (EBS) design, thermal management, performance assessment (PA), materials longevity, cost, and fuel cycle system impacts. Each of these worksheets or sets of worksheets guides the user through the process of developing internally consistent design options, and documenting the thought process. The worksheets interact with each other to transfer information and identify inconsistencies to the user.

In some cases, the worksheets are stand-alone, and in other cases (such as PA), the worksheets refer the user to another tool, with the user being responsible to transfer summary results into the DSEF worksheet. For example, the DSEF PA worksheet will have

only a minimal 1D analytic transport model, and will rely on the more sophisticated models such as those being developed by the Generic Disposal System Environment (GDSE) work packages in the UDF Campaign. Researchers at Sandia National Laboratories (SNL), Argonne National Laboratory (ANL) and Los Alamos National Laboratory (LANL) are developing Generic Disposal System Environment (GDSE) performance assessment models using the *GoldSim* software package (Goldsim 2009) for salt, clay, and granite repository environments, respectively (Wang and Lee 2010, Chu et al 2011, Freeze and Lee 2011, Wang 2011, Lee et al 2011, Nutt et al 2011). The DSEF documents the inputs going to, and the results coming from such GDSE performance assessment models. LLNL and SNL have licenses for GoldSim and are able to execute the GDSE PA models directly. Other laboratories may request SNL or LLNL to execute the GDSE PA model. It should be noted that the GDSE model interfaces with an input spreadsheet and with a parameter database. The DSEF user will use those same tools for the GDSE calculation. The user will document in the DSEF the pertinent inputs and results from GDSE, as well as configuration management information (GDSE version and GDSE parameter database version) and GDSE files (input spreadsheet, and output files). In the PA area, the DSEF documents and integrates results, rather than generating the results directly.

A second example of DSEF interface with more sophisticated models is thermal analysis. As described in more detail in Section 8, the DSEF (or its auxiliary software) will be capable of efficient calculations using simplified conceptual models. LLNL (as part of the Thermal and EBS work packages) is also developing an interface to its sophisticated finite element thermal code that was developed (and is maintained) by the weapons program. This tool will be available to all the UFD participants, including the GDSE PA development team, which currently does not incorporate a sophisticated thermal model. The DSEF also will document results from the user's home organization thermal codes, should those be used. Again, the DSEF will document the thermal calculations, but will not duplicate development or calculation results done by other UFD work packages.

Finally, the DSEF includes several top-level worksheets, including inputs & results, interface parameters, and knowledge management (i.e. references to reports, models, and publications). These sheets enable the user to see the overall picture on only a few summary worksheets, while developing the design option systematically using the detailed worksheets.

2. EXCEL FILE ARCHITECTURE

The DSEF *Excel* file architecture is designed for two types users. Each realization or instance of the file corresponds to a single repository conceptual design. The developer of the realization (i.e., *the repository designer*) is led through a logical process to develop an internally consistent conceptual design for a given waste form and geologic environment, that respects known geometric and thermal constraints. This requires carefully crafted worksheets for each aspect of the repository design, as well as a substantial body of information taken from the literature and organized to assist the repository designer. The other type of user is someone seeking to understand the design (*the post-design user*). This type of user needs to quickly see the inputs, constraints, design decisions, and results (performance, cost, footprint, etc.). The post-design user needs well-organized high-level information suitable to enable comparison of multiple designs. The post-design user will be able to obtain the information from the top-level worksheets in an *Excel* file documenting a single realization, as well as from the *Access* database that collects the results from multiple realizations. To meet the goals of the two types of users, the DSEF *Excel* file is organized into top-level worksheets and detail worksheets as described in Section 2.1. Because use of the DSEF will occur during its development, well-documented revision control is essential, so that post-design users can determine if comparison of results from different versions of the DSEF are valid, or if early results need to be rerun before the comparison is valid. Revision control is described in Section 2.2.

2.1 ARCHITECTURE

Figure 2.1-1 shows the high level structure of the DSEF. At the top level, there are two elements of the DSEF. The *Excel* workbook is a user-friendly interface for data entry, documentation of repository designer decisions, and the results (performance, cost, etc.). It is designed for use by both the repository designer (and thus contains substantial background material for the designer's use) and by those seeking to understand the design (post-design users). Each design corresponds to a single realization of the *Excel* workbook, and the workbooks will be collected and archived. The *Access* database collects the results from multiple realizations, and is an alternative to examining individual *Excel* files, for post-design users. The functionality of a relational database greatly expands the capabilities of the post-design users, allowing searches for combinations of input parameters or for

combinations of results (e.g., find all designs that had a performance better than a specified standard, or rank all designs by cost).

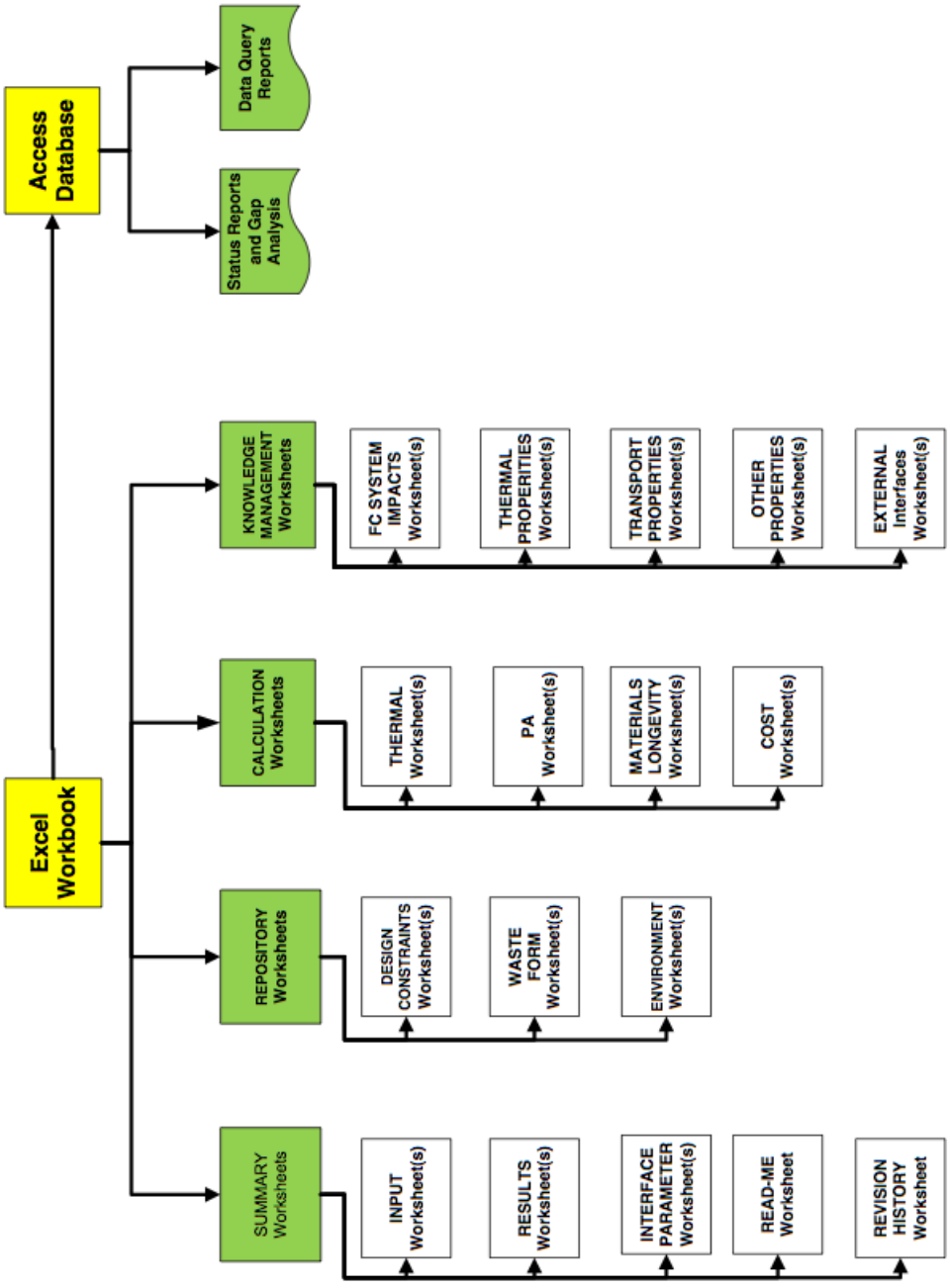

Figure 2.1-1 DSEF architecture schematic diagram

For the *Excel* workbook, the worksheets are grouped into categories. The *Summary* category includes the *Input*, *Results*, and *Interface Parameter* worksheets. The *Input* worksheet guides the user through the input process and prompts the user to go to other worksheets during the design process. The *Results* worksheet documents the results of the design. The *Interface Parameter* worksheet documents all parameters that are passed from worksheet to worksheet, facilitating extraction of pertinent information to the *Access* database, and reducing the potential for hard-wired changes to mask differences between revisions of the DSEF. Finally, the *Read-me* and *Revision History* worksheets document the DSEF itself, and provide an entry point for users.

The *Repository* category of worksheets includes upper-level worksheets that show the D*esign Constraints* (e.g., temperature limits), the *Waste Form* options, and the *Geologic Environments*. As the repository designer progresses through these worksheets, decisions will be made to accept pre-loaded information (e.g., the decay heat curve for a given waste form), or to use alternative information provided by the user. These decisions will be documented on both the individual worksheet and on at least one of the *Summary* category worksheets.

The *Calculation* category of worksheets documents the key aspects of the repository design. The *Thermal* worksheet uses the geometric decisions, along with the waste-form and environment properties, to determine if thermal design constraints are met. The user can iterate this process until an acceptable design is found. The *Results* worksheet will allow the user to capture the results of the failed thermal iterations, as well as the final iteration, to assist subsequent users (both post-design users and users developing alternative designs). The *Thermal* worksheet provides the user a number of options to calculate temperatures. These will include look-up tables of previous calculations, simple analytic models (located in separate files), more complex finite element models (located in separate files), or to documentation of calculations performed with the user's own model.

The *PA* worksheet uses the geometric decisions, the waste form, the environment, and the thermal results to estimate repository performance. The worksheet will include look-up tables of previous calculations, simple analytic models (located in separate files), and pointers to the Generic Disposal System Environment (GDSE) models available for use. The *PA* worksheet will document the PA calculation selected by the user, including inputs to

GDSE models from the DSEF file. Results will also be documented on at least one of the *Summary* worksheets.

The *Materials Longevity* worksheet will document the engineered material chosen for the design, and will evaluate the viability of the selected materials in the repository environment.

The *Cost* worksheet uses unit costs (e.g., cost per unit length of a tunnel of a specified size in a specified geologic medium) taken from more detailed designs in the literature. The DSEF will prompt the user to develop the set of parameters needed to generate subsystem costs (tunnels, waste packages, etc.) for the design. Results will be documented on both the *Cost* worksheet and at least one of the *Summary* worksheets.

The *Knowledge Management* category of worksheets includes properties used by the other worksheets and interfaces of the design with other NE campaigns. The *Thermal Property* and *Transport Property* worksheets provide the property values to be used by the *Calculation* worksheets. Properties vary with environment type (e.g., clay vs. salt) and within an environment type (e.g., boom clay vs. Opalinus clay). Further, the literature often provides a range for a given property, due to material heterogeneity and measurement uncertainty. These worksheets show the user the options (including the ranges), and clearly document the user's choices, both on the *Property* worksheet and at least one of the *Summary* worksheets. The *Property* worksheets (thermal and transport) include the upper level worksheet in which property values are selected, mid-level worksheets that show how the property ranges were developed, and reference-level worksheets that show or hyper-link to the underlying property data.

The *Fuel Cycle System Impacts* worksheet develops parameters to be provided to other NE campaigns, including the *Systems Analysis* and *Systems Engineering* campaigns. Figure 12-1 in Section 12 shows the relationship of the DSEF to the other fuel cycle models in the model pyramid. Finally, the External Interfaces worksheet shows information to be provided to (or taken from) other work packages within the *Used Fuel Disposition* Campaign.

Section 3 shows more detail of the interaction among these worksheets.

2.2 REVISION CONTROL

Because DSEF inputs and outputs will change with each execution of the framework for differing scenarios, it is vital to clearly document revisions within the workbook itself. A *Revision Control* worksheet within the DSEF workbook will summarize (in text form) information on the system (clay, salt, granite etc), the waste form, and key inputs together with the date, time and *DSEF Developer* information. *Repository Design* users will also be required to enter notes documenting their usage of the file (date, time) on the *Input* worksheet, which will automatically be replicated on the *Revision Control* worksheet. This will provide a unique and transparent log of activities performed for each realization. The worksheet will also include a "to-do" list, in which the *Repository Design* user can identify previous realizations that need to be re-run with updated inputs. A "suggested improvement" list will allow any user to document their ideas for future runs.

The filename of the DSEF workbook includes characters that will be used to document revisions. The filename will be modified each time a revision is made such that traceability exists between current and previous workbooks, and such that no worksheets or results are overwritten. The filename will follow the following nomenclature:

DSEF-R#.#m-AA-NN-*yyyymmmdd-Run##*.xlsx

where #.# are the revision numbers, and *m* is the minor revision letter for the DSEF version. For the run itself, AA is the 2-letter code for the users institution, NN is the user's initials, yyyy*mmmdd* is the four digit year, 3 character month, and two digit day of the run, and Run## starts with 01 for the first run of the day by that user. A uniform filename structure will allow automated manipulation and abstraction of data from multiple DSEF workbooks, and logical sequencing of files in the DSEF archive of files.

Similar to the notations used within the NE Project Management system, AA should be replaced with AN for Argonne National Laboratory, IN for Idaho National Laboratory, LA for Los Alamos National Laboratory, LB for Lawrence Berkeley National Laboratory, LL for Lawrence Livermore National Laboratory, OR for Oak Ridge National Laboratory, PN for Pacific Northwest National Laboratory, SN for Sandia National Laboratories, etc. For example, the second model run of the day at LLNL by Harris Greenberg on April 1, 2012, using DSEF version 3.2a, would have file name:

DSEF-R3.2a-LL-HG-2012Apr01-Run02.xlsx

2.3 CONFIGURATION MANAGEMENT

Configuration management (CM) will be documented in a file stored on the LLNL GS Server, in path

"Programs – E/Nuclear Fuel Cycle/DSEF"

The CM file name is

"READ-ME-DSEF Configuration Management-R#.docx"

This file will be periodically updated as configuration management (CM) processes evolve. When that occurs, the CM file updater will increase the R# in the CM file name and move the prior version of the CM Read-me file to the

"Archive CM"

folder in the above path. The file updater will also add a line to the Revision History table (Table 2.3-1).

Table 2.3-1 Revision History

Revision	Updater	Date/time	Description of the Change
0	J. Blink	5/11/11	Initial file

The LLNL UFD-EBS work package manager will appoint a Responsible Individual and an Alternate Configuration Management of DSEF files. At the time of this deliverable report, Harris Greenberg is the Responsible Individual and James Blink is his Alternate.

The repository for DSEF files is the LLNL GS Server, in the above path. This server is regularly backed-up by LLNL-GS-IT staff. In addition, Harris Greenberg will maintain a duplicate set of folders on his PC.

LLNL staff with access to the GS Server can obtain DSEF software from the above path and write modified software files and DSEF realizations to the above path. Only Harris Greenberg or Jim Blink are allowed to delete files from the above path or to move them between folders. Staff (at LLNL or elsewhere) without access to the GS Server can obtain DSEF software from Harris Greenberg or Jim Blink, and can provide realization files to

Harris or Jim Blink for storage in the above path. Once DSEF has matured, a user version may be placed on a UFD-accessible site such as the INL Portal or SNL SharePoint.

The following folders have been established in the above path. The purpose of each folder is listed after the folder name. For grouped files, see the note following the list of folders.

- "Superseded CM READ-ME files" – This folder stores prior versions of this file.
- "Current Software" – This folder stores the latest version of the DSEF *Excel* file (with version number #.#m in file name, which has the format

  DSEF-R#.#*m*-AA-NN-*yyyymmmdd-Run##*.xlsx,

  where the first two fields are numbers and the third is a lower case letter). It also has the latest version of the DSEF *Access* file and the latest versions of auxiliary software files (such as *Mathcad* files)
- "Superseded Software Versions" – This folder stores all prior versions of the DSEF *Excel*, *Access*, and auxiliary (such as *Mathcad*) files
- "DSEF Realizations" – This folder stores completed realizations of the DSEF *Excel* and auxiliary files.
- "Superseded DSEF Realizations" – This folder stores *DSEF Excel* and auxiliary files. The file name will be the original name, with "-superseded" inserted prior to the extension (e.g., prior to ".xlsx" for *Excel* files). In the "Input" worksheet of DSEF *Excel* files, and at or near the top of auxiliary files, the following will be placed: "superseded by file *name*", where *name* is the file name of the superseding file.

A note on file grouping: In some cases, a DSEF realization will include the *Excel* file and one or more auxiliary files. These files will be placed in a subfolder in "DSEF Realizations" or "Superseded DSEF Realizations". The subfolder will be named as if it were a standalone DSEF *Excel* file (with no extension), i.e.,

DSEF-R#.#*m*-AA-NN-*yyyymmmdd-Run##*

The determination of when a series of minor revisions (the "m" in "#.#m") is complete will be made by Harris Greenberg or Jim Blink. At that time, the final file will be archived in "Superseded Software Versions". The same file will remain as the current file in "Current

Software, with the second "#" being incremented, and the lower case letter changed to "a". Similarly, when a series of revisions is complete and the next major release is due, the final file will be archived, and the current file (same content as the file being archived) will be named with the first # incremented and the second # and letter being "0a". Thus, the first release of DSEF will have name "DSEF-R0.0a.xls", and all realizations using that release will have names beginning with "DSEF-R0.0a".

3. INPUTS AND RESULTS

Figure 3-1 shows the flow of information through the DSEF *Excel* file. The remainder of this section discusses that information flow.

The *Inputs* worksheet is the starting point for the DSEF user (the repository concept developer). Upon entry to the worksheet, the user is asked to save the DSEF file with a name that meets the requirements of Section 2.3 (those requirements are repeated in the worksheet. Then, the user is asked to describe the repository concept being documented by this DSEF file. That description cell and the filename will be propagated to all the worksheets, so that printouts will be easily identifiable.

The *Inputs* worksheet then leads the user through a set of decision steps designed to elicit as much information as possible about the repository design being developed. The first step is to determine the geologic environment, the waste form, and the design and thermal constraints to be applied. This is done with a succession of list boxes. The choices made in early boxes tailor later boxes. For example, if the user selects a clay environment, there will be a subsequent list of types of clay (e.g. boom clay) to assist the user in selecting properties to be used in thermal and other analyses.

As the user further defines the repository design, opportunities are presented that allow choices among pre-loaded options. For example, if the user has selected boom clay, available thermal property values will be presented, including available minimum, maximum, and representative values from one or more references. In addition to having the option to select one of these numbers, the user is presented with the option to use their own number. The DSEF will clearly document, in the *Results* worksheet, the actual numbers used, as well descriptions of each number (e.g., *number provided by user with comment "___"*, or *representative value from reference "author, date"*). After the *Inputs* worksheet has led the user through the choices available in the *Environments*, *Waste Forms*, and *Design Constraints* worksheets (supported by the *Thermal Properties* and *Transport Properties* worksheets, it will send the user to the *Thermal* worksheet, where the user will use internal DSEF tools or auxiliary software to develop temperature histories. The *Thermal* worksheet also leads the user to compare the temperatures to the design constraints and decide if the design (aging time, number of assemblies or canisters per waste package, waste package emplacement geometry, waste package spacing in boreholes/alcoves/drifts, and borehole/alcove/drift spacing) meets the constraints. If it does not, the user is prompted to

enter the pertinent information in a table documenting iterations (which will be mirrored in the *Results* worksheet) and to modify the design parameters and run another iteration. When the user is satisfied that the constraints are met, the user is prompted to return to the *Inputs* worksheet.

The *Inputs* worksheet, after some clarification actions, sends the user to the *Materials Longevity* worksheet, which will address coupled processes and EBS materials performance. Again, iteration is permitted, including iteration back to the *Inputs* and *Thermal* worksheets.

When the *Materials Longevity* worksheet actions are complete, the user is sent to the Inputs worksheet and then on to the *PA* worksheet. The *PA* worksheet will function similarly to the *Thermal* worksheet, offering the user the opportunity to interpolate from prior results, to use a simple analytic transport model in auxiliary software, or to use the GDSE software being developed in other UFD work packages. Again, iteration is permitted, including iteration back to the *Inputs*, *Thermal*, and *Materials Longevity* worksheets.

When the *PA* worksheet actions are complete, the user is sent to the *Inputs* worksheet and then on to the *Cost* worksheet. A similar iterative process is followed there, and the user ends up back at the *Inputs* worksheet to finalize the DSEF realization. At this point, the *Results* worksheet has automatically pulled results in from the four *Calculation* worksheets (*Thermal*, *Materials Longevity*, *PA*, and *Cost*), and the *Interface Parameters* worksheet has recorded all information passed between among those four *Calculation* worksheets. As part of the finalization actions, the *Inputs* and *Results* worksheets provide information to the *FC Systems Impacts* and *External Interfaces* worksheets, where it will be recorded in the format requested by the external organizations.

The DSEF *Access* Database will draw information directly from the *Inputs* and *Results* worksheets, and if appropriate, from the *Interface Parameters* worksheet.

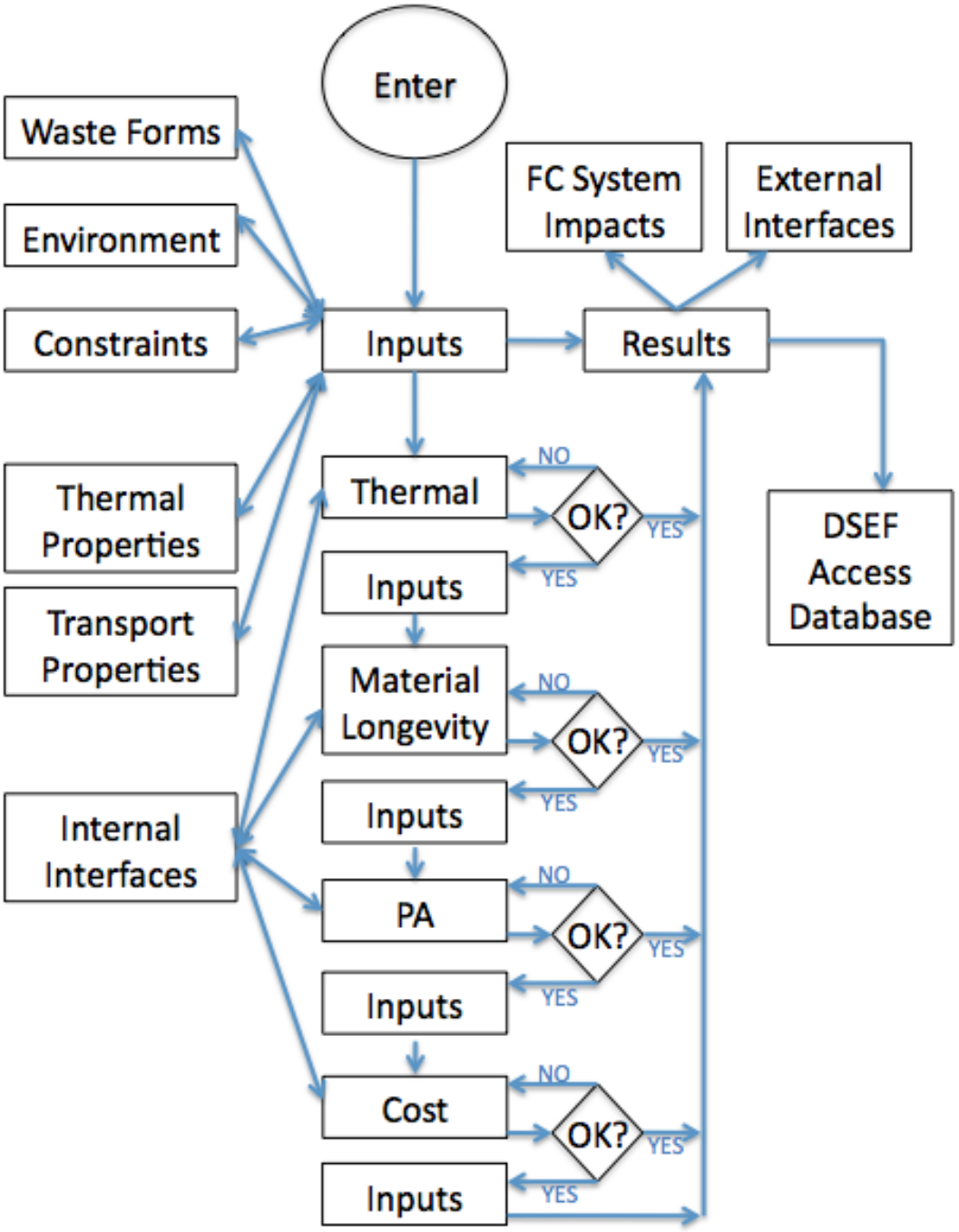

Figure 3-1 Information flow through DSEF Excel workbook

4. INTERFACE PARAMETERS

As described in Section 2.1, the *Interface Parameter* worksheet documents all parameters that are passed from worksheet to worksheet (other than the *Inputs* and *Results* worksheets), facilitating extraction of pertinent information to the *Access* database, and reducing the potential for hard-wired changes to mask differences between revisions of the DSEF.

Interfaces between worksheets within DSEF are considered internal interfaces, and interfaces to other UFD work packages and to other DOE-NE campaigns are considered external interfaces.

4.1 INTERNAL INTERFACES

Calculation worksheets will require interface with information from a number of other worksheets. To ensure that these interfaces are easily understood and documented, the information passing between worksheets (other than the *Input* and *Results* worksheets) will pass through the *Interface Parameters* worksheet. For example, a thermal property could pass to the *Input* and *Interface Parameters* worksheets and then be read by the *Thermal* worksheet.

Figure 4.1-1 is an Input-Process-Output diagram that provides an example of how the DSEF worksheets and external programs interface and work together to evaluated repository alternatives.

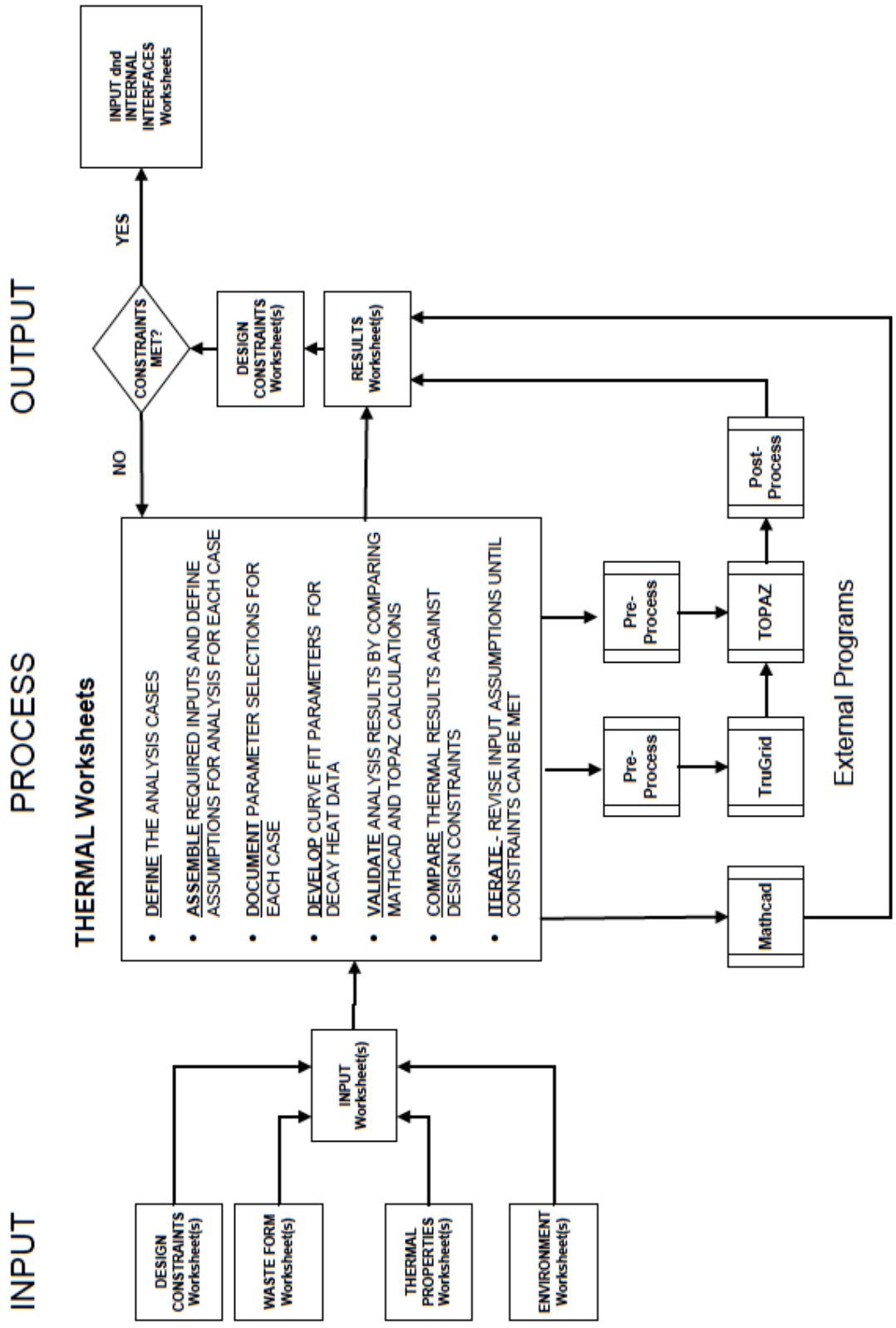

Figure 4.1-1 Interface Parameters – thermal worksheet input-process-output example

On the left hand side of the figure several working-level worksheets feed information into the Inputs worksheet as follows:

Design Constraints:

- Repository Layout / Geometry
- Engineered Barrier Configuration / Materials
- Repository Environment Description
- Constraints – Thermal, Mechanical, Chemical, etc.

Waste Form:

- General Physical Description
- Radionuclide Inventory
- Decay Heat Data
- Canister Volume and Dimensions

Thermal Properties:

- Host Rock Properties
- Engineered Barrier Material Properties
- Mean values, Ranges / Distributions
- QA Status / Confidence in Data
- Limitations / Assumptions

Environment

- Host Rock Type
- Geologic Stratigraphy Assumed
- Porosity / Saturation Assumed
- Expected Chemical Environment

The central area of the figure shows the process steps addressed in the *Thermal* worksheet, and shows the external programs and interfaces where data are passed to *Mathcad* (Mathcad 15.0) and *TOPAZ3D* (Wemhoff et al, 2007), as described further in Section 8 of this report.

Mathcad has an *Excel* component that can read and write directly to the DSEF worksheets. However, pre-processing and post-processing interface programs are currently being developed to allow the DSEF user to set up and run *TOPAZ3D* (and its gridding pre-processor, *TrueGrid*) directly from the DSEF worksheets.

The *Thermal* worksheet will pass the following kinds of information to these external programs:

To *Mathcad*:

- Decay Heat
- Material Properties
- Other Problem Definition Data

To the *TrueGrid* grid generation tool (and its simplified interface being developed as part of DSEF):

- Geometry
- Mesh Spacing
- Material Zone Boundaries
- Boundary Conditions

To *TOPAZ3D* finite element code (and its simplified interface being developed as part of DSEF):

- Decay Heat
- Material Properties
- Other Problem Definition Data

The right-hand side of the figure shows the data passed from the external thermal analysis programs and the *Thermal* worksheet to the *Results* worksheet, and the operation of checking the results against the *Constraints*. If the results do not meet the constraints, then the design user modifies the input and performs additional iterations until the constraints are met. Once the constraints have been met, the successful combination of inputs and results are returned to the *Input* worksheet and passed to the *Interface Parameters* worksheet.

Data passed from the *Thermal* worksheet to *Results*:

- Definition of Cases Evaluated
- Waste Form and Canister Parameters
- Surface Storage Time
- Geologic Environment
- Repository Design Parameters

Data passed from the external analysis programs to *Results*:

- Peak and Transient Temperature Results for Each Analysis Case for
- Waste Form
- Canister Surface
- EBS Components
- Host Rock

4.2 External Interfaces

As described in Section 4.1, the *Interface Parameter* worksheets in DSEF will document information passing from one element of the DSEF to another element. This is similar function to that provided by the Information Exchange Documents (IED) on the Yucca Mountain Project, which tracked information passed between elements of the repository design and between the design and the performance assessment. The *Interface Parameter* worksheet provides a standard, common location to exchange information between the DSEF elements. Similarly, external interface worksheets are included to exchange information with other Work Packages in the Used Fuel Disposition Campaign and between the UFD Campaign and other DOE-NE Campaigns (Figure 4.2-1). The DSEF worksheets that will be specifically tailored for other organizations are the *FC System Impacts* worksheet (tailored for the Systems Analysis Campaign) and the *External Interfaces* worksheet.

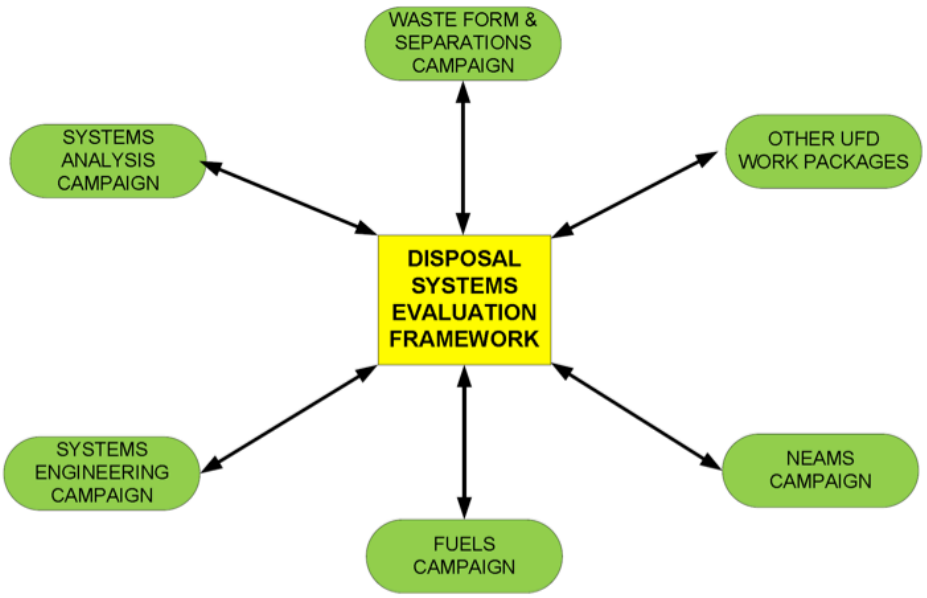

Figure 4.2-1 Schematic showing DSEF interfaces with other UFD campaigns

5. WASTE FORMS

The DSEF began with a catalog (developed by the larger UFD Campaign team for Features, Events and Processes (FEPs) development and by other DOE-NE Campaigns) of potential waste forms (Freeze et al 2010). These include the generic waste forms summarized in Table 5-1. More specific information on the radionuclide inventory within each of the waste form types can be found in (Carter and Luptak 2010).

The DSEF is integrated with the FEPs development and also with work in the thermal design work packages. The latter effort is integrated with the waste form work packages and has developed three base case fuel cycles with specific waste forms (Carter, et al., 2011), summarized in Table 5.1 and Table 5.2. Each fuel cycle consisting of light water reactors (LWRs), specifically pressurized water reactors (PWRs). The 3 fuel cycle options are shown in Figures 5-1, 5-2 and 5-3.

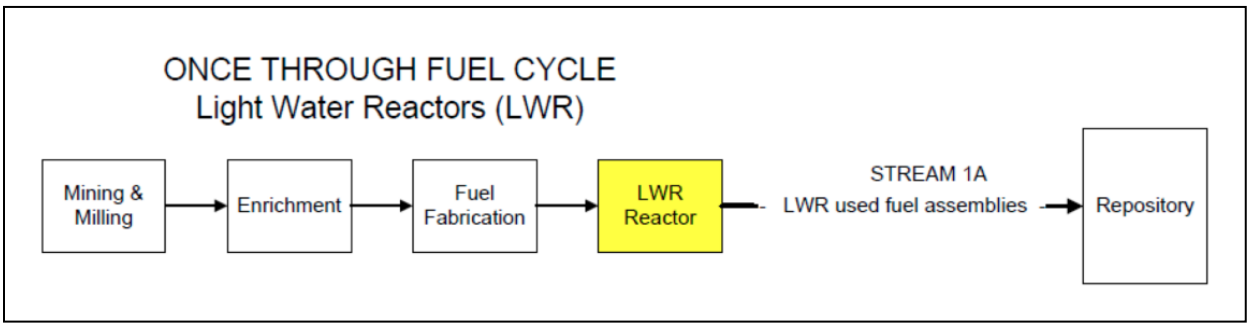

Figure 5-1 Once Through Fuel Cycle Waste Stream

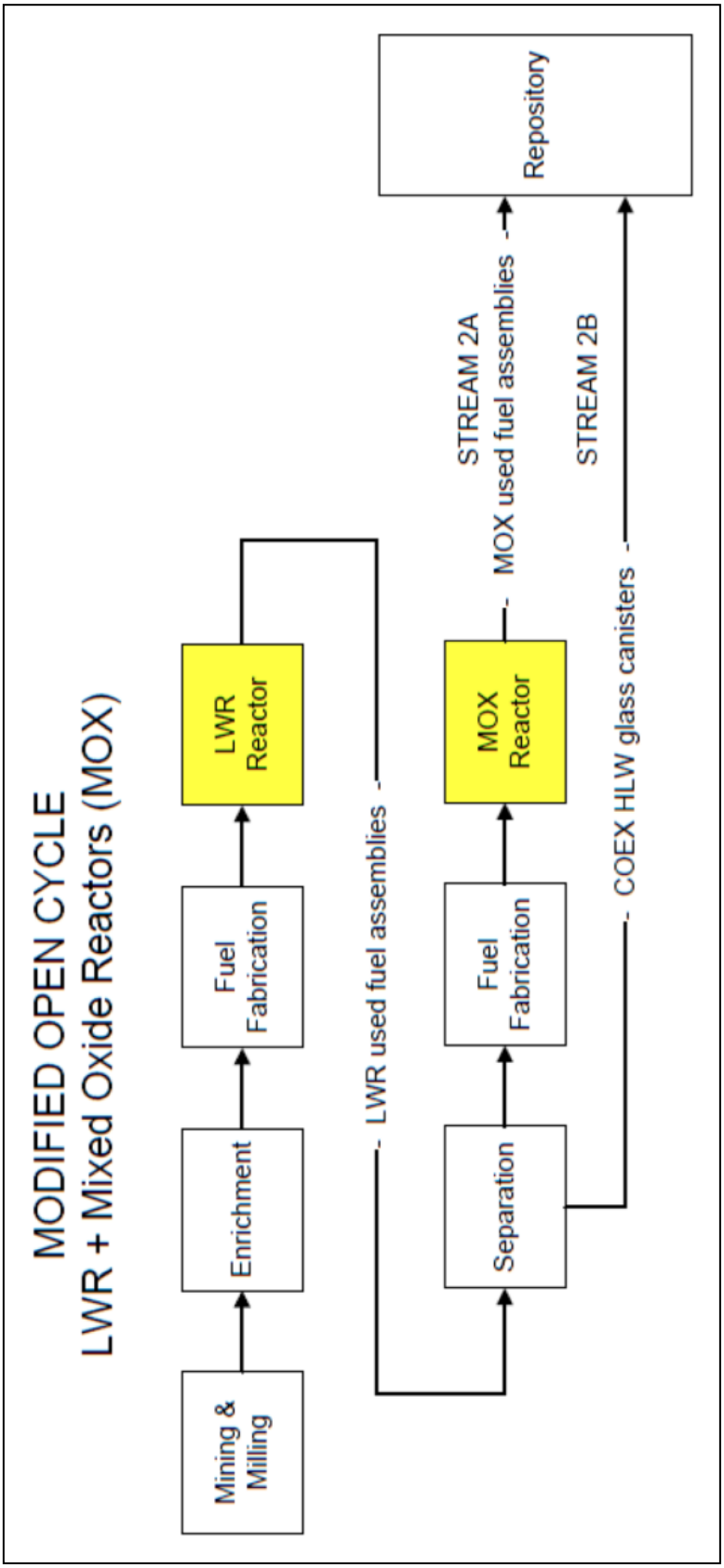

Figure 5-2 Modified Open Cycle Waste Streams

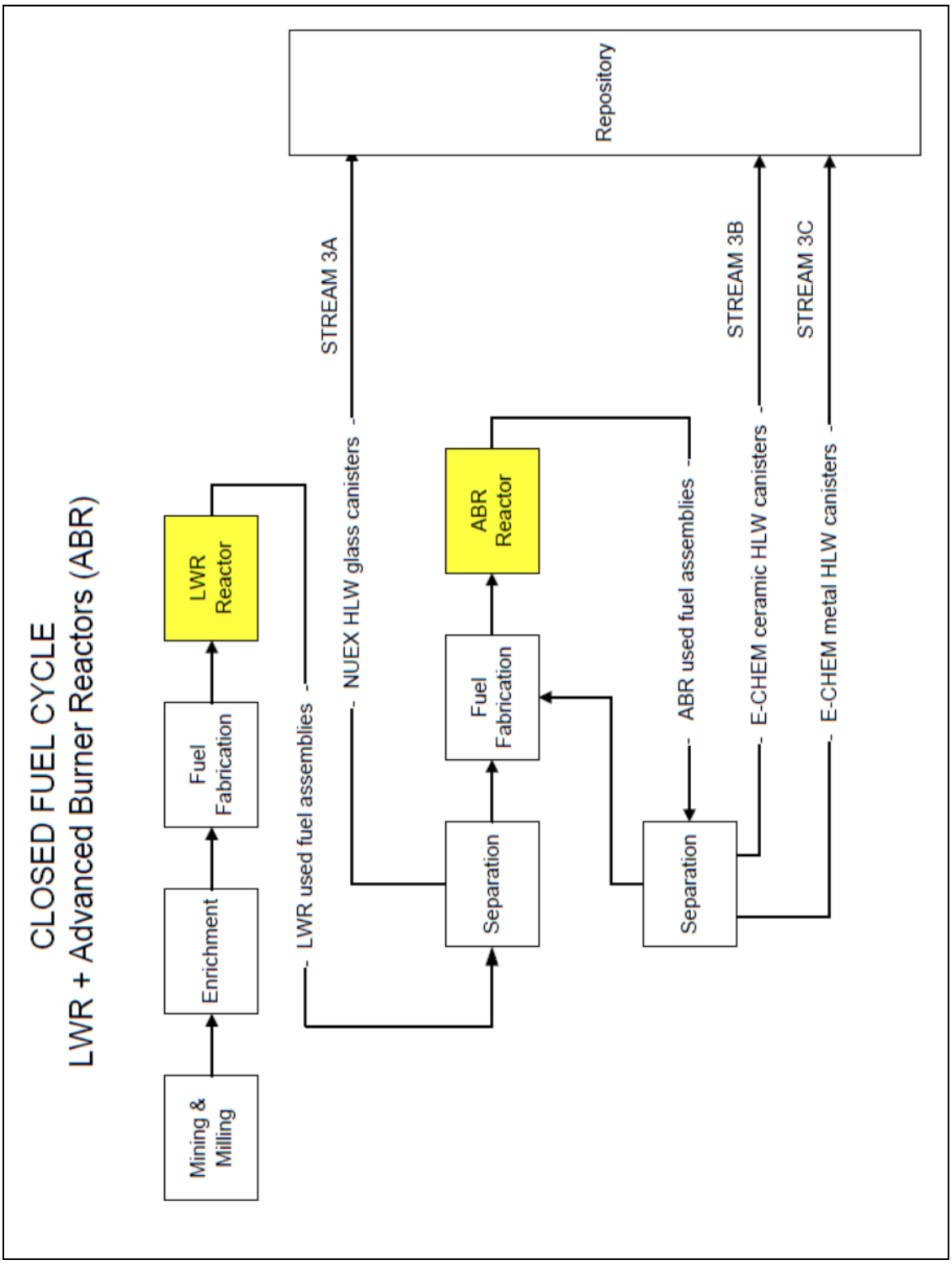

Figure 5-3 Closed Fuel Cycle Waste Streams

An open fuel cycle consists of light water reactors (LWRs), specifically pressurized water reactors (PWRs), with all waste going to storage and disposal.

In the modified open cycle (MOC), the LWR used fuel is reprocessed with Co-Extraction (COEX) aqueous processing similar to the current generation of deployed technology (e.g., the Rokkasaho Reprocessing Facility). In COEX, uranium and plutonium are recovered together (no pure plutonium separation), producing 108.9 kg of mixed oxide fuel (MOX) for each metric ton (MT) of LWR fuel, based on an average plutonium enrichment of 10.74%. The principal fission product waste including the minor actinides are combined with the undissolved solids (UDS) and recovered technetium into a single COEX borosilicate glass waste form. The total burnup of the cycle, per MT of original LWR fuel, is $BU_{UOX} + BU_{MOX} * (MT_{MOX}/MT_{LWR}) = 56.4$ GWt-days/MT_{UOX}. The remaining waste stream from the MOC does not produce a significant amount of heat. Nevertheless, physical accommodation of that waste stream will be addressed in the DSEF, based on the information in Carter, et al. (2011), and repository concept development will consider co-disposal of that waste in the repository footprint.

For a closed fuel cycle (CFC), all used fuel is reprocessed with New-Extraction (NUEX) aqueous processing that recovers all transuranic (TRU) elements for reuse. According to Carter, et al. (2011), NUEX will include Transuranic Extraction (TRUEX) and the Trivalent Actinide Lanthanide Separation by Phosphorus-based Aqueous Komplexes [sic.] (TALSPEAK) process for complete TRU recovery. The principal fission product wastes are combined with the UDS and separated technetium into a single NUEX borosilicate glass waste form. In this base-case closed fuel cycle, the recovered transuranic elements from the LWR used fuel (0.6142 MT per MT of LWR fuel) will fuel Advanced Burner Reactors (ABRs) that are sodium cooled, produce 1 GW_t, use U-TRU-Zr metal alloy fuel, have a TRU conversion ratio of 0.75. The used fuel from the ABRs is reprocessed using an electro-chemical (EC) process that is a dry process using conductive molten salt baths to recover all TRU elements. In this process, the fission products are split between three waste streams. Elements more noble than uranium (e.g., cladding and noble metal fission products) remain as metals and are incorporated into a metal alloy waste form. Elements less noble than uranium are converted to chloride salts. The lanthanide elements are recovered from the salt by electrolysis and converted to a lanthanide glass. Excess salt is purged, and the chloride is absorbed by zeolite and bonded with glass to make the final waste form (termed

EC-Ceramic in the DSEF). After a short period, the heat from the EC lanthanide glass is negligible, and thus only the NUEX glass, the EC-metal, and the EC-Ceramic waste forms are considered in the thermal aspects of the DSEF. The remaining waste streams from the NUEX reprocessing and the EC reprocessing do not produce a significant amount of heat. Nevertheless, that waste stream will be quantified in the DSEF, based on the information in Carter, et al. (2011), and repository concept development will consider co-disposal of that waste in the repository footprint.

Table 5-1 Base case waste forms for once-through, modified open and closed fuel cycles.

Cycle	**WF type**	**Canisters per GW_e-yr cycle**	**Width diameter, m**	**Length, m**	**Mass, kg**	**Burnup GW_{td}/MT**
OC	SNFA	39.2	0.22	4.07	470	60
MOC	COEX (UOX)	3.7	0.6096	4.572	2,900	51
	SNFA (MOX)	4.5	0.22	4.07	470	50
	Total	8.2	NA	NA	NA	56.4
CFC	NUEX	0.97	0.6096	4.572	2,900	51
	EC-Ceramic	4.9	0.6096	4.572	2,900	99.6
	EC-Metal	6.6	0.6096	3.048	3,600	
	Total	12.47	NA	NA	NA	112.2

The three fuel cycles described above produce the following waste forms that are considered in the thermal aspects of the DSEF.

The thermal decay curves from the six heat-producing waste forms (1 from the Open Cycle, 2 from the MOC, and 3 from the CFC) are shown in Figure 5-4. It is important to note that these curves are based on the time after the fuel is removed from the neutron flux in the reactor that produced it, rather than the time after reprocessing.

There are other modified open and closed fuel cycles that are similar to those above. The DSEF developers treat the above base cases as representative of those many possibilities, but will follow the progress in the DOE-NE Separations and Waste Forms Campaign and add options accordingly. In addition, there are more "exotic" waste forms that have historically been proposed. Many of these waste forms require spent nuclear fuel to be reprocessed and separated prior to encapsulating in a waste form. Examples include glass encapsulated silver zeolite, functionalized silica aerogels, chalcogenide aerogels, silicon carbide, iron

phosphate glass, glass ceramics, cermets, epsilon metals and bentonite clay with copper. Some of these will be added to future DSEF versions.

The DSEF assembles summary information about waste form and waste package combinations. Waste form parameters include heat/volume ratio, heat/mass ratio, and heat/electrical-energy (from which the waste was derived) ratio, as well as the mass and half lives of the radionuclides in the waste. This information will interface with the FCT Systems Engineering Campaign fuel cycle catalog, the FCT Systems Analysis Campaign "VISION" model of nuclear fuel cycles and material flows, and the Separations and Waste Forms Campaign waste stream and waste form descriptions, as well as with the Waste Form, EBS, Natural Systems and FEPS work packages in the UFD Campaign.

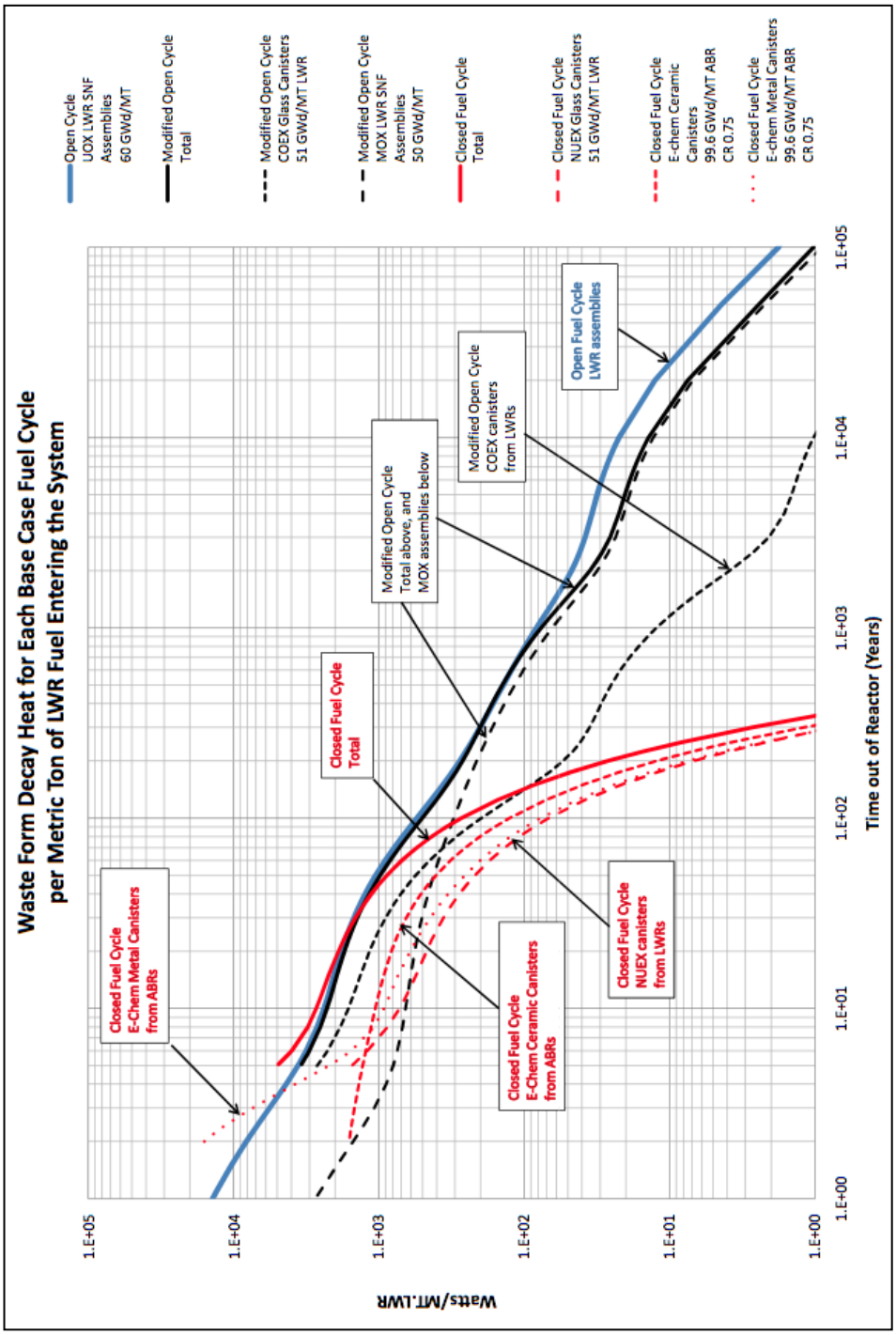

Figure 5-4 Thermal decay curves from the six heat-producing waste forms (OC, MOC, CFC)

Table 5-2 FEPs-identified waste forms

Category	Sub-category
Used Nuclear Fuel (UNF)	Commercial Spent Nuclear Fuel (CSNF) with nominal burnup: Uranium (U) & mixed oxide (MOX) from Light Water Reactors (LWRs)
	CSNF with high burnup: U & MOX, >50% burnup without reprocessing, such as in some fusion-fission hybrids
	High Temperature Gas Reactor (HTGR) fuel using TRISO/graphite elements: Large volume, low volumetric heat, and higher burnup than LWRs
	DOE Spent Nuclear Fuel (DSNF): U metal from N-reactor, and carbides & oxides
High-Level Waste (HLW) Glass	Current borosilicate glass: Includes processing chemicals from original separations, with U/Pu removed, but minor actinides and Cs/Sr remaining
	Potential borosilicate glass: No minor actinides and/or no Cs-137/Sr-90. Mo may be removed to increase glass loading of radionuclides. This waste form has a lower volumetric heat rate
HLW Glass Ceramic / Ceramic	Glass-bonded sodalite from Echem processing of EBR-11, and from potential future Echem processing of oxide fuels
	An advanced waste form that includes iodine volatilized during chopping, which is then gettered during head-end processing of used fuels
HLW Metal Alloy	Metal alloy from Echem: Includes cladding as well as noble metals that did not dissolve in the Echem dissolution
	Metal alloy from aqueous reprocessing: Includes undissolved solids (UDS) and transition metal fission products
Lower Than HLW (LTHLW)	Includes Classes A, B, and C, as well as Greater Than Class C (GTCC)
Other	Molten salt, electro-chemical refining waste, new waste forms, and radionuclides removed from other waste forms (e.g. Cs/Sr, I-129, C-14, H-3 and Kr-85)

6. DISPOSAL SYSTEM ENVIRONMENTS

Seven specific disposal environments have been identified (in the FEPs work packages) for further investigation (Freeze et al 2010), in addition to other possible environments such as deep seabed, and carbonate rocks. These environments are summarized in Table 6.1. Historical perspectives on each of the disposal systems can be found in (Sutton et al 2011). The first two of these (Surface Storage and Shallow Disposal) are being studied by the Storage and Transportation work packages in the UFD Campaign, and will be integrated into a future version of the DSEF. The third environment in Table 6.1 (Unsaturated Hard Rock) has been studied extensively for the Yucca Mountain Site. The results of those studies will be used to validate the architecture and algorithms for the DSEF, during its development. The thermal design work packages have identified the next four environments in Table 6.1 for development of base cases for UFD. These are salt, clay, saturated hard rock, and deep boreholes.

Table 6-1 FEPs-identified disposal system environments

Category	**Description**
Surface Storage	Long-term interim storage at reactors or at centralized sites
Shallow Disposal	Depths ≤ 100 m (e.g., near-surface disposal, LTHLW sites)
Mined Geologic Disposal (Hard Rock, Unsaturated)	Unsaturated Zone (UZ): Granite/crystalline or tuff (Depths > 100 m)
Mined Geologic Disposal (Hard Rock, Saturated)	Saturated Zone (SZ): Granite/crystalline or tuff (Depths > 100 m)
Mined Geologic Disposal (Clay/Shale, Saturated)	SZ: Clay/shale (Depths > 100 m)
Mined Geologic Disposal (Salt, Saturated)	SZ: Bedded or domal salt (Depths > 100 m)
Deep Borehole Disposal	Granite/crystalline (Depths ~ 1000 m or deeper)
Other	Examples include deep seabed, and carbonates

Thermal design constraints for each of the disposal environments are discussed in section 7 of this report, and material property requirements are discussed in section 9.

7. DESIGN CONSTRAINTS

The three base-case fuel cycles described in Section 5 produce six total waste forms with sufficient heat output to significantly influence the repository design. The four base-case environments described in Section 6 result in 24 combinations of waste forms and environment. The thermal design for a repository is based on thermal power, which declines with aging time; hence, a range of aging times needs to be considered for each of these cases. Initially, the thermal design work packages planned to investigate three aging periods for each combination. A minimal aging period (5 yr), a medium aging period (50 yr), and a long aging period (100 yr) were initially selected for investigation. This would result in 72 combinations of waste form composition, environment, and aging time. The thermal design investigators (from SNL, ORNL, SRNL, and LLNL) decided that an adequate range of designs would result if some combinations were eliminated (i.e., minimal aging for very high initial power waste forms, and long aging periods for very low initial power waste forms). The result is shown in Table 7-1, which shows 24 combinations of waste form composition, environment, and aging time. These, in addition to the validation cases of YMP and WIPP, will be the base cases for the DSEF. The 24 fuel cycle cases and the 2 validation cases will be prioritized rather than being developed and executed in parallel.

Table 7-1 Fuel cycle, disposal environment, and aging time for 24 base case combinations

Fuel Cycle	**Hard Rock, Saturated**	**Clay/Shale, Saturated**	**Salt, Saturated**	**Borehole**
Once Through (SNFA)	Moderate Aging Extended Aging	Moderate Aging Extended Aging	Moderate Aging Extended Aging	Moderate Aging Extended Aging
Modified Open Cycle (COEX from UOX and MOX SNFAs)	Short Aging Moderate Aging	Short Aging Moderate Aging	Short Aging Moderate Aging	Short Aging Moderate Aging
Closed Fuel Cycle (NUEX from UOX, and EC-Ceramic and EC-Metal from ABRs)	Short Aging Moderate Aging	Short Aging Moderate Aging	Short Aging Moderate Aging	Short Aging Moderate Aging

With a number of repository designs and environments being evaluated in countries across the world, data on proposed thermal constraints are available for many of the environments listed in Table 7-1.

For a repository in granite various limits have been proposed. The French designs have thermal limits of <100°C at the canister surface, to minimize the vaporization/condensation processes that could cause corrosive salts to deposit on the surface of the copper waste package. Packages are separated by 12-15 m and have a maximum heat output of 1.6 kW/can UOX and 1.1 kW/can MOX (ANDRA 2005b). In Finland, the maximum heat output in granite is limited to 1.7 kW/can (Posiva Oy 2010). Swedish repository designs at Forsmark and Laxemar in granite assume an initial thermal output of 1.7 kW/can and use a waste package separation of 7.4 m to limit the temperature on the surface of a waste package to <100°C. Additionally the buffer temperature should not exceed 100°C to minimize dehydration and chemical alteration (SKB 2006).

For clay repositories in France and Belgium, the maximum temperature is generally limited to less than 100°C based on mineral stability. Temperatures close to or above 100°C tend to dry out the clay and cause deformation cracks and subsequently fast pathways for potential radionuclide release to the biosphere. Thermal constraints in France are <100°C in argillite, with canisters spaced at 7.5 m parallel and 10.3 m perpendicular, and maximum heat outputs of 1.6 kW/can UOX and 1100 W/can MOX (ANDRA 2005a). In Belgium, canisters are spaced 3 m apart, and temperatures of HLW and SNF are limited to <400°C and <350°C respectively, with 188 W/can UOX and 905 W/can MOX (NIROND 2001). These values were chosen because HLW glass undergoes structural and mechanical changes at 500°C and to prevent excessive pressure buildup via He in fuel (NIROND 2001). In Switzerland thermal constraints are limited to 125°C in emplaced bentonite with canisters spaced 3 m apart with a maximum heat output of 1.5 kW/can (NAGRA 2002).

For engineered backfill, Swiss studies have demonstrated the dehydration and illitization of bentonite buffer EBS material above 120-150°C in wet conditions, although dry conditions require higher temperatures (perhaps up to 350°C (P. Wersin, L.H. Johnson and I.G. McKinley, Performance of the bentonite barrier at temperatures beyond 100°C: A critical review, Physics and Chemistry of the Earth, Parts A/B/C, Volume 32, Issues 8-14, 2007, Pages 780-788). In Belgium, temperature constraints are limited to <100°C in the backfill to prevent physico-chemical alteration of the backfill and any significant disturbance of the local hydraulic system from buildup of interstitial pressures (NIROND 2001).

Studies of a conceptual salt repository in the US led to a waste package spacing of 7.5 m. The maximum glass temperature, cladding temperature and salt temperature were 500°C,

375°C and 250°C respectively, and the maximum heat output was 6.6 t kW/can containing 12 PWR assemblies (BMI 1985, DOE 1987). A more recent study found that maintaining waste package temperatures below 500°C and salt bed below 200°C would reduce the disposal concept's uncertainty (AFCI 2009). Salt tends to decrepitate above 200°C and melts above 800°C. Intact salt creep is exponentially related to temperature and creep occurs without forming fractures with salt deformation being dominated by plastic behavior at elevated temperatures (Hansen and Leigh 2011).

Thermal constraints also exist for waste package material. Long-range order transformations in Alloy C22 are not expected at 200°C over very long timescales (Turchi et al 2007). Low temperature sensitization of some stainless steels occurs over long time periods above 400°C (Sutton et al 2010, Farmer 1988). Copper alloys have been shown to remain stable up to at least 300°C (Sutton et al. 2010, Farmer 1988).

8. THERMAL

There are two thermal model systems within the DSEF: analytic and finite element. There will also be tables of prior results (which will be updated in later versions based on realizations using the early versions); these tables can be used to interpolate results for new cases, if most of the input parameters are suitably similar.

As described in the subsections of Section 8.1, the analytic models in the DSEF will use a variety of source and environment geometries that have existing published analytic solutions. Source geometries (all in an infinite medium) include a point heat source, a finite line source, an infinite line source, an array of finite line sources, a finite plane source, a semi-infinite plane source, an infinite plane source, and an infinite cylinder source. These solutions can be extended (by superposition of reflected geometries) to a semi-infinite medium bounded by an isothermal surface and an infinite region bounded by two parallel isothermal surfaces. The analytic models can be executed in commercially available off-the-shelf (COTS) software such as *Microsoft Excel*, *Mathcad* (Mathcad 15.0 2010) or *Mathematica* (WRI 2010). These models use textbook empirical equations to solve heat flow in a variety of geometries and offer a simple and quick examination of a unit cell. For the DSEF, *Mathcad* models will be included as auxiliary software. These models can be run at the appropriate point in the development of the repository design, and documented in the *Thermal* worksheet of the DSEF.

The finite element models (Section 8.2) within DSEF evaluate heat flow within a more complex geometry using specifically designed thermal transport software such as *TOPAZ3D* and an input mesh that more accurately describes the waste package and unit cell (or repository region). These models are more complex than analytic models and require more effort to perform. During the remainder of FY11, the application of TOPAZ3D to address complexities not addressed by the analytic models will be tested.

Section 8.3 is a report of the initial comparison of analytic and finite element models. Section 8.4 concludes the thermal section with a description of the decay heat formulation to be input to these models.

8.1 ANALYTIC MODELS

There are a number of analytical solutions that are potentially applicable as a basis for the planned UFD thermal design analyses. There are several basic references that document the analytical solutions for a wide class of conduction heat transfer problems, but the most widely cited is Carslaw and Jaeger (1959, Section 8.1.3).

Analytic solutions that were developed in *Mathcad*, and used on the Yucca Mountain Project have been used to some extent in developing the suite of analytical solutions documented below (Chipman et al. 2004).

The finite line and plane source solutions are derived from the transient solution for a continuous point source (q(t)) in an infinite homogeneous media (Carslaw and Jaeger 1959, Section 10.4, p261). In the following sections, the radial distance from the point source is r, and the initial temperature is zero.

8.1.1 SOLUTION FOR A POINT SOURCE IN AN INFINITE MEDIUM

This solution is based on linear superposition in a conduction only heat transfer environment (Duhamel's theorem, Carslaw and Jaeger 1959, Section 1.14). The following equation is a convolution integral of a transient heat source q(t).

$$T_{point}(t,r) = \frac{1}{8\cdot\rho\cdot Cp\cdot(\pi\cdot\alpha)^{\frac{3}{2}}}\cdot\int_0^t \frac{q(t')}{(t-t')^{\frac{3}{2}}}\cdot e^{\frac{-r^2}{4\cdot\alpha\cdot(t-t')}}\,dt'$$

(Carslaw and Jaeger 1959, Section 10.4 equation (1))

If q(t) is a constant = q_0, then the result simplifies to:

$$T_{point}(t,r) = \frac{q_0}{4\pi\cdot(\rho\cdot Cp)\cdot\alpha\cdot r}\,erfc\left(\frac{r}{\sqrt{4\cdot\alpha\cdot t}}\right)$$

(Carslaw and Jaeger 1959, Section 10.4 equation (2)); where *erfc* is the complementary error function.

The conversion from the spherical coordinates of the solution to the Cartesian coordinates of the repository is:

$$r^2 = (x-x0)^2 + (y-y0)^2 + (z-z0)^2$$

Where the source is located at (x0, y0, z0)

8.1.2 Solution for a Finite Line Source in an Infinite Medium

The line source solution is obtained by applying the differential transform:

$$q_L(t)\cdot dy0 = q(t)$$

We then integrate y0 over the length of the line source (with line length L). When the line source is centered at y=0, the line source solution becomes:

$$T_{line}(t,x,y,z) = \frac{1}{8\cdot\rho\cdot Cp\cdot(\pi\cdot\alpha)^{\frac{3}{2}}}\cdot\int_0^t \frac{q_L(t')}{(t-t')^{\frac{3}{2}}}\cdot e^{\frac{-\left[(x-x0)^2+(z-z0)^2\right]}{4\cdot\alpha\cdot(t-t')}}\cdot\left[\int_{\frac{-L}{2}}^{\frac{L}{2}} e^{\frac{-(y-y0)^2}{4\cdot\alpha\cdot(t-t')}}\,dy0\right]dt'$$

The definite integral over dy0 is recognized as a form of the error function. The coordinate (x0, z0) is set to (0, 0). The line source solution reduces to:

$$T_{line}(t,x,y,z) = \frac{1}{8\cdot\pi\cdot k}\cdot\int_0^t \frac{q_L(t')}{t-t'}\cdot e^{\frac{-\left(x^2+z^2\right)}{4\cdot\alpha\cdot(t-t')}}\cdot\left[\operatorname{erf}\left[\frac{1}{2}\cdot\frac{\left(y+\frac{L}{2}\right)}{\sqrt{\alpha\cdot(t-t')}}\right]-\operatorname{erf}\left[\frac{1}{2}\cdot\frac{\left(y-\frac{L}{2}\right)}{\sqrt{\alpha\cdot(t-t')}}\right]\right]dt'$$

8.1.3 Solution for an Infinite Line Source in an Infinite Medium

The solution for a constant heat flux infinite line source q_{0L} along the y-axis is:

$$T_{infinite\_line}(t,x,z) = \frac{q_{0L}}{4\cdot\pi\cdot k\cdot t}\cdot e^{\frac{-\left(x^2+z^2\right)}{4\cdot\alpha\cdot t}}$$

(Carslaw and Jaeger 1959, Section 10.3 equation (1));

The equivalent convolution integral solution for a time varying line source was applied on the Yucca Mountain Project (DOE 2008a, equation 6.1-2) and is defined as:

$$T_{infinite\_line}(t,x,z) = \frac{1}{4\cdot\pi\cdot k}\cdot\int_0^t \frac{q_L(t')}{t-t'}\cdot e^{\frac{-\left(x^2+z^2\right)}{4\cdot\alpha\cdot(t-t')}}\,dt'$$

8.1.4 Solution for Multiple Finite Line Sources in an Infinite Medium

The temperature field for multiple line sources is obtained by the linear addition of single line sources. In the equation below, it is assumed that we have one source at the coordinates (z=0, x=0) and that there is a plane of symmetry at x=0. The variable Ns is the number of additional line sources on one side of the plane of symmetry. Hence, Ns =0 produces a single source, Ns =1 produces 3 sources, Ns =2 produces 5 sources, and so on.

$$T_{line\_mult}(t,x,y,z,N_s) = T_{line}(t,x,y,z)\ \ldots + \sum_{ns=1}^{N_s}\left(T_{line}(t,x-ns\cdot L_{offset},y,z)+T_{line}(t,x+ns\cdot L_{offset},y,z)\right)$$

$$T_{line\_mul}(t,x,y,z,N_s) = \sum_{ns=-Ns}^{Ns} T_{line}(t,x-ns\cdot L_{offset},y,z)$$

$$T_{line\_m}(t,x,y,z,N_s) = \frac{1}{(8\cdot\pi\cdot k)}\cdot\int_0^t\left[\frac{q_L(t')}{t-t'}\cdot coef_x(x,t,t')\cdot coef_y(y,t,t')\cdot e^{\frac{-z^2}{4\cdot\alpha\cdot(t-t')}}\right]dt'$$

Where

$$coef_x(x,t,t') = \sum_{ns=-Ns}^{Ns} e^{\frac{-\left[\left(x-ns\cdot L_{offset}\right)^2\right]}{4\cdot\alpha\cdot(t-t')}}$$

$$coef_y(y,t,t') = erf\left[\frac{y+\frac{L}{2}}{2\cdot\sqrt{\alpha\cdot(t-t')}}\right] - erf\left[\frac{y-\frac{L}{2}}{2\cdot\sqrt{\alpha\cdot(t-t')}}\right]$$

8.1.5 Solution for a Finite Plane Source in an Infinite Medium

The plane source solution is obtained by applying a differential transform to the solution for a finite line (length L):

$$q_P(t)\cdot dx0 = q_L(t)$$

and integrating x0 over the width of the plane source (W_P). When the plane source is centered at x=0, the plane source solution becomes:

$$T_{plane}(t,x,y,z) = \frac{1}{8\cdot\pi\cdot k}\cdot\int_0^t \frac{q_P(t')}{t-t'}\cdot e^{\frac{-z^2}{4\cdot\alpha\cdot(t-t')}}\cdot\left[\operatorname{erf}\left[\frac{1}{2}\cdot\frac{y+\frac{L}{2}}{\sqrt{\alpha\cdot(t-t')}}\right]\ldots + -\operatorname{erf}\left[\frac{1}{2}\cdot\frac{y-\frac{L}{2}}{\sqrt{\alpha\cdot(t-t')}}\right]\right]\cdot\int_{\frac{-W_P}{2}}^{\frac{W_P}{2}} e^{\frac{-(x-x0)^2}{4\cdot\alpha\cdot(t-t')}}\,dx0\,dt'$$

The definite integral over dx0 is recognized as a form of the error function. When the plane is centered about x=0, the solution reduces to:

$$T_{plane}(t,x,y,z) = \frac{\alpha}{8\cdot k\cdot\sqrt{\pi\cdot\alpha}}\cdot\int_0^t \frac{q_P(t')}{\sqrt{t-t'}}\cdot coef_x(x,t,t')\cdot coef_y(y,t,t')\cdot e^{\frac{-z^2}{4\cdot\alpha\cdot(t-t')}}\,dt'$$

Where

$$coef_x(x,t,t') = \operatorname{erf}\left[\frac{x+\frac{W_P}{2}}{2\sqrt{\alpha\cdot(t-t')}}\right] - \operatorname{erf}\left[\frac{x-\frac{W_P}{2}}{2\sqrt{\alpha\cdot(t-t')}}\right]$$

$$coef_y(y,t,t') = \operatorname{erf}\left[\frac{y+\frac{L}{2}}{2\sqrt{\alpha\cdot(t-t')}}\right] - \operatorname{erf}\left[\frac{y-\frac{L}{2}}{2\sqrt{\alpha\cdot(t-t')}}\right]$$

8.1.6 Solution for a Semi-infinite Plane Source in an Infinite Medium

When the plane source is of infinite length, but finite width, the solution reduces to

$$T_{semi\_infinite\_plane}(t,x,z) = \frac{\alpha}{4\cdot k\cdot\sqrt{\pi\cdot\alpha}}\cdot\int_0^t \frac{q_P(t')}{\sqrt{t-t'}}\cdot coef_x(x,t,t')\cdot e^{\frac{-z^2}{4\cdot\alpha\cdot(t-t')}}\,dt'$$

Where

$$coef_x(x,t,t') = erf\left[\frac{x+\frac{W_P}{2}}{2\sqrt{\alpha\cdot(t-t')}}\right] - erf\left[\frac{x-\frac{W_P}{2}}{2\sqrt{\alpha\cdot(t-t')}}\right]$$

8.1.7 Solution for an Infinite Plane Source in an Infinite Medium

The solution for an infinite plane source with a constant heat flux is given in Carslaw and Jaeger (1959, Section 10.3 equation (2)). The equivalent convolution integral solution for a time varying heat flux is:

$$T_{infinite\_plane}(t,z) = \frac{\alpha}{2\cdot k\cdot\sqrt{\pi\cdot\alpha}}\cdot\int_0^t \frac{q_P(t')}{\sqrt{t-t'}}\cdot e^{\frac{-z^2}{4\cdot\alpha\cdot(t-t')}}\,dt'$$

8.1.8 Solution for an Infinite Medium Internally Bounded by a Cylinder

The thermal response of an infinite medium internally bounded by a cylinder (of radius a) subject to a constant flux Q (Carslaw and Jaeger 1959, Section 13.5, equation (17)) is defined as

$$T_{cylinder}(r,a,t) = -2\cdot\frac{Q}{\pi\cdot k}\cdot\int_0^\infty \left(1-e^{-\alpha\cdot u^2\cdot t}\right)\cdot\left[\frac{(J0(u\cdot r)\cdot Y1(u\cdot a)) - Y0(u\cdot r)\cdot J1(u\cdot a)}{u^2\cdot\left(J1(u\cdot a)^2 + Y1(u\cdot a)^2\right)}\right]du$$

The convolution integral for a time varying Q is therefore:

$$T_{cylinder}(r,a,t) = \frac{-2}{(\pi\cdot k)}\cdot\int_0^t\int_0^\infty Q(t')\cdot\left[1-e^{-\alpha\cdot u^2\cdot(t-t')}\right]\cdot\left[\frac{(J0(u\cdot r)\cdot Y1(u\cdot a)) - Y0(u\cdot r)\cdot J1(u\cdot a)}{u^2\cdot\left(J1(u\cdot a)^2 + Y1(u\cdot a)^2\right)}\right]du\,dt'$$

Where:

J0 is the zero order Bessel function of the first kind

J1 is the first order Bessel function of the first kind

Y0 is the zero order Bessel function of the second kind

Y1 is the first order Bessel function of the second kind.

This solution was applied on the Yucca Mountain Project (BSC 2004, Equation 6-57, page 6-25), where the equation was first put into dimensionless form, and evaluated at the drift wall (r = a) to predict the drift wall temperature transient. The drift wall temperature was subsequently used to evaluate the ventilation air stream, waste package surface, and cladding temperature transients.

For the Yucca Mountain case, the project simulated the convolution integral with a series summation of finite differences based on one-year time increments (BSC 2004). Section 6.4 of BSC 2004 describes the use of two ANSYS numerical models and the analytic solution model applied to calculate the ventilation system heat removal efficiency as well as the component temperatures. Section 6.6 of BSC 2004 presents the results of the two approaches and provides evidence of the effectiveness of the analytical solution in Table 6-7 on page 6-39. The ventilation system removal efficiency for a 600 m drift with 50 years of ventilation was calculated by the "ANSYS-LA-Coarse" model as 88.3% (documented in DTN: M00406MWDLACVD.001), and the same result was calculated by the "Analytical-LA-Coarse" model as 88.0% (documented in DTN: M00406MWDAC8VD.001). The reference provides a similar comparison of results for an 800 m drift with the ANSYS and analytical model results of 85.8% and 86.0% respectively. The ANSYS model was then validated against a quarter-scale ventilation test as documented in the reference (Section 7 and Appendix XII). A pulse response to an assumed 1-year duration pulse was approximated by taking the solution above for a constant flux of Q, and subtracting a second solution for an assumed flux of –Q shifted in time by one year. A convolution integral solution was then approximated by a series summation approach using an exponentially decaying heat source Q(t) convolved with the "pulse" solution.

8.1.9 Extension of Analytic Solutions to a Semi-infinite Domain Bounded by One Isothermal Surface

The analytic solutions for an infinite domain are extended to the case of a semi-infinite domain by the method of images (Carslaw and Jaeger 1959, Section 10.10, page 273). A sink of strength equal to the source is reflected across the isothermal plane at z=ZG (ground surface). The solution is based on the sum of the source and sink fields (superposition), shown in Figure 8.1-1.

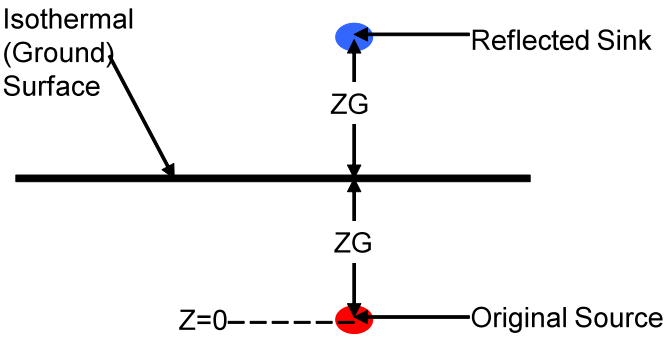

Figure 8.1-1 Application of the Method of Images for a Single Isothermal Surface

The technique is applicable to all of the line and plane source solutions derived above. Hence,

$$T_{line\_1iso}(t,x,y,z) = T_{line}(t,x,y,z) - T_{line}(t,x,y,z-2\cdot ZG)$$

$$T_{line\_mult\_1iso}(t,x,y,z,N_s) = T_{line\_mult}(t,x,y,z,N_s) - T_{line\_mult}(t,x,y,z-2\cdot ZG,N_s)$$

$$T_{plane\_1iso}(t,x,y,z) = T_{plane}(t,x,y,z) - T_{plane}(t,x,y,z-2\cdot ZG)$$

8.1.10 Extension of Analytic Solutions to a Semi-infinite Domain Bounded by Two Parallel Isothermal Surfaces

The source/sink pair constructed above can then be reflected to create the lower (water table) isothermal condition. This, however, compromises the effectiveness of the first (ground) isothermal surface. The newly added sources and sinks are reflected about the plane z=ZG to reestablish the first (ground) isothermal. This double reflection (first about z=-ZW and then about z=ZG) is termed a "paired" reflection in this document, shown in Figure 8.1-2.

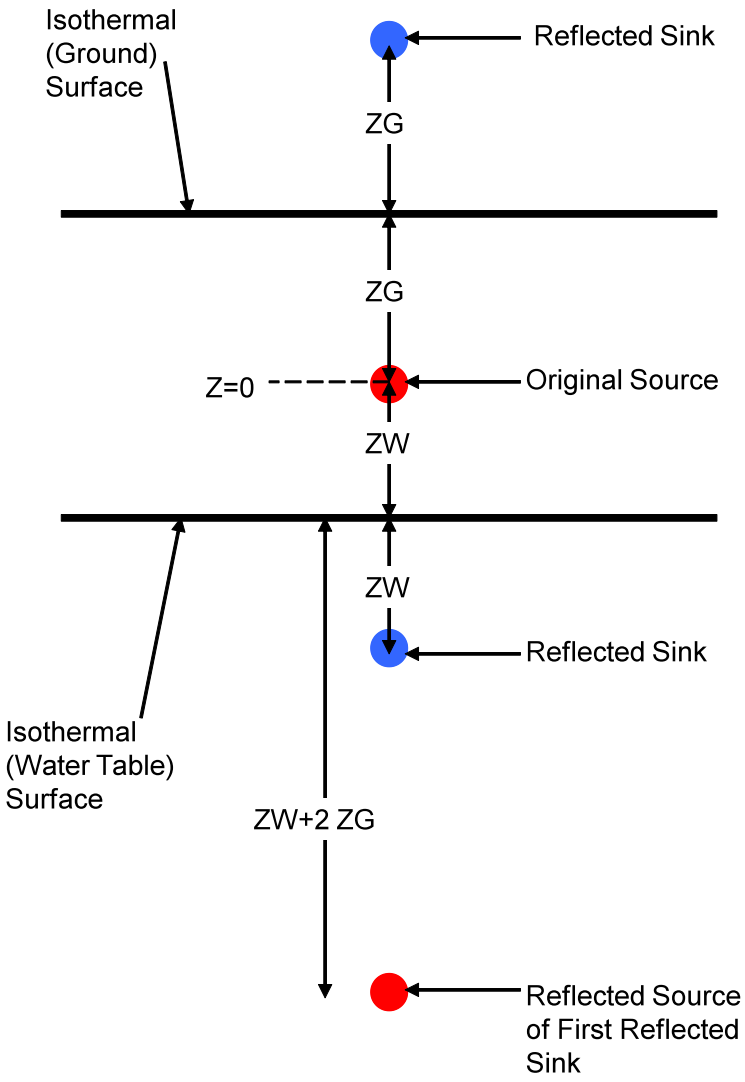

Figure 8.1-2 Application of the method of images to two isothermal surfaces (the ground and water table surfaces)

Continuation of the process produces an infinite series of sources and sinks. Because the series is convergent, a finite number of terms are used to approximate the solution. The series, derived by induction, always maintains the ground surface as a true isothermal surface. Increased numbers of paired reflections (Nr) produce successively closer approximations of an isothermal surface at the water table.

8.2 FINITE ELEMENT MODELS

Among the capabilities of DSEF is the interface with the *TOPAZ3D* (Wemhoff 2007) finite element heat transfer code. *TOPAZ3D* solves for the steady state or transient temperature field on three-dimensional geometries and allows for temperature-dependent material properties, either isotropic or orthotropic. The code accepts a variety of time and temperature dependent boundary conditions, including temperature, flux, convection and radiation. Additional features include thermal contact resistance across an interface, bulk fluids, phase change and energy balances. The DSEF interface will read the required input data from a worksheet and translate them in the *TOPAZ3D* input format. Even for relatively simple geometries the setup of the mesh is a complex task; therefore, the DSEF interface will rely on the *TrueGrid* (Rainsberger 2006) mesh generator. This section illustrates the input data and the formatting required to generate a mesh using the *TrueGrid* code. In this preliminary stage, three representative geometries were selected: (1) multi-layered parallelepiped; (2) multi-layered parallelepiped with inclined layers; and (3) concentric cylinders. The geometries that DSEF will handle are expected to be a combination of the three selected.

8.2.1 PARALLEL MULTI-LAYER

The `block` command within the *TrueGrid* input file generates a rectangular mesh according to the input parameters. Its generic form is given as:

```
block i-list; j-list; k-list;
      x-list; y-list; z-list;
```

The i-, j-, and k-list define boundary nodes in three directions, and x-, y-, and z-list define the corresponding boundary dimensions (the units are defined by the user; for clarity we will assume meter throughout).

This example illustrates the case of a stack of three layers of constant thickness. Each layer is made of a different material. The input file for *TrueGrid* is:

```
block 1 5; 1 7; 1 10 18 30;
      0. 4.; 0. 5.5; 0. 4. 10. 15.;
```

Here, 5 equally spaced nodes and 4 elements are generated in the x-direction between 0 m and 4 m; 7 nodes and 6 elements in the y-direction between 0 m and 5.5 m; 10 nodes and 9 elements between 0 m and 4 m, 9 nodes and 8 elements between 4 m and 10 m, 13 nodes and 12 elements between 10 m and 15 m (total 30 nodes and 29 elements) in the z-direction. The lists also define partitions (n) with the block in the example above composed of one partition in the x- and y-direction, and three in the z-directions. Partitions can be referred to directly using the position of the boundary nodes in the block definition—reduced indices. For example, the second partition in the z-direction is bounded by node 10 and 18 that are in position 2 and 3 in the k-list; when a command requires a partition input, partition 2 in the z direction will be defined using reduced indices: 2 3.

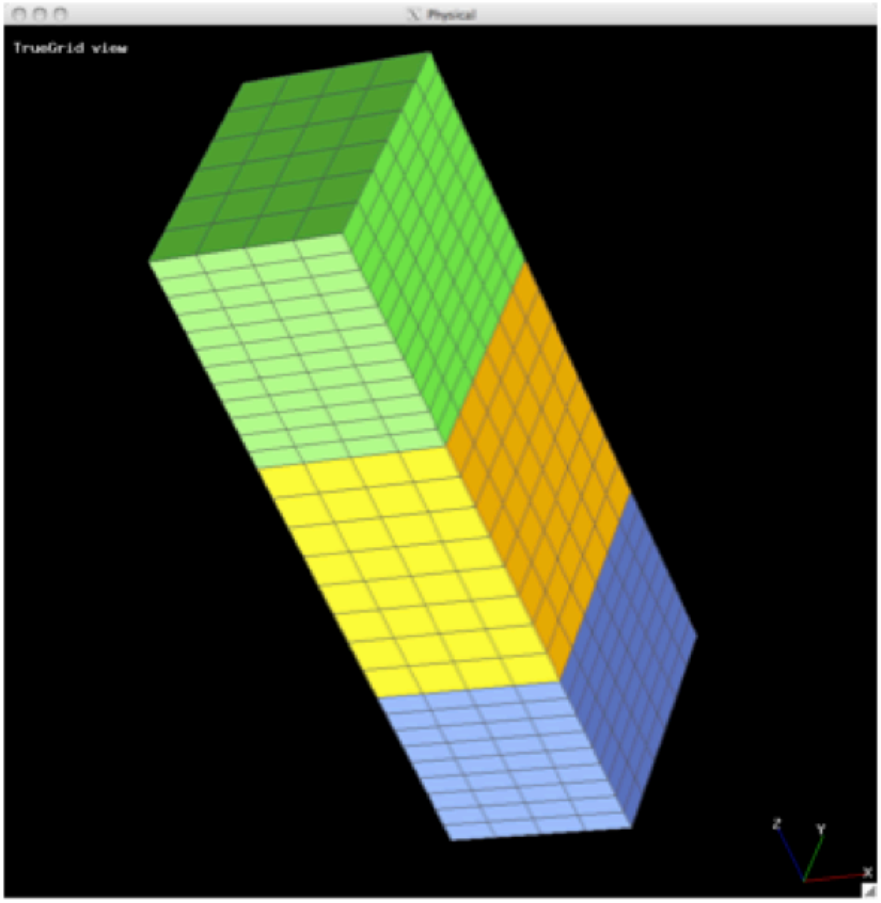

Figure 8.2-1 Example of a configuration with three parallel layers

The mesh size is uniform within a partition, but can vary from a partition to another. The number of nodes within a partition can be modified without changing the partition indices using the *mseq* command.

The three partitions in the z-direction enable the possibility to assign a different material to each of them. Two options are available for specifying the material. The *mt* command uses the reduced indices of the boundary nodes to identify a partition and assign to it a material—this is called the "region" method:

```
mt   1 1 1   2 2 2   1
mt   1 1 2   2 2 3   2
mt   1 1 3   2 2 4   3
```

The first three integers are the minimum reduced indices in the three directions; the following three integers are the maximum reduced indices, and the last integer is the material number assigned to the partition.

The *mti* command, instead, uses the so-called "progression" method where a partition is still identified using reduced indices, but as follows:

```
mti  1 2; 1 2; 1 2; 1
mti  1 2; 1 2; 2 3; 2
mti  1 2; 1 2; 3 4; 3
```

The three pairs of integers separated by a semicolon identify the minimum and maximum reduced index of the partition in x-, y-, and z-direction, respectively. The last integer is the material number. The *mti* command allows assigning the same material to multiple zones in a single line.

Figure 8.2-1 shows the mesh structure as generated by *TrueGrid* for a parallelepiped with dimensions 4 x 5.5 x 15 m. Each color corresponds to a different material. Material properties will be defined at a later stage in the *TOPAZ3D* input.

All commands that identify a partition using the "region" method have a counterpart (same command with an *i* at the end) that uses the "progression" method. As the latter command allows a more compact syntax, it will be the preferred choice from this point on.

8.2.2 INCLINED MULTI-LAYER

This second example refers also to a stratified configuration, but now with uneven layers. The input file for *TrueGrid* is the following:

```
block 1 5; 1 7; 1 10 18 30;
0. 4.; 0. 5.5; 0. 4. 10. 15.;
mbi -1; 1 2; -3; z 2.8
mbi -1; 1 2; -2; z -1.
mti  1 2; 1 2; 1 2; 1
mti  1 2; 1 2; 2 3; 2
mti  1 2; 1 2; 3 4; 3
```

The block definition is the same as in the previous example. The inclination is obtained by translating all the vertices on the edge of a partition using the *mbi* command. An edge, in the progression method, is identified by holding constant (negative sign) the reduced indices over two directions. Finally, the direction and size of the offset are provided. In this example the offset is in the z-direction and it is 2.8 m in the first case, negative 1 m in the second case. The resulting mesh structure is shown in Figure 8.2-2 for a parallelepiped with dimensions 4 x 5.5 x 15 m.

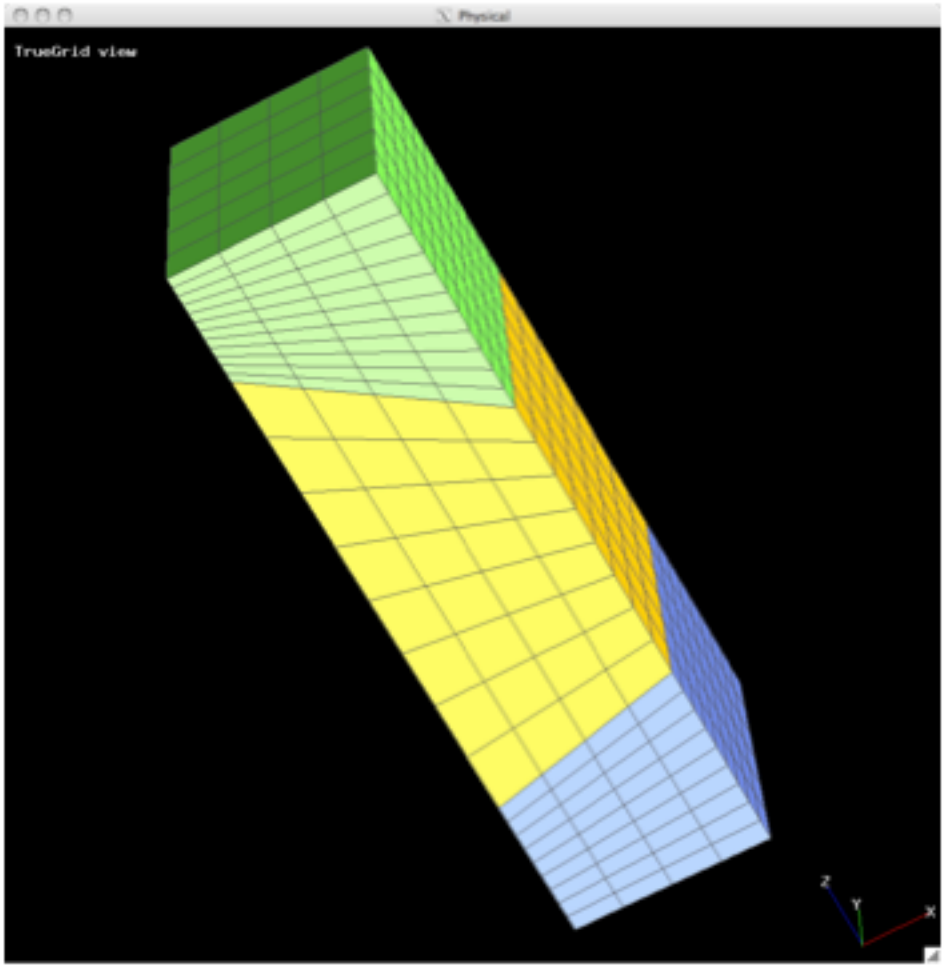

Figure 8.2-2 Example of a configuration with three non-parallel layers

8.2.3 CONCENTRIC CYLINDERS

This example considers a configuration with two concentric cylinders. Two different approaches apply to this situation and are illustrated here. In the first approach the basic initial mesh structure is a simple block as for the examples above. The mesh is then deformed (or projected) on cylinders to resemble the desired geometry. The input file for *TrueGrid* is the following:

```
block 1 5 14 18; 1 5 14 18; 1 30;
 0. 1. 3. 4.; 0. 1. 3. 4.; 0. 15.;
sd 1 cyli 2. 2. 0.  0 0 1  2
sd 2 cyli 2. 2. 0.  0 0 1  1
```

```
sfi -1 -4; -1 -4; 1 2; sd 1
sfi -2 -3; -2 -3; 1 2; sd 2
mti 1 2 0 3 4; 1 2 0 3 4; 1 2; 1
mti 2 3; 2 3; 1 2; 2
```

After the block is defined, two surfaces are introduced with the ***sd*** command. The first entry in this command is the surface number, followed by the surface type (cylinder). The next six entries are: three Cartesian coordinate of a point on the cylinder's axis; three coordinates of the directional unit vector parallel to the cylinder's axis (the z-axis in this case). The last entry is the cylinder radius. The ***sfi*** command deforms the mesh, projecting the boundary surfaces of a partition (selected using the progression method) onto one of the cylinders. The resulting mesh is illustrated in Figure 8.2-3, where the diameter of the inner and outer cylinders are 2 and 4 m respectively, and a length of 15 m.

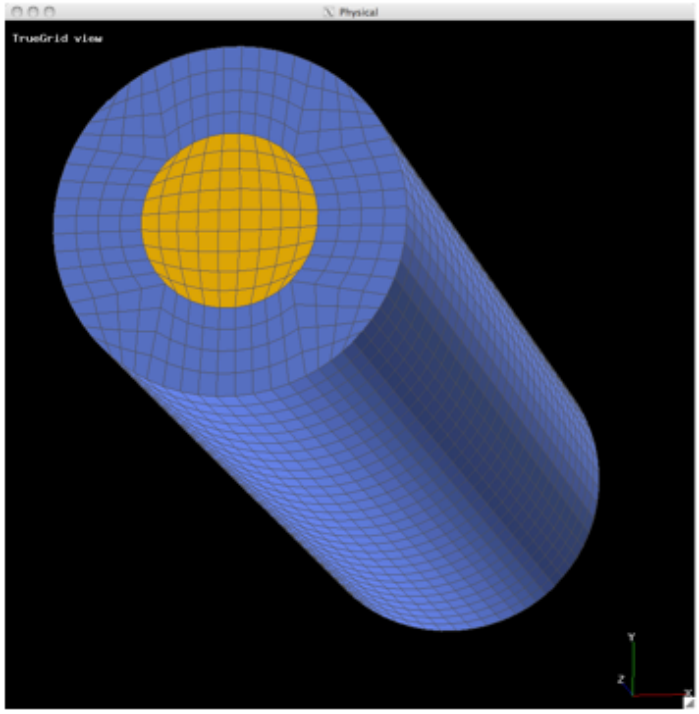

Figure 8.2-3 Example of a configuration with two concentric cylinders

In the second approach the initial mesh structure is cylindrical rather than a block. The input file for *TrueGrid* is the following:

```
cylinder 1 10 19; 1 20; 1 30;
    0. 1. 2.; 0. 360.; 0. 15.;
mti 1 2; 1 2; 1 2; 2
mti 2 3; 1 2; 1 2; 1
```

The *cylinder* command is similar to the *block* command, but refers to a cylindrical coordinate system (r,θ,z), where r is the radial coordinate, θ is the azimuthal coordinate and z is the height. The resulting mesh is illustrated in Figure 8.2-4. The mesh structure is regular with *cylinder* and irregular with *block* commands. In both cases the cylinders are approximated by quadrilateral elements (Figure 8.2-5). Cylinders in both Figure 8.2-4 and 8.2-5 have inner and outer diameters of 2 and 4 m respectively, and length of 15 m. Typically, even complex geometries are carved out of a single structure for which the *block* command is preferred.

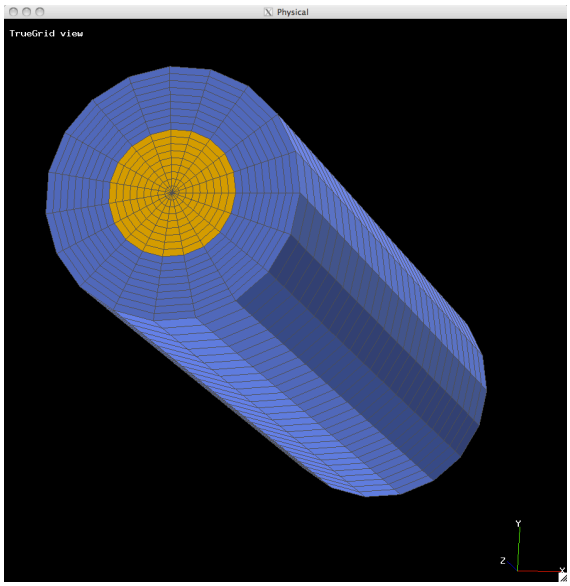

Figure 8.2-4 Example of a configuration with two concentric cylinders and cylindrical mesh

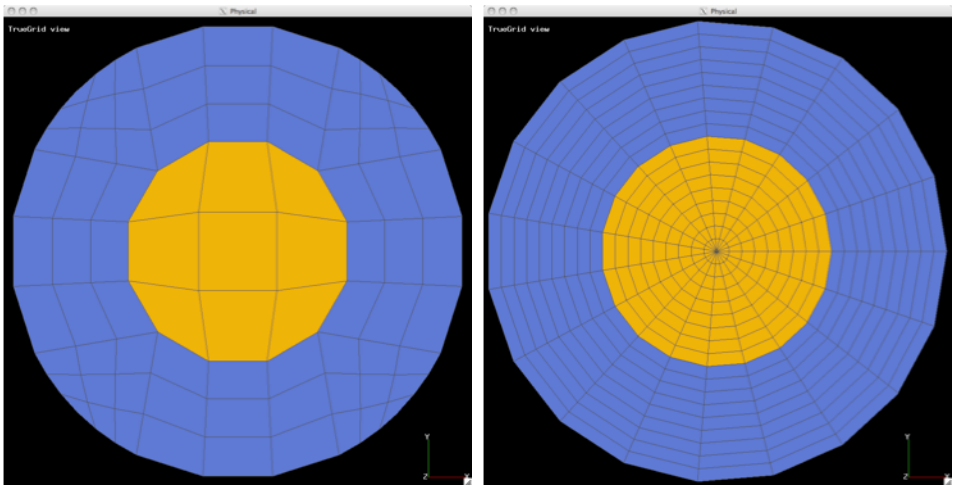

Figure 8.2-5 Mesh structure generated using the block (left) and the cylinder (right) structure

8.3 MODEL TESTING

Analytic models and finite element models were developed with a realistic thermal analysis case. Models were then prepared in *Mathcad* and *TOPAZ3D*. The model testing described below resulted in good agreements between both approaches.

8.3.1 APPROACH

To test the viability of the thermal modeling approach of using the thermal analyzer *TOPAZ3D* to check and extend thermal analyses using analytical models developed in *Mathcad*, a simple simulation of a temperature transient in a 3-dimensional solid parallelepiped was used.

Mathcad was used to prepare an analytical solution to a transient defined as follows:

- Object analyzed – a solid parallelepiped of aluminum, measuring 2 cm x 2 cm x 8 cm
- Initially at a constant temperature of 25°C
- At time zero all exposed surfaces incur a step change to 100°C
- *Mathcad* was used to predict the transient temperature at the centroid of the solid, and the transient average temperature of the solid.

A *TOPAZ3D* model was developed for the same scenario, and variations in gridding and other input variables were tested until agreement with the analytical solution was demonstrated.

8.3.2 DESCRIPTION OF MATHCAD ANALYSIS

The solution for the temperature transient for a 1-dimensional case where a semi-infinite slab is exposed to a step change in temperature from T0 to TS is given in Carslaw and Jaeger (1959, Section 3.4, equation (4), page 100). An analysis using dimensionless parameters was used to duplicate Figure 11 in Carslaw and Jaeger to confirm the validity of the one-dimensional *Mathcad* model (see Figure 8.3-1). Using 10,000 series terms produced good agreement with the figure.

$$\Theta(t,x) := 1 - \frac{4}{\pi}\left[\sum_{n=0}^{10000}\left[\frac{(-1)^n}{2n+1} e^{-(2n+1)^2 \pi^2 \frac{Fo(t)}{4}} \cos\left(\frac{2n+1}{2}\pi\,\xi(x)\right)\right]\right]$$

Where

$\Theta(t,x)$ was a dimensionless temperature change, such that the temperature

Temp(t,x) = T0 + (TS – T0)Θ(t,x)

T0	initial temperature
TS	final surface temperature after time zero.
Fo	dimensionless time = thermal diffusivity*t/(slab thickness)^2
Ξ(x)	dimensionless length = x/(slab thickness)

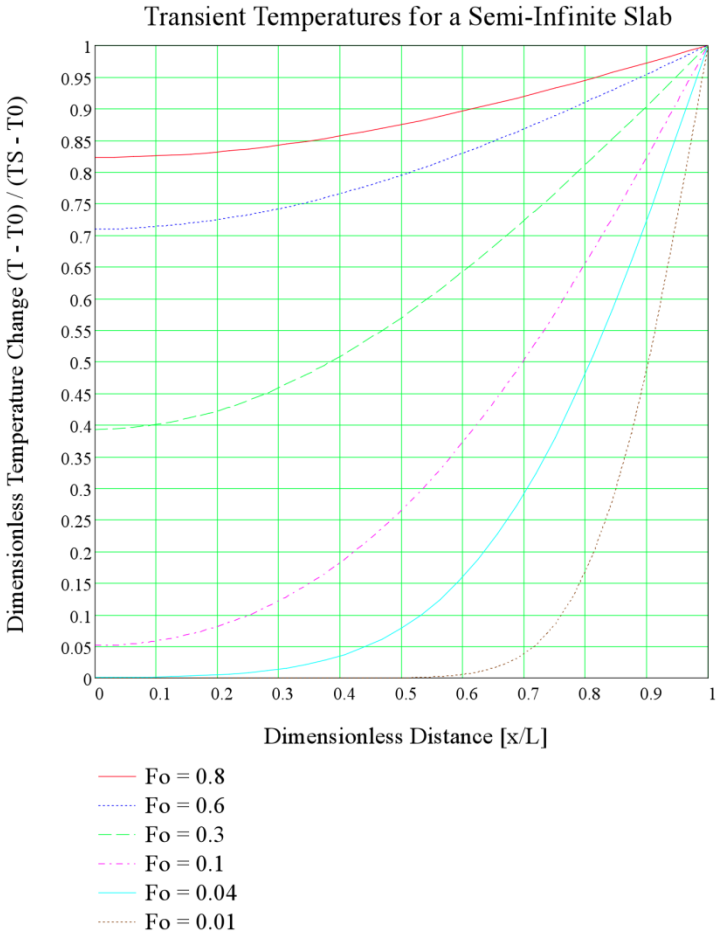

Figure 8.3-1 Mathcad model reproduction of Carlsaw and Jaeger (1959, figure 11)

The equation for the average temperature of the slab at time t (Carslaw and Jaeger 1959, Section 3.3, equation (10), page 97) is given as:

$$\Theta_{avg}(t) := \frac{8}{\pi^2} \cdot \sum_{n=0}^{10000} \left[\frac{1}{(2n+1)^2} e^{-(2n+1)^2 \pi^2 \cdot \frac{Fo(t)}{4}} \right]$$

Both centroid and average dimensionless temperature transients were checked against Carslaw and Jaeger, Figure 12 as shown in Figure 8.3-2.

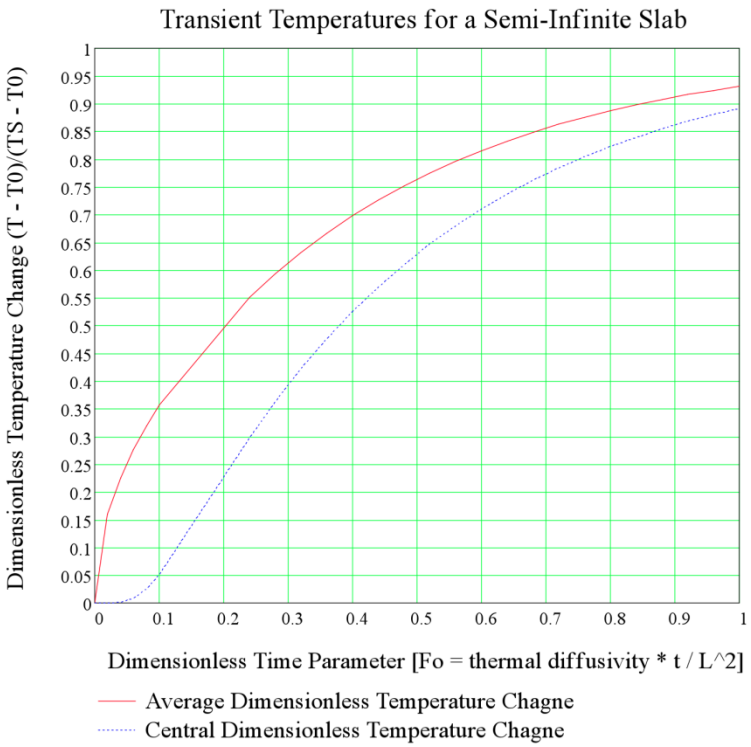

Figure 8.3-2 Mathcad model reproduction of Carslaw and Jaeger (1959, figure 12)

The 3-dimensional problem of the parallelepiped subjected to a step change in surface temperature at time zero is based on the Handbook of Heat Transfer, Second Edition (Rohsenow et al 1998), page 4-87. The transient 3-dimensional solution for a number of solid geometry cases can be expressed in terms of the product of the one-dimensional slab solutions. The solution for various geometries is given in Rohsenow et al (1998 Table 5 *Product Solutions for Internal and Central Temperatures in Solids with a Step Change in Surface Temperature*).

The temperature transients developed in this manner were compared against a *TOPAZ3D* model of the aluminum parallelepiped as described in Section 8.3.3.

8.3.3 DESCRIPTION OF THE TOPAZ3D ANALYSIS

The temperature transients developed in the previous Section were compared against a *TOPAZ3D* model of the same aluminum parallelepiped. This model used material properties and assumptions coherent with the *Mathcad* model:

- Density 2,700 kg/m^3
- Thermal conductivity 238.5 W/m-K
- Specific heat 920.5 J/kg-K
- Initially the sample is at a uniform temperature of 25°C; a step change is applied on the exposed surfaces (100°C) at time 0.

Figure 8.3-3 shows a comparison of the analytical solution and the *TOPAZ3D* solution for the temperature at the centerline of the parallelepiped as a function of time. The *TOPAZ3D* solution is very sensitive to the mesh size. The solution obtained applying a 21 x 11 x 11 nodes mesh is close to the analytical solution, whereas a coarser mesh (9 x 3 x 3 nodes) is inadequate for this problem. Further mesh refining was attempted, but led to a computational stall. That issue is currently under investigation. The time step size was optimized to guarantee a converged solution. Figure 8.3-4 shows the temperature distribution at the center of the parallelepiped of dimensions 2 x 2 x 8 cm (see p.47) for selected time steps.

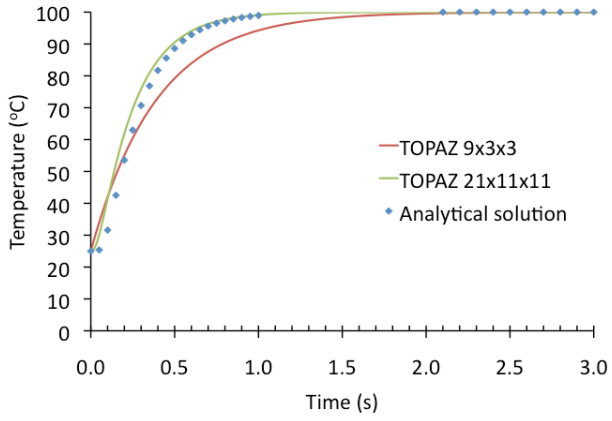

Figure 8.3-3 Comparison of the temperature at sample centerline as a function of time obtained with TOPAZ3D and dimensionless analysis

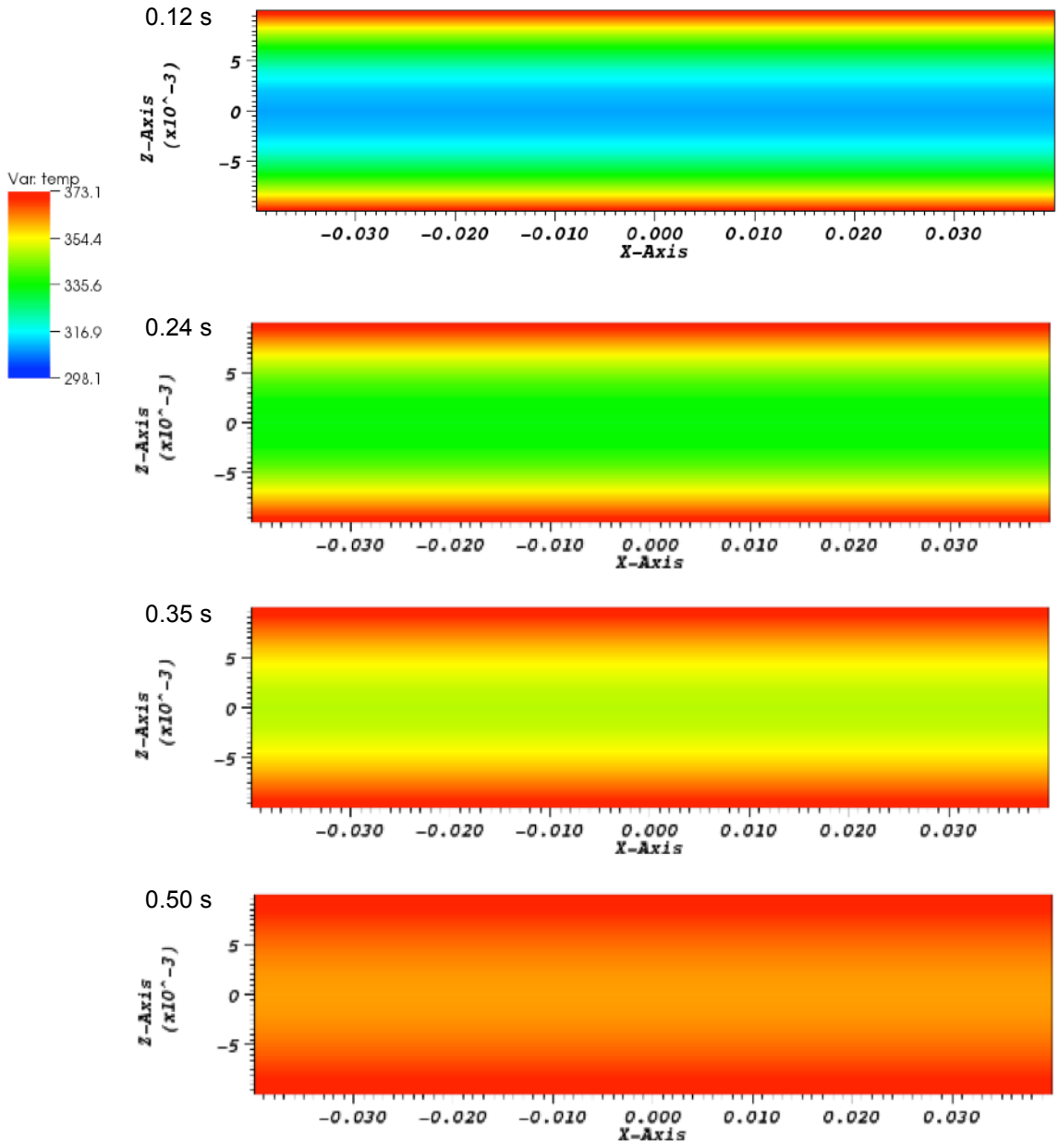

Figure 8.3-4 Fuel temperature distribution (K) for a central cross section of a 2 x 2 x 8 cm parallelepiped at selected time steps

(x and z axis dimensions in meters)

8.4 DECAY HEAT

The decay heat data to be used in DSEF relies on data developed in Carter et al 2011, which models specific radionuclide inventory data in each of the waste forms for the once-through (Figure 5-1), open-cycle (Figure 5-2), and closed-cycle (Figure 5-3) waste streams for various burnup and process time assumptions.

8.4.1 APPROACH

The approach used to model the decay heat data for used nuclear fuel on the Yucca Mountain Project DOE 2008a and BSC 2004 was to fit the detailed decay heat data (developed using ORIGEN or other codes that tracked radioisotope decay and in-growth for the specific waste streams) to a series of three or four exponential terms of the form:

$$Q_{decay\_heat}(t) = A1 \cdot \exp(-B1 \cdot t) + A2 \cdot \exp(-B2 \cdot t) + A3 \cdot \exp(-B3 \cdot t) + A4 \cdot \exp(-B4 \cdot t)$$

In DOE 2008a and BSC 2004 the curve fit was performed by using the SOLVER Add-in in *Excel* to minimize the error based on the sum of the squares of the difference between the actual data and the curve fit equation. That approach worked well, but care was needed in selecting the initial guess for the process, to obtain convergence.

The approach taken here is to use the GENFIT function included in *Mathcad* to perform the curve fit operation. This approach was successfully tested against the decay heat data shown in the Yucca Mountain Repository License Application (DOE 2008b) Figure 1.5.1-6 *Thermal Power after Discharge: Comparison of Pressurized Water Reactor and Boiling Water Reactor*. The same issue of selecting an adequate initial guess in order to obtain convergence applies to the *Mathcad* approach as to the *Excel* SOLVER Add-in approach.

8.4.2 WASTE STREAM DECAY HEAT DATA DEVELOPMENT

- The decay heat from all of the waste forms resulting from each of these potential fuel cycles is being addressed. The priority for running each waste form model is being evaluated based on input from the R&D Roadmap and related work packages such as Thermal and Waste Form.

Initial data provided in an *Excel* workbook by SRNL includes data based on assumed fuel cycle radionuclide inventory data and analysis using ORIGEN. The SRNL workbook's function is to determine the process wastes derived from reprocessing Used Nuclear Fuel and its properties especially the isotopic content of the products and wastes. The results of the workbook are documented in FCRD-USED-2010-00031 Rev 3. Alternate waste streams for potential future nuclear fuel cycles, including:

- Future Open Cycle - Light Water Reactor used nuclear fuels at higher burnup
- PWR used fuel data at 40, 51, 60, and 100 GWd of burnup
- BWR used fuel data at 30 and 50 GWd of burnup
- Partial Recycle – MOX fuel – at 50 GWd of burnup
- Full Recycle waste streams using different processes
- COEX glass and COEX BWR
- UREX glass and UREX BWR
- NUREX glass and NUREX BWR
- E-Chem – Glass, Zeolite (ceramic), and Metal

From the extensive set of possible fuel cycles and waste streams analyzed by SRNL, a subset of representative burnup, waste forms, and waste containers have been chosen to represent each of the proposed fuel cycles. Figure 8.4-2 shows the decay heat in units of W/canister or W/assembly to be utilized in modeling the repository design cases including:

- LWR fuel assemblies
- MOX fuel assemblies
- COEX glass HLW canisters
- NUEX glass HLW canisters
- E-CHEM ceramic HLW canisters
- E-CHEM metal HLW canisters

The *Excel* workbook includes the mass inventory of each of the radionuclide species as a function of time and develops decay heat data for each constituent and the total for all of the waste forms.

For analysis purposes curve fits will only be developed for the total decay heat for each of the waste streams analyzed.

Because of the wide variety of reactor types, fuel cycles and waste streams, for comparison purposes the data has been normalized to Megawatts Electric produced by the fuel. With this approach the waste volumes and decay heat generated by a given fuel cycle which produced an equivalent amount of electricity can be compared.

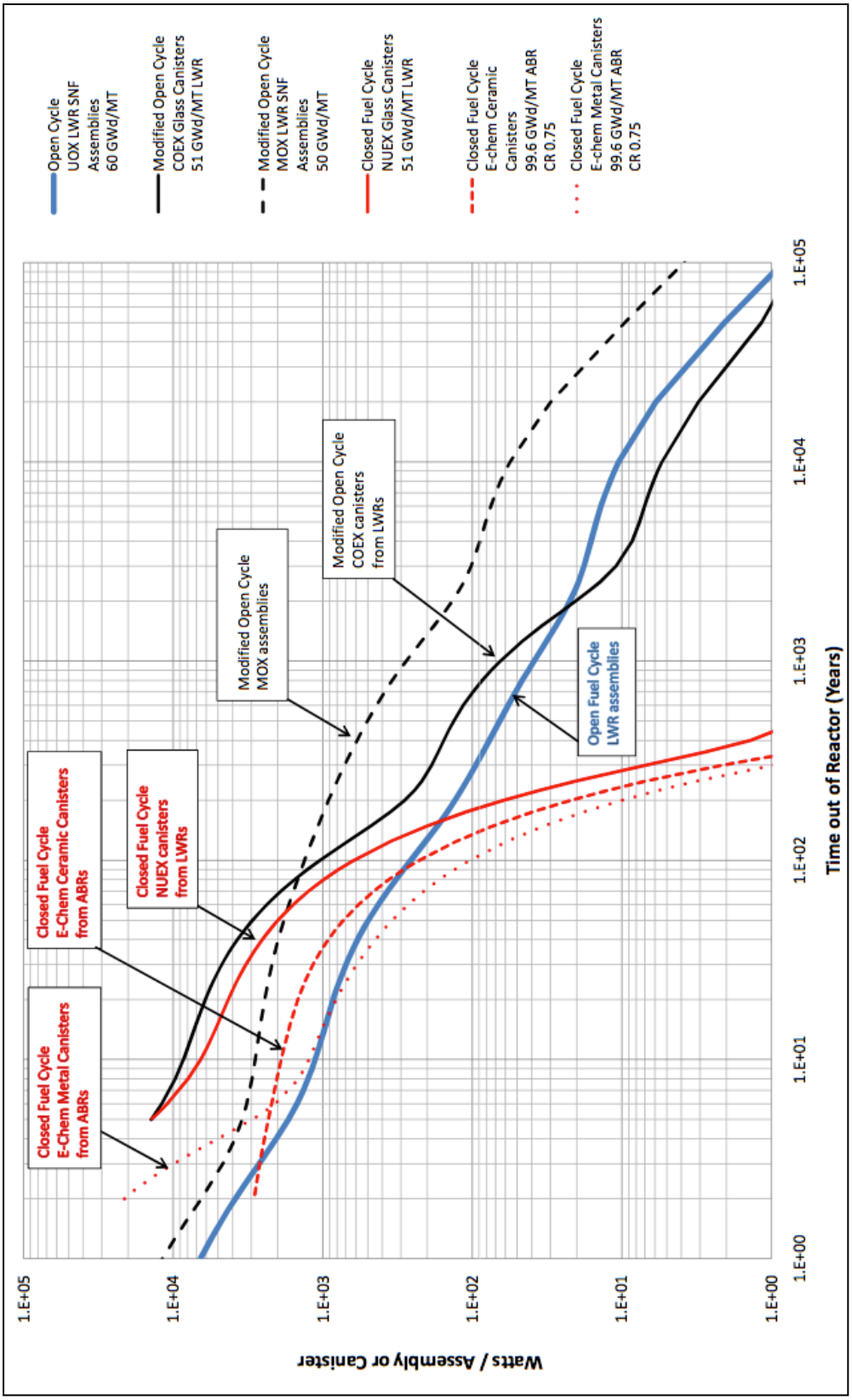

Figure 8.4-1 Long-term waste form decay heat for each base case fuel cycle per canister assembly or canister

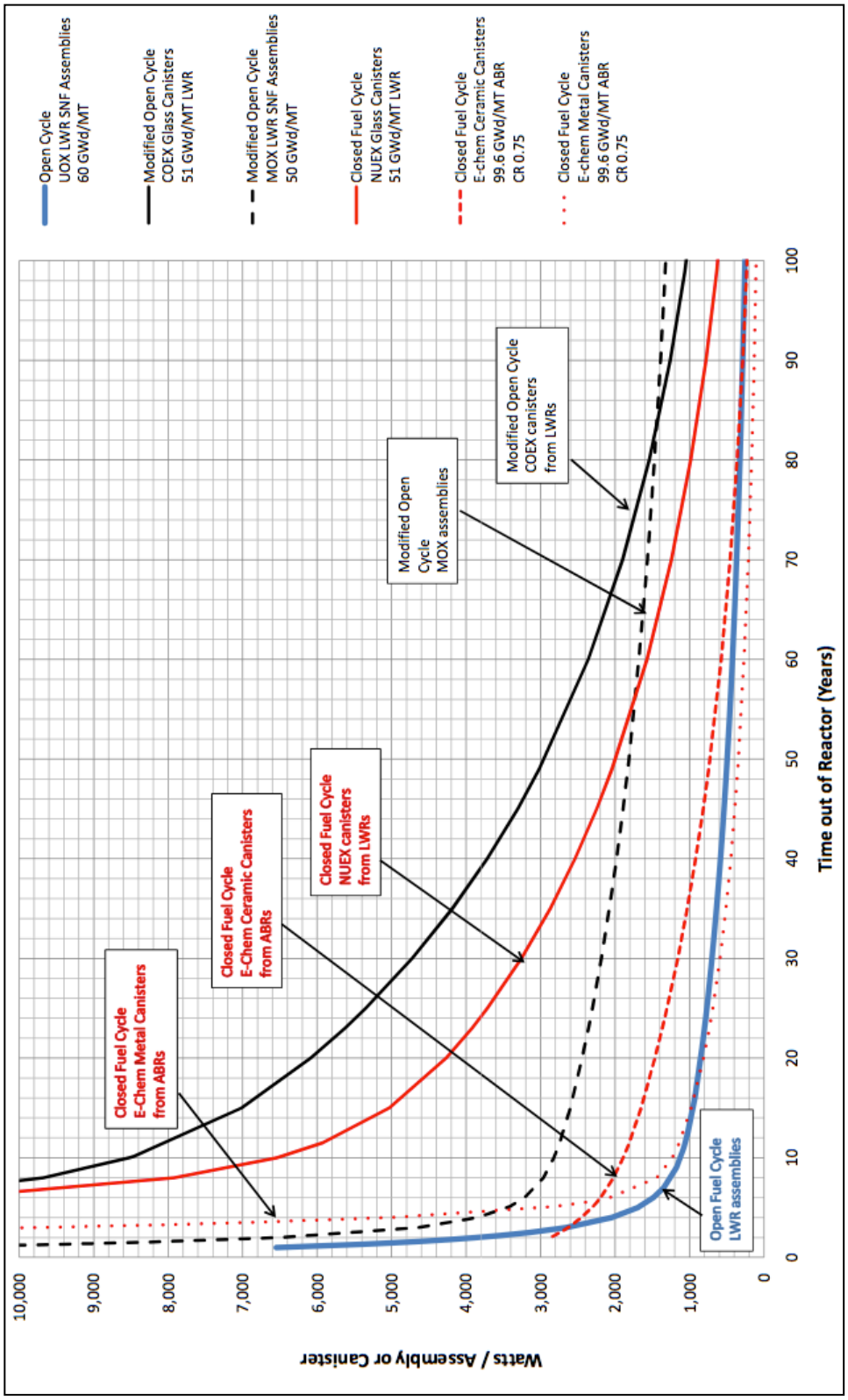

Figure 8.4-2 Short-term waste form decay heat for each base case fuel cycle per canister assembly or canister

9. MATERIAL PROPERTIES

The material property data in the DSEF *Knowledge Management* worksheets (shown in Figure 2.1-1) include properties for both the natural environment (shown in Table 6-1 from Blink et al. (2011), Table 2) and the engineered barrier system components for the various repository options considered in by UFD, as shown in Table 9-1 (Blink et al. 2011, Table 3).

Table 9-1 Engineered Barrier System (EBS) concepts and components

Category	Sub-category
EBS Emplacement Options	Large waste packages in drifts
	Horizontal or vertical borehole emplacement from drifts
	Deep boreholes
EBS Barrier Options	Waste form
	Cladding
	Barriers internal to the waste package
	The waste package itself
	Drip shields
	Backfill
	Buffer materials
	Sorptive materials
	Seals above deep boreholes
EBS Reactive Properties	Material porosity, tortuosity, bulk density and saturation
	Infiltrating and conditioned water chemistries
	Radionuclide solubilities
	Radionuclide sorption distribution coefficients, k_d
	Radionuclide diffusion
	Groundwater pore velocity

9.1 EXAMPLE STRUCTURE AND DATA INCLUDED IN THE THERMAL AND TRANSPORT PROPERTY WORKSHEETS

The *Thermal Property* data worksheets are structured as follows:

- Rows
    - Sections of groups of rows
        - Host Rock, Engineered Materials (includes buffers, plugs, liners for now)
    - Groups of rows for media types
        - Clay, Salt, Granite, Basalt, Limestone, Sandstone, Subseabed,Tuff
        - Cementitious Buffer, Stainless Steel Liner, Cementitious Backfill, Concrete Lining, Compacted Clay Backfill, Sand, Soil

    - Rows for specific media (e.g. Opalinus clay, Boom clay, etc.)
- Each row includes:
    - Overall reference information for the medium
    - Property mean and ranges (in columns)
    - Comments and citations (for each property)
- Properties in the columns
    - Bulk thermal conductivity, dry thermal conductivity, wet thermal conductivity, matrix porosity, total porosity, saturation, volume % water, bulk density, dry density, wet density, specific heat, volumetric heat capacity, thermal diffusivity (usually calculated)

In addition to the primary data worksheet, the *Thermal Properties* worksheets (some of which may be stored in an auxiliary file) include other worksheets as follows:

- References (full list of those cited on the sheets)
- Material sheets (key tables and figures from the cited references, sometimes equations and critical discussion sections)
    - Clay
    - Salt
    - Granite
    - Basalt
    - Tuff
    - Subseabed
    - EBS Materials
    - General

It should be noted that the tuff environment has been well covered by the Yucca Mountain Project and is included in the DSEF for validation purposes. Basalt and granite are two examples of hard rock (Table 7-1). Subseabed is not being considered in the DSEF but the properties were available in compilations reviewed and hence were captured for completeness.

The *Transport Property* worksheets utilize the same basic organization and structure as the *Thermal Property* worksheets, but address the following material properties: Permeability,

Hydraulic Conductivity, Porosity, Effective Porosity, Coefficient of Molecular Diffusion, Longitudinal Hydrodynamic Dispersion

9.2 Data Evaluation and Selection of Input Values to Use as Representative Data for Analysis

The Material (*Thermal and Transport Property* worksheets provide a central assemblage of relevant material references and source data. However, before the information can be used in a thermal or radionuclide transport model calculation, the wide range of raw data needs to be evaluated to develop representative properties for use in the calculations.

Depending on the extent of the data available it may be treated differently, for example

- Very limited data – a bounding value may be assumed, with justification provided
- Small sample of data – a mean value and an uncertainty band may be developed for use
- Extensive data – a mean value with uncertainty band, or a parameter distribution function may be appropriate

This evaluation will be performed in the *Thermal* worksheets and the representative material properties for the selected natural environment and engineered barrier components will be summarized in the *Input* and/or *Interface Parameters* worksheets for potential reference in other worksheets within DSEF and in the *External Interface* and *FC System Impacts* worksheets for external organizations (see Figures 2.1-1, 2.1-2, and 4.2-1).

9.3 Materials Longevity

The Material (*Thermal and Transport Properties* and *Materials Longevity* worksheets will pull data from the *Knowledge Management* worksheets based on the selections made by the DSEF user and will feed waste form degradation and waste package degradation data to the *PA* worksheet. Information from historical degradation mode surveys (e.g. Farmer 1988, Sutton 2010) together with more recent publications and data will be maintained such that the user can select the most appropriate container material for the repository environment and can determine the maximum corrosion rate. The rate of dissolution of waste form and

waste package for a given repository environment is typically modeled using yearly fractional degradation rates.

The near-field volume is the volume of potentially saturated space inside the repository footprint that would be available for radionuclides to dissolve into. The bulk volume is defined as the repository footprint multiplied by the height. A reasonable assumption is that the near-field volume is comprised of 3 "compartments" (a) void space in the repository tunnels, (b) available pore space in the degraded EBS (including waste form, waste package, backfill), and (c) available pore space in the host rock. The near-field volume available for dissolved radionuclides to mix with is then defined as the porosity of each compartment multiplied by the available volume of each compartment. In some cases (e.g. salt repositories), the space between the waste package and the tunnel walls will be negligible, since the salt walls creep towards the waste package. For salt repositories, the tunnel height is assumed to be the diameter of a waste package, while for granite and clay the height is assumed to be twice the diameter of the waste package (Wang and Lee 2010). The data on area, height and porosity of EBS materials and host rock is fed to the *PA* worksheet from the Material *(Thermal and Transport) Properties* worksheets based on the selection of the repository design, waste package material and waste form within the DSEF workbook.

10. PERFORMANCE ASSESSMENT

The Performance Assessment (*PA*) worksheet within DSEF will allow users to document and in some cases calculate various portions of the PA process. Factors that will be accounted for in the PA process will follow the FEPs process and should include:

- Waste package material and waste form degradation (corrosion rates in appropriate chemical and temperature environment)
- Near-field volume
- Radionuclide solubility and transport through the EBS (with defined EBS conditions and radionuclide solubility and sorption calculations, THCMBR processes)
- Radionuclide solubility and transport through the geosphere (ambient chemical far-field conditions, THCMBR processes
- Radionuclide transport and uptake in the biosphere, and dose assessment.

Relevant data and worksheets within the Material (*Thermal and Transport) Properties* and *Materials Longevity* worksheets will feed the *PA* worksheet based on the selections for repository environment, repository design and thermal requirements made by the DSEF user for both the EBS and geosphere media.

The DSEF contains a simple, high-level 1-D transport code, and a dose calculation worksheet. Radionuclide concentration exiting the EBS will be transferred to a model predicting radionuclide concentration in the geosphere, subsequently the biosphere and dose calculations can be performed using either an undisturbed or human intrusion assumption. However, the *PA* worksheet will encourage the user to use more complex PA models in *GDSE*, which uses the *GoldSim* software package (Goldsim 2009).

Whether a high-level simple PA is calculated inside DSEF or a more complex PA is developed in an external code such as GDSE or GoldSim, the inputs, constraints, outputs and discussion of each run will be documented in DSEF. This will allow consistent comparison between many different scenarios for each base case model.

Initially, the PA portion of DSEF will evaluate and compare the 24 base case systems shown in table 7-1 for six waste forms, 4 repository environments and two aging times. Initially, the baseline cases comparable to YMP and WIPP will be evaluated to provide confidence in the models. Subsequently, to provide maximum benefit to the UFD Campaign and decision-

makers, the priority in which the remaining cases would be evaluated will then be decided based on the immediate needs of the Campaign. Beyond those base cases, users will continue to build a library of PA outputs that can be drawn upon to improve the repository design. It is expected that in FY12, DSEF will prove a useful capability in performing site-selection work.

11. COST

The *Cost* worksheet will develop a rough estimate of the repository cost based on published unit costs developed by repository programs from around the world. It is recognized that cost models are relatively easy to develop, but are nearly impossible to validate. For that reason, the cost models will be most useful in comparing design options for a given waste form and environment, and less accurate in comparing design options for different waste forms and environments. Results of these high level cost models should not be used to try to establish the actual cost for use in developing an actual facility; detailed cost models should be developed specifically for such a facility.

Two of the DSEF team members followed the Yucca Mountain life cycle cost exercises over the years. In 2008, one of the DSEF team members obtained a more detailed cost breakout for Yucca Mountain and used it to develop a costing algorithm for a repository designed to dispose of ultra-high-burnup waste from laser fusion-fission hybrid reactors. That algorithm will be extended for the DSEF during the remainder of FY11.

Costs, at a high level, have been obtained for the WIPP repository, and more detailed costs area being sought. The international literature will also be surveyed to obtain other cost data for various repository media. Published cost comparisons will be most valuable, because they will enable linkage of multiple studies and a determination of whether unit cost estimates should be increased or decreased from a particular reference.

The cost algorithm will be based on unit costs for waste packages of a specified size and material, drilling costs, etc. In some cases, published unit costs are available, and in other cases, they will be estimated using raw material costs and/or material properties. This approach was implemented in the hybrid reactor study noted above.

The other three *Calculation* worksheets in the DSEF (*Thermal*, *Materials Longevity*, and *PA*) can complete their calculations based on a unit cell approach. The *Cost* worksheet will need to go beyond a single unit cell to estimate the repository footprint for a specified repository capacity. To facilitate cost comparisons, a reference capacity will be chosen to represent a fleet of reactors producing a specified amount of power for a specified period of time. A fuel cycle with higher burnup and less waste volume and/or heat will then be comparable to other fuel cycles on an even basis.

The DSEF will clearly record the unit costs used as inputs to the cost calculations, to allow updating of estimates if additional cost data become available.

12. KNOWLEDGE MANAGEMENT

Section 4.2.4 of the UFD R&D Roadmap (FCR&D, 2011) describes Knowledge Management as applied to UFD as follows:

> The collection, categorization, and dissemination of information regarding disposal system performance is essential as the U.S. embarks on the investigation of a variety of potential geologic media and repository concepts for the disposal of SNF and HLW that could be generated under advanced fuel cycles.

This applies to the U.S. program in that both a range of geologic environments and also a range of potential future nuclear fuel cycles and associated waste streams are being investigated.

In this chapter, we discuss the various levels of knowledge management within DOE-NE/UFD, and provide information on what role a LLNL knowledge management system has with respect to DSEF.

12.1 LEVELS OF KNOWLEDGE MANAGEMENT

There is a hierarchy of knowledge management systems. At the highest level, the DOE-NE knowledge management system (which was discussed at the October 2010 PI meeting) is still being developed, and will subsequently be populated. The team at LLNL is supportive of this NE-wide repository of information.

Below the NE-wide knowledge management system is the INL document management system. Here, controlled documents, records and a library are available for the various Fuel Cycle Technology (FCT) campaigns. The INL system was created (and is maintained) in accordance with the DOE-NE-FCT QA program.

The UFD campaign-specific knowledge management system is SharePoint, managed by SNL. This resource is very similar to the YMP SharePoint created by SNL for sharing program documents, results and records. While useful, this system requires the researcher to be on-line and logged in with a secure account. The structure and population of the SNL UFD SharePoint system are still under development. The SNL UFD SharePoint knowledge management system is related (but not identical) to the UFD-Natural Barrier System

knowledge management system, which is currently proposed by the NBS team within UFD and which may be more of a database than a collection of documents.

Each individual National Laboratory participant houses a reference collection, which contain archived material, journal articles, books, notebooks, reports etc. There is a certain degree of overlap between each Laboratory's libraries, but the material is available without a network connection and without log-in credentials, day and night. The material is also readily shared between National Laboratory partners. In some cases the material is electronic, in other cases it is a hard copy. This is where the DSEF knowledge management tool fits within the framework. Similar to the UFDC specific level, the YMP had a formal system of documents and records, and their system is still available to some degree through the DOE office of legacy management, where we have successfully obtained source files of DTNs and files from AMRs for use, in addition to highly valuable lessons learned material.

12.2 LLNL DSEF-SPECIFIC KNOWLEDGE MANAGEMENT

The DSEF is designed to be a flexible systematic analysis and knowledge-management framework for evaluation of disposal system options for a wide range of potential future nuclear fuel cycles and used fuel disposition alternatives (see Figure 12.2-1 taken from Blink et al. 2011, and the DSEF Architecture diagram, Figure 2.1-1). The *Excel* worksheets serve as a user-friendly data entry and retrieval system, and the *Access* database is used for generation of status reports and gap analyses. The *Access* database also serves as a query tool for data mining and extraction of specific technical information stored within DSEF.

This knowledge-management framework also serves as a valuable communication tool for the community of producers and users of knowledge. Figure 2.1-1, the DSEF Interface Architecture diagram shows how other Office of Fuel Cycle Technology (OFCT) campaigns interface with DSEF in its knowledge-management role.

The DSEF will: (1) facilitate integration of UFDC process and system models and data, (2) enhance the UFDC interface with other OFCT elements (see Figure 12-2 taken from Blink et al. 2011), and (3) provide rapid response capability to address information requests from DOE or other organizations. The DSEF will establish a UFDC knowledge management system to organize high-level information, data, and assumptions, thereby facilitating consistency in high-level system simulation and economic analyses.

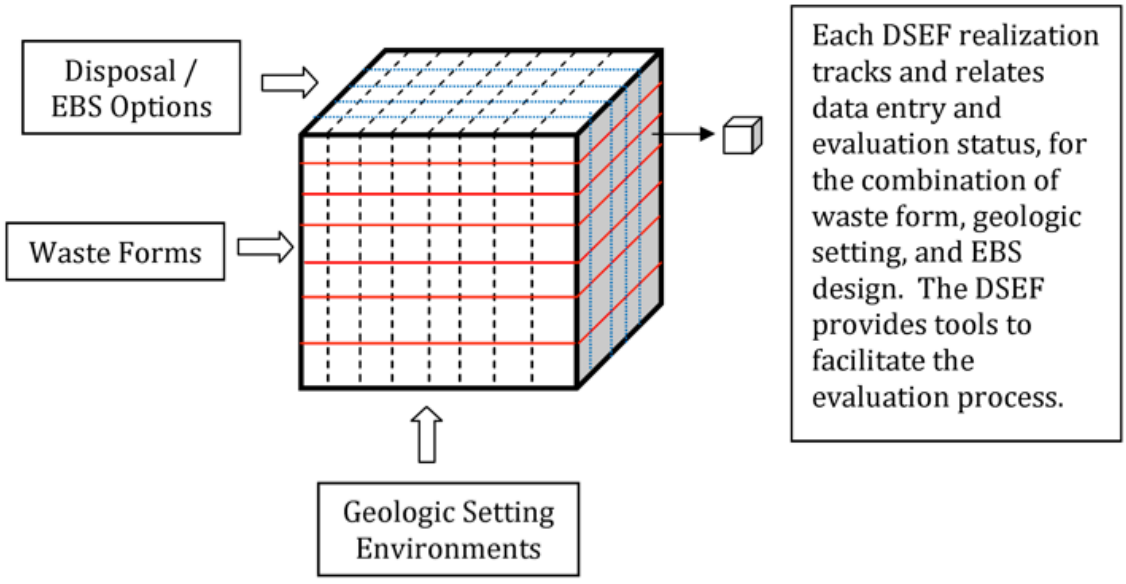

Figure 12.2-1 The DSEF addresses combinations of waste form, geologic setting, and repository design

The material properties assembled to define the geologic settings shown in Figure 12.2-1 were described in Section 11. The knowledge management aspect of that data assemblage provides for the traceability of the data and references used to populate the *Excel* worksheets containing those material properties.

Specifically, where a reference provides a table of properties, which is then cited as a primary reference, where possible that reference will be readily accessible, and hyperlinked to the worksheet if it is available in electronic form. If the primary reference assembled the data and cited secondary references as the original source of the data, the full citation to the secondary reference will also be included in the DSEF worksheets. In this manner the traceability of the numbers used in analysis can be clearly tied to the original sources of the data.

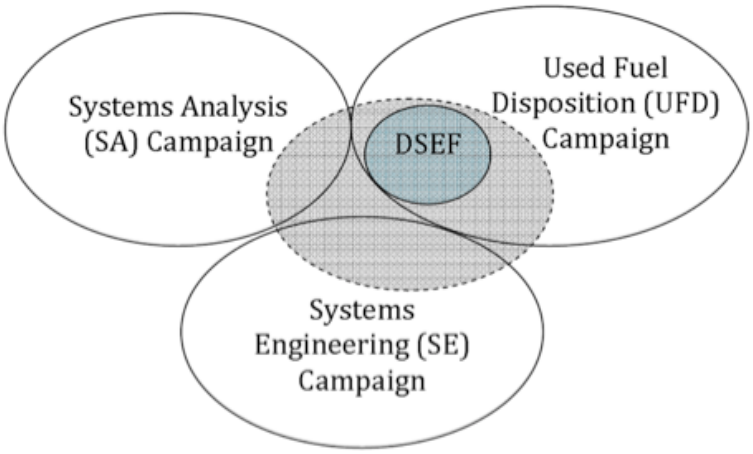

Figure 12-2 The relationship between DSEF and the SA, SE, and UFD campaigns

13. FUEL CYCLE SYSTEM IMPACTS

As a framework for integrating the technical behavior of waste streams in differing disposal pathways, the DSEF is designed to serve as part of the waste management interface with the rest of the fuel cycle. In this role, it is intended to make the DSEF compatible with the information flows and the other models used in other parts of fuel cycle analysis, and to enable iterative analysis between disposal impacts and the rest of the nuclear fuel cycle.

The FCT Systems Analysis campaign serves the function of integrating models and analyses across the entire fuel cycle, and maintains interfaces with the various technical parts that comprise a complete fuel cycle, and builds and utilizes fuel cycle system models. Systems Analysis employs a "model hierarchy" as shown in Figure 13-1. In this hierarchy, fundamental process models form the base layers and are owned, developed and used by the technology R&D campaigns. In UFD, these would include process models such disposal environment thermal-hydrology, corrosion, waste form dissolution, radionuclide migration, etc. The middle portion of the hierarchy contains models for fuel cycle wide material flows (FIT) and dynamic nuclear energy facility evolution (VISION), and energy supply and demand models are at the top.

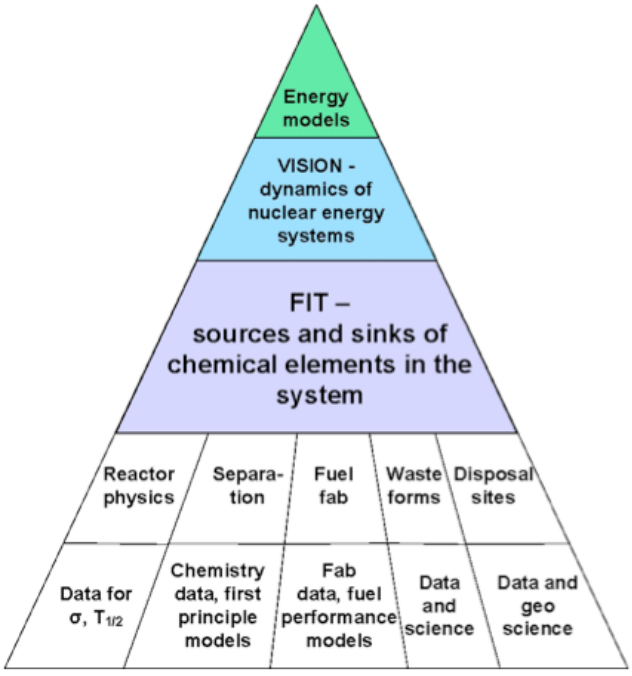

Figure 13-1 Hierarchy of nuclear fuel cycle models

The role of the DSEF in this hierarchy includes integration of certain process models within the UFD campaign at the 'lower-right' corner of the hierarchy, connection to waste form models from the Waste Form and Separations campaign, and connection to the material flow models at the 'middle-right' edge.

Another interface for the DSEF development is with FCT Systems Engineering, where there is an ongoing activity to build a catalog of potential fuel cycles and their characteristics. Eventually, this catalog could be both a source of waste stream information and a place for DSEF to feed back disposal consequences to the rest of the nuclear energy enterprise. An example fuel cycle summary flows being developed for this catalog is shown in Figure 13-2 for the LWR once-through fuel cycle. The DSEF should be able to continue this flow into specific disposal pathways for the waste stream, and provide feedback on disposal implication.

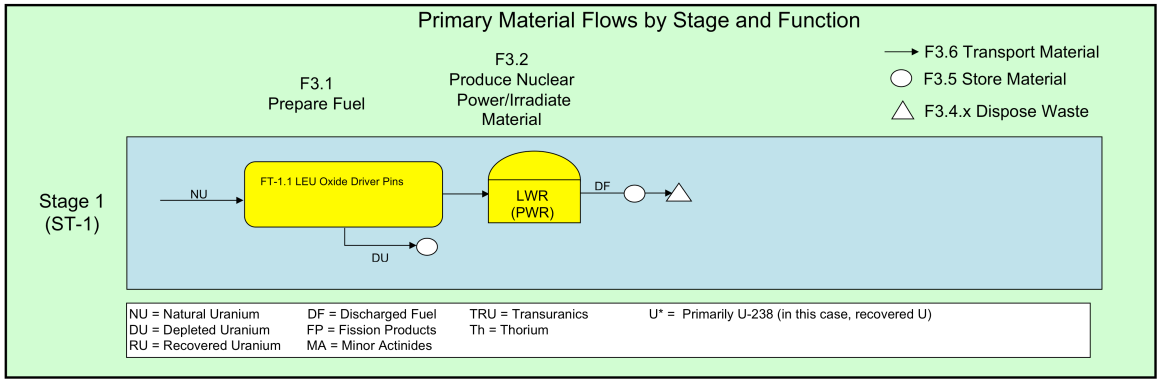

Figure 13-2 Systems Engineering Catalog - Fuel Cycle O-T/R.1 PWR UOX – Once-through

Also, in the recently completed Systems Engineering "Initial Screening of Fuel Cycle Options" [Sevougian et al 2011], the disposal aspects of the fuel cycle were represented parametrically, without specific disposal pathways being considered or technologies evaluated. In future screenings, it is desired to be able to include more specific disposal behaviors tied to waste streams and disposal alternatives. This could be enabled through DSEF analysis.

14. SUMMARY OF CURRENT STATUS AND LOOK AHEAD

DSEF work is expected to continue through FY11 into FY12.

14.1 CURRENT STATUS

At the present time, significant progress has been made in the thermal modeling of materials of various geometries. The structure of DSEF, the flow of information within worksheets of the DSEF workbook, and the flow of information in and out of DSEF have been designed and evaluated. Information on waste form properties (including heat) have been gathered and analyzed, and design constraints are being evaluated.

14.2 LOOKING AHEAD IN FY11 AND FY12

In the remainder of FY11, we plan to:

- Complete DSEF structure and prepare initial prototype of DSEF *Excel* workbook(s)
- Talk to potential users and define requirements for *Access* database
- Finish populating *Thermal Properties* worksheets and develop representative repository thermal parameters for use in thermal calculations
- Run initial realizations for thermal analyses of repository design, waste form, and decay/storage option cases coordinating with the Repository Science / Thermal Load Management / Design Concepts work packages

For FY12, we plan to:

- Continue to assemble and populate realizations of DSEF worksheets for different evaluations
- Update DSEF *Excel* worksheet operation and capabilities based on user feedback and capability requests
- Develop specification for and prototype of the DSEF *Access* database

- In a deliverable report, document the validation of the DSEF software model using YMP and WIPP data and compare to other work package results, e.g., GDSE, THMC, Thermal Management, etc.
- Run realizations utilizing priority configurations from the R&D Roadmap.

15. RECOMMENDED AREAS OF INTERNATIONAL COLLABORATION AND PARTICIPATION

At a level more comprehensive than the EBS work package, LLNL has provided the UFD International Collaboration Coordinator (Jens Birkholzer) with information pertaining to current LLNL international collaborations in the nuclear waste area and a suggested new collaboration.

This area will be developed for the September 2011 LLNL deliverable in the EBS work package. Particular emphasis will be placed on identifying potential collaborations in the areas of thermal performance and stability and longevity of engineered components including canisters and buffer materials.

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