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Disposal Systems Evaluations and Tool Development - Engineered Barrier System Evaluation (Work Package LL1015080425)

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Used Fuel Disposition Campaign

Disposal Systems Evaluations and Tool Development – Engineered Barrier System Evaluation (Work Package LL1015080425)

Milestone M4508042501 (MS Level 4, QRL 3)

Mid FY Progress Report on Evaluation of EBS

Lawrence Livermore National Laboratory

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Introduction

This document is the cited LLNL Level 4 milestone shown in the FCPICS planning system. It is a summary of LLNL work during the first half of the 2010 fiscal year in this work package.

LLNL worked with Carlos Jove-Colon, the SNL Lead, and other participating organizations on organizing the overall conduct of work in this area, and co-developed the presentation on the work organization to the Used Fuel Disposition Campaign (UFDC) workshop in Albuquerque, January 28-29, 2010. LLNL work in this area is included in the presentation materials which have been posted to the UFDC website maintained by INL.

Subsequent to the workshop, LLNL conducted brainstorming sessions to develop specific tasks that define the scope of the work package as well as to ensure that the LLNL scope was integrated with the scopes of the other organizations in this area. The result of the brainstorming sessions was a recommendation to develop a **Disposal Systems Evaluation Framework (DSEF)**. That recommendation was discussed with colleagues and managers at ANL and SNL, and LLNL was authorized to include an initial description of the DSEF concept in this milestone. The recommendation was also discussed with colleagues at INL in the DOE-NE Fuel Cycle Research and Development (FC-R&D) Systems Analysis Campaign.

A team was formed to begin development of the DSEF. The goal is to have a working prototype that has been exercised on a few examples by the end of the FY. The team initially includes Jim Blink, Tom Buscheck, Bill Halsey, and Tom Wolery at LLNL; Ted Bauer, Jim Cunnane, Tom Cotton (subcontractor), and Mark Nutt at ANL; and Carlos Jove-Colon at

SNL. This milestone is the result of discussions with team members; however, the ANL and SNL team members were not provided the opportunity to review this written milestone due to schedule constraints. It is intended that the review be completed in time for the SNL Level 4 milestone M4508042601, Mid FY10 Progress Report, due April 15, 2010, in work package SN1015080426, Disposal Systems Evaluations and tool Development – Engineered Barrier System Evaluation.

The DSEF is intended 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. This knowledge-management framework will also serve as a valuable communication tool for the community of producers and users of knowledge. The capability to solicit feedback from users is essential; such feedback can, in turn, be used to improve the structuring of information and the manner in which it is presented. Hence, an iterative process is envisioned wherein the DSEF will evolve into a powerful, objective tool supporting decision making.

The DSEF can facilitate integration of UFDC process and system models and data, enhance the UFDC interface with other FC-R&D elements, and provide rapid response capability to address information requests from DOE Management or other organizations such as the Blue Ribbon Commission on America's Nuclear Future (BRC).

Overview of the DSEF

The DSEF will use a logical process for developing one or more disposal system concepts (also referred to as repository system in this report) for any given waste form and geologic setting combination.

In the Features, Events, and Processes (FEPs) group of work packages, there are seven categories of waste forms and eight categories of geologic setting being studied. Each of these categories could be subdivided as studies become more detailed:

- Waste Forms
  - Once-Through Used Fuel: This includes subcategories
    - Commercial Spent Nuclear Fuel (CSNF)-nominal burnup: Uranium (U) & mixed oxide MOX)
    - CSNF-high burnup (U & MOX, >50% burnup without reprocessing, such as in some fusion-fission hybrids)
    - High Temperature Gas Reactor (HTGR) fuel - TRISO/graphite: Large volume, low volumetric heat, and burnup higher than Light Water Reactors LWRs)

    - DOE Spent Nuclear Fuel (DSNF): U metal from N-reactor, and carbides & oxides
  - Borosilicate Glass: This includes subcategories
    - 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/Sr; Mo may be removed to increase glass loading of radionuclides; it has a lower volumetric heat rate
  - Glass Ceramic: This is glass-bonded sodalite from Echem processing of EBR-II, and from potential future Echem processing of oxide fuels
  - Metal Alloy: This includes subcategories
    - 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 and transition metal fission products
  - Advanced Ceramic: An advanced waste form that includes iodine volatilized during chopping, which is then gettered during head-end processing of used fuels
  - Lower Than High Level Waste (LTHLW): Includes Classes A, B, and C, as well as Greater Than Class C (GTCC)
  - Other: Examples include radionuclides removed from other waste forms (e.g., Cs/Sr, I, C), as well as new waste forms such as a salt waste form

- Disposal-System Environments
  - Surface Storage: At reactor, or at centralized sites
  - Near Surface: e.g., LLW disposal sites
  - Mined Hard Rock, Unsaturated Zone (UZ): Tuff or granite, for example
  - Mined Hard Rock, Saturated Zone (SZ): Tuff or granite, for example
  - Mined Salt
  - Mined Clay or Shale
  - Deep Borehole: In Crystalline rock
  - Other: Examples include deep seabed, and carbonates

The DSEF encompasses several decision-support analysis categories (note that the framework can provide links to the corresponding analysis toolkits).

- High-level simulator of waste-isolation performance of the disposal system. This is not a Total System Performance Assessment (TSPA), which will be developed separately. This tool looks at waste hazard durations, regulatory requirements, and existing performance assessments to give a very high-level rough estimate of performance
- Sorter of disposal-system attributes (pros and cons). It is anticipated that the DSEF will be exercised for multiple disposal system concepts for many of the combinations of waste forms and disposal-system environments listed above. Thus, a compilation of pros and cons for each situation will aid in grouping and contrasting various options.

- High-level estimator of disposal-system cost. This will use high-level estimating tools benchmarked to existing detailed cost estimates or actual costs.
- High-level thermal-analysis toolkit to assess geometric requirements (footprint, drift and waste-package spacing) for the disposal system, based on specified thermal criteria (e.g., limits on peak temperatures of engineered components and the near-field). Once a geologic setting and waste form are selected for evaluation, thermal analysis is key to defining potential disposal-system layouts (single level, multi-level, in-drift, horizontal borehole, vertical borehole, deep borehole from the surface, etc.) and EBS concepts (capillary barrier, clay barrier, etc.). Early attention will be focused on the thermal tools (see below).
- High-level assessment of overall system impacts of a disposal concept. The disposal system is one component of the overall fuel cycle. As such, it must interface with other components that may influence the disposal system design requirements. One goal of the DSEF is to integrate with higher-level systems analysis tools being used and developed in the FC-R&D arena (see below).

The DSEF will also 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. This system will likely be housed with the INL-based documentation system. Attention will be given to lessons learned from the systems used at the Waste Isolation Pilot Plant (WIPP) and the Yucca Mountain Project (YMP). Where reference material from other programs (e.g., international) is used or cited, the knowledge-management system will import the reference material directly or refer to it in bibliography form. Alternative data sets (e.g., from other programs) will also be utilized to evaluate their influence on DSEF analyses for given waste form and disposal-system combinations. The knowledge-management system can also be used to maintain the results of DSEF realizations, enabling the comparison and ranking of various waste-form/disposal-system-environment/disposal-system-design options. Finally, the UFDC knowledge-management system will be able to provide a compendium of "templates" that can be utilized, in a labor-efficient fashion, to build parallel DSEF analyses (e.g., "one offs").

The DSEF will not be a stand-alone, push-the-button and wait for the results, item of software. It will use software (probably EXCEL, initially), to guide the team members through a logical process of evaluating combinations of waste-form, disposal-system-environment, and disposal-system design. In later stages, it will utilize software developed in the field of knowledge engineering and knowledge-management systems (Umeki et al. 2009). At certain points in the logical process, the DSEF software will point the evaluator to other software tools to do analyses needed to move the process forward. In the development of the DSEF, we will be mindful to make it no more complex than necessary to evaluate the system being considered. The DSEF will organize and document the work such that multiple realizations for different combinations can be compared and contrasted.

Waste Forms

The DSEF team will develop a catalog of potential waste forms, and will assemble information about waste form and waste package combinations. Waste form parameters include heat/volume ratio, heat/mass ratio, and waste density, as well as the mass and half-lives of the radionuclides in the waste. ANL and LLNL will jointly assemble the information.

This information will interface with the Systems Analysis Campaign "VISION" model of nuclear fuel cycles and material flows, the Separations and Waste Forms Campaign waste stream and waste form descriptions, as well as the Waste Form, EBS, Natural Systems and FEPS work packages in the UFDC.

Geologic Setting

The DSEF team will determine geologic parameters (such as thermal conductivity) for the disposal-system setting that are needed to calculate thermal performance. These parameters will be used to determine (see below) whether a disposal-system concept provides sufficient heat removal to respect temperature limits of the waste form, EBS components, and near-field. The DSEF team will assemble other geologic parameters for each disposal-system setting, which are needed for a rough estimate of disposal-system performance. These parameters include porosity, permeability, and rock composition.

Disposal-System Concept and the EBS

A number of options for disposal-system concept will be considered, including surface storage (prior to disposal, or in some cases, until a short-lived waste form has decayed), near-surface burial (for low hazard, short-lived waste), single or multi-level geologic mined systems, and deep boreholes. EBS emplacement options include large waste packages in drifts, horizontal or vertical borehole emplacement from drifts, and deep boreholes. The barrier options in the EBS include the waste form, cladding, barriers internal to the waste package, the waste package itself, capillary barriers, drip shields, backfill, buffer materials, sorptive materials, and seals above deep boreholes. Further, the size of the waste package (capacity) and the spacing (between waste packages and between drifts or deep boreholes) are a key factor to meeting thermal limits.

The combination of waste form parameters and geologic setting parameters will be used to compile a set of disposal-system design options for that waste form and geologic setting combination. Each option of the set will be treated as a separate realization of the DSEF.

LLNL will develop a thermal-analysis toolkit to perform this evaluation, in a labor- and computationally-efficient fashion, for various geologic media, during FY10 and will refine and apply the tool in FY11. Options that will be evaluated include a simplification of the YMP multiscale model (discretized), the YMP waste emplacement flexibility model (uses analytic solutions to simplified geometries), and the model developed by ANL for GNEP and AFCI. LLNL and Ted Bauer of ANL will develop the thermal toolkit. Initial thoughts on the thermal toolkit are included as Appendix A, below.

The results of the thermal analysis will determine the required disposal-system (e.g., repository) footprint for that waste form (type and quantity) and geologic setting. In turn, the disposal-system footprint and design provide much of the information needed for a high-level cost estimate. LLNL, Tom Cotton (supporting ANL), and Carlos Jove-Colon of SNL will develop the concepts.

A catalog of candidate materials for the engineered barriers will be developed by LLNL. Metals will be evaluated based on an extension of the LLNL Degradation Mode Surveys developed for Yucca Mountain. Other barrier materials (clay, backfill, etc.) will initially use information developed in other repository programs worldwide.

Cost and Performance

Costs of WIPP and cost estimates of YMP will be used to envelop a high-level cost estimate for the barriers and for disposal-system construction, for each option evaluated. LLNL and Carlos Jove-Colon of SNL will develop the cost-estimation component of the DSEF.

An initial selection of included FEPs will be determined from the UFD FEP work package list. The FEP list will be the basis of a preliminary high-level model to be developed jointly by Mark Nutt of ANL and LLNL. This model will be an extension of models developed by ANL for GNEP, ASCI, and other FC-R&D programs during the last several years. The model will consider natural and human-caused initiating events appropriate for the geologic setting. The FEPs will be selected by LLNL, Carlos Jove-Colon of SNL, and Mark Nutt of ANL.

The DSEF team will identify the key impacts of the disposal-system concept on the pre-disposal waste management system, using tools developed by the Systems Analysis Campaign.

LLNL will study the Uncertainty Quantification tools from Stockpile Stewardship, NIF, Climate, ASCEM, etc. for their applicability to the DSEF. This will be accomplished by the middle of FY11.

Siting Criteria

The result of the above steps will be a preliminary set of siting criteria for this geologic setting, waste form, and disposal-system concept. These can be used to iterate through the process with more specific geologic setting information based on generic application of the siting criteria. Here, we define generic as distinguishing between major categories of the same medium, without specifying any particular geographic location.

For a generic disposal-system setting, the ensemble of DSEF evaluations will identify the envelope of waste-form options that could be potentially accommodated. Equally important, the evaluations will identify the envelope of waste-form options that *could not* be potentially accommodated, by the combination of geologic setting, and disposal-system concept.

Metrics

Metrics to be considered during the thought process include cost, performance, and licensability. Pre-disposal system impacts include

- Flexibility with respect to future changes in waste streams
- Range of potential waste forms that could use the disposal-system concept, and geologic setting, evaluated for a single waste form

The metrics will be refined by LLNL and Tom Cotton (supporting ANL).

Interface Between DSEF and Fuel Cycle Systems Models

In addition to providing a framework to organize and integrate disposal-system information within the UFDC, the DSEF should also provide a working interface with other parts of the program, and with the rest of the nuclear energy production system. A primary interface is with the Systems Analysis models for static and dynamic nuclear energy systems (VISION, SLAM, and the hierarchy of model that support them). These models gather mass flow and waste stream information from other elements of the nuclear fuel cycle (fuel fabrication, reactors, separations & waste forms, etc.) for any given nuclear energy system scenario. This provides an avenue for DSEF to receive comprehensive and internally consistent waste stream information for a given nuclear energy scenario. DSEF can then provide feedback to the system and economics models on disposal implications such as storage requirements, disposal alternatives and disposal-system (e.g., repository) size and performance parameters. With a working lineage to the broader system models, DSEF will provide a functional 'back end' capability to evaluate the wide range of disposition alternatives currently under consideration.

DSEF will replace the constrained "YM-like" repository parametric analysis that has been a useful working model for disposal impacts in prior FC-R&D systems analyses. With the broad range of fuel cycle options, and wide variety of disposal pathways alternatives, a simple parametric model is no longer adequate.

A starting list of potential exchange parameters between DSEF and VISION/SLAM include:

Inputs from Systems to DSEF:

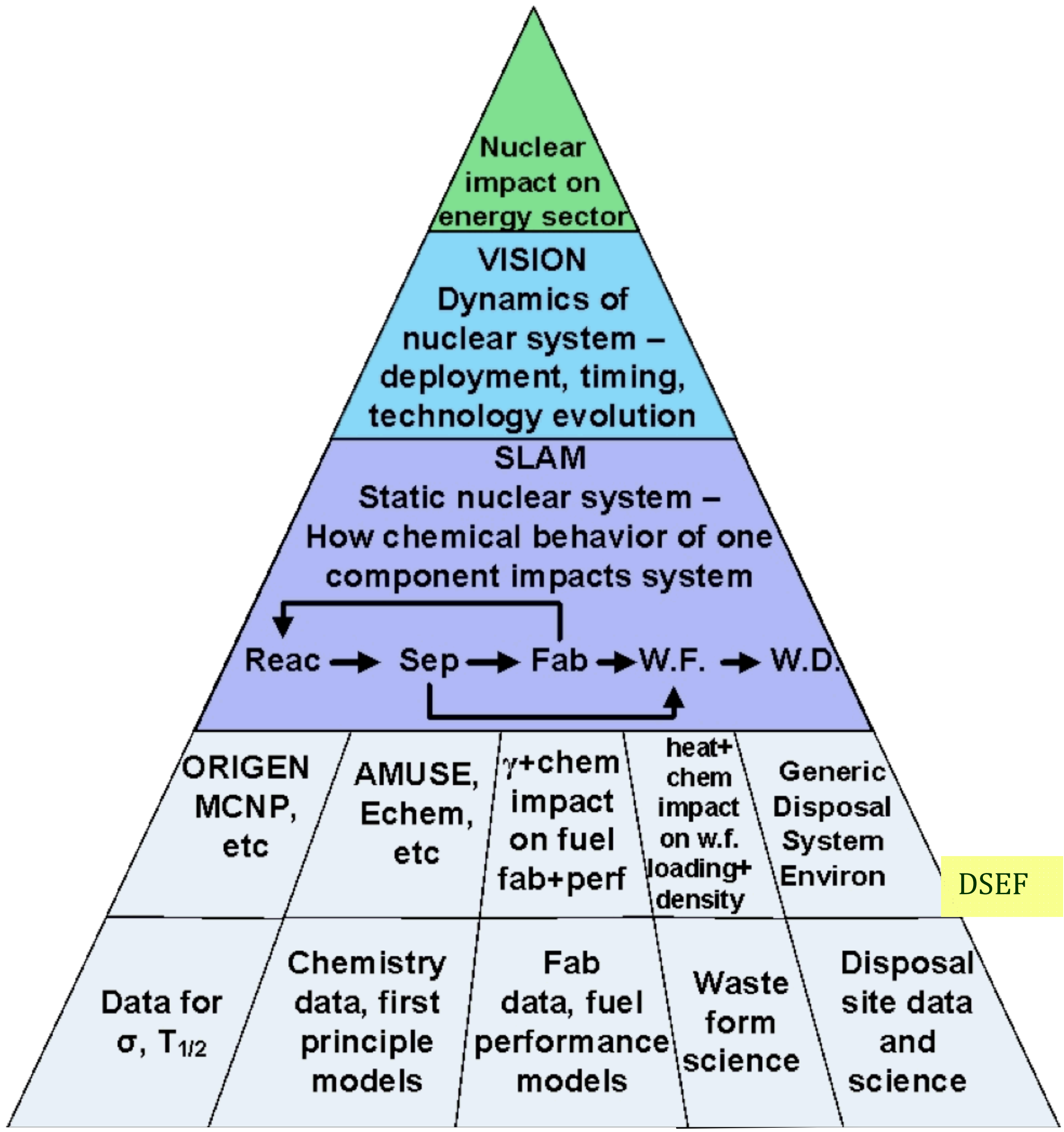
- Waste stream partitions (and alternatives) and normalized mass flows
- Radionuclide content
- Waste forms, characteristics, and alternatives
- Timing relationships

Feedback from DSEF to Systems:

- Waste categorization and potential disposition pathways
- Storage requirements/characteristics
- Disposal alternatives
- Disposal-system characteristics: footprint, drift length, package count, …
- Isolation performance factors

A conceptual mapping of DSEF onto the evolving Systems Model hierarchy is shown in Figure 1. Details of the interface will develop as both DSEF and SLAM evolve.

Figure 1. The Systems Model Hierarchy interface with the DSEF.



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Appendix A: Thermal Analysis Toolkit

A key aspect of evaluating potential used-fuel-disposition (UFD) alternatives is determining space requirements for the engineered barrier system (EBS). While much of the application of this tool will be for geologic disposal systems, it is also intended to address a broader range of disposal-system concepts, such as shallow burial systems and surface-storage facilities. The primary physical constraint in determining the space requirement for a given quantity of used fuel is heat dissipation in the host environment, in conjunction with the thermal criteria of the EBS components and natural barriers. Typically, thermal criteria are expressed as temperature limits; however, they may also include temporal and spatial temperature gradients, if those gradients are steep enough to lead to phenomena detrimental to barrier performance. Heat dissipation primarily depends on the heat source (time dependent, for the used fuel per unit mass or volume), the geometry of the EBS, and the thermal conductivity of the EBS components (e.g., backfill) and host rock. EBS geometry covers a wide range of possibilities, from the simplest geometries, such as the diameter and spacing of deep disposal boreholes, to very complex geometries, such as level spacing; drift diameter, length, and spacing; borehole diameter, length, and spacing; and waste-package diameter and length. If thermal criteria are achieved with margin for a UFD/EBS alternative, it is possible to decrease spacing between the relevant EBS components (e.g., boreholes, emplacement drifts, emplacement boreholes, etc.), which increases the areal density of the used fuel, and is equivalent to reducing the disposal system space requirements.

The Thermal Analysis Toolkit is designed to be a flexible, computationally- and labor-efficient software package to conduct thermal analyses for a wide range of potential UFD/EBS alternatives. In its initial stage of development, one option for this toolkit is to use the thermal-conduction version of the NUFT code (Nitao, 1998), a catalog of EBS concepts, a catalog of thermal properties for the engineered and natural barriers, and a catalog of heat-generation histories for USD alternatives. Another option is to use analytical solution approaches developed in the YMP and elsewhere. Protocols will be established for the importing and reviewing of thermal property and UFD heat-generation-history data. Users will be given the option of specifying their own thermal-property and heat-generation-history input data; however, the preferred approach is to utilize data that has a confirmed pedigree. Within the available range of EBS concepts, the user will be able to specify EBS geometric parameters, such as drift diameter and spacing (both vertical and horizontal), borehole diameter and spacing, etc. Users will initially be given the option of developing additional EBS concepts by utilizing an existing template from the EBS-concept catalog and making revisions specific to the new EBS concept. In a later stage of development, a more flexible mesh-generation capability may be available to facilitate generating new EBS concepts.

The first generation version of the Thermal Analysis Tool will apply the conservative assumption that heat flow in the EBS is dominated by thermal conduction. For geologic disposal, this assumption is reasonably conservative, since convection tends to dissipate temperature buildup, and thermal radiation tends to smooth out variations in the EBS between hotter and cooler regions. The first generation version will focus on geologic disposal. For surface-storage and near-surface burial facilities, it will be necessary to address atmospheric convection, using appropriately selected values of the heat-transfer coefficient, as well as a reasonable means to represent thermal radiation. The first generation version will also assume lateral and longitudinal symmetry, which is to say that lateral and longitudinal heat loss at the edges of the disposal system (e.g., repository edges) is negligible. Thus, this tool will be applicable to the center of the disposal system where temperatures and temperature gradients are highest. The benefit of assuming lateral and longitudinal symmetry is that the 3-D model of the disposal system can be of a representative region, which is infinitely repeated in the plan view.

If necessary, future generations of the Thermal Analysis Tool could address the influence of thermal convection in a fashion similar to that applied in the Multiscale Thermohydrologic Model (Buscheck et al. 2006). Application of the Multiscale Thermohydrologic Model methodology also allows for relaxing the assumption about lateral and longitudinal symmetry.

The NUFT option for the first generation version of the Thermal Analysis Toolkit will consist of three software modules:

1. **Thermal-Analysis Pre-Processor:** This script (possibly written in MATLAB) reads in (1) the user-selected EBS concept from the EBS-Concept catalog, (2) the user-specified geometric parameters for the EBS concept of interest, and (3) the user-selected thermal properties from the Thermal-Property catalog or user-specified thermal properties, and generates the input file for the thermal-analysis simulator (e.g., NUFT code).
2. **Thermal-Analysis Simulator:** Utilizing the thermal-conduction version of the NUFT code and an input file generated by the thermal-analysis pre-processor, this

simulator generates temperature output wherever thermal criteria are specified (e.g., waste-package surface).

3. **Thermal-Analysis Post-Processor:** Applying user-specified thermal criteria, this processor determines whether (or when and where) thermal criteria are exceeded.