

# FCT Quality Assurance Program Document

## Appendix E FCT Document Cover Sheet

Name/Title of Deliverable/Milestone: Beta Version of UNF Database  
 Work Package Title and Number: UNF Data and M&S Toolset Development and Demonstration – ORNL FT-13OR091406  
 Work Package WBS Number: 1.02.09.14  
 Responsible Work Package Manager: John Scaglione **John M. Scaglione**  
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 Date: 2012.12.21 14:36:16 -05'00'  
 Date Submitted: 12/21/2012

Quality Rigor Level for Deliverable/Milestone	<input type="checkbox"/> QRL-3	<input type="checkbox"/> QRL-2	<input type="checkbox"/> QRL-1 <input type="checkbox"/> Nuclear Data	<input checked="" type="checkbox"/> N/A*
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# FCT Quality Assurance Program Document

## Appendix E FCT Document Cover Sheet

Name/Title of Deliverable/Milestone Complete Initial Version of UNF M&S Toolset  
 Work Package Title and Number UNF Data and M&S Toolset Development and Demonstration –  
ORNL FT-13OR091406  
 Work Package WBS Number 1.02.09.14  
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Date Submitted 12/21/2012

Quality Rigor Level for Deliverable/Milestone	<input type="checkbox"/> QRL-3	<input type="checkbox"/> QRL-2	<input type="checkbox"/> QRL-1 <input type="checkbox"/> Nuclear Data	<input checked="" type="checkbox"/> N/A*
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Rob Howard

Peer Review

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## EXECUTIVE SUMMARY

This report documents work performed supporting the Department of Energy (DOE) Office of Nuclear Energy (NE) Fuel Cycle Technologies Nuclear Fuel Storage and Transportation (NFST) Planning Project under work breakdown structure element 1.02.09.14, CX *Used Nuclear Fuel Assessment Capabilities*. In particular, this report documents completion of the M2 milestone M2FT-13OR0914066, *Complete Initial Version of UNF M&S Toolset*, and the M4 milestone M4FT-13OR0914065, *Beta version of UNF database* within work package FT-13OR091406 – UNF Data and M&S Toolset Development and Demonstration. Both of these milestones represent components within an integrated computational framework that automates nuclear safety evaluations for discharged commercial nuclear fuel assemblies for individual assembly evaluations and cask-specific evaluations.

A centralized, comprehensive, and integrated data and analysis tool system is being developed to facilitate modeling and analysis capabilities for existing storage and transportation cask systems. The analysis system is referred to as the used nuclear fuel (UNF) Integrated Data, Experiments, and Analysis System (IDEAS). Initial work documented in this report is focused on building the system infrastructure and integrating existing data and analysis capabilities that form the nucleus of UNF-IDEAS. The nucleus is referred to as the UNF modeling and simulation (M&S) System, which provides key technical data and analysis capabilities for demonstrating compliance with regulatory requirements and assessing technical issues related to the aging and safety of discharged nuclear fuel.

The UNF database and the M&S toolset are developed simultaneously in a consistent manner. Technical data collection and its synthesis into appropriate formats are based on the SCALE and COBRA-SFS input requirements for depletion, criticality, and thermal analysis. Model templates for the computer codes utilize fuel assembly and storage cask information from the UNF database. A set of matrices illustrating existing UNF M&S System status and completion percentages is presented in Appendix B.

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# Nuclear Fuel Storage and Transportation Planning Project

## *Used Nuclear Fuel Modeling and Simulation System*

### 1. INTRODUCTION

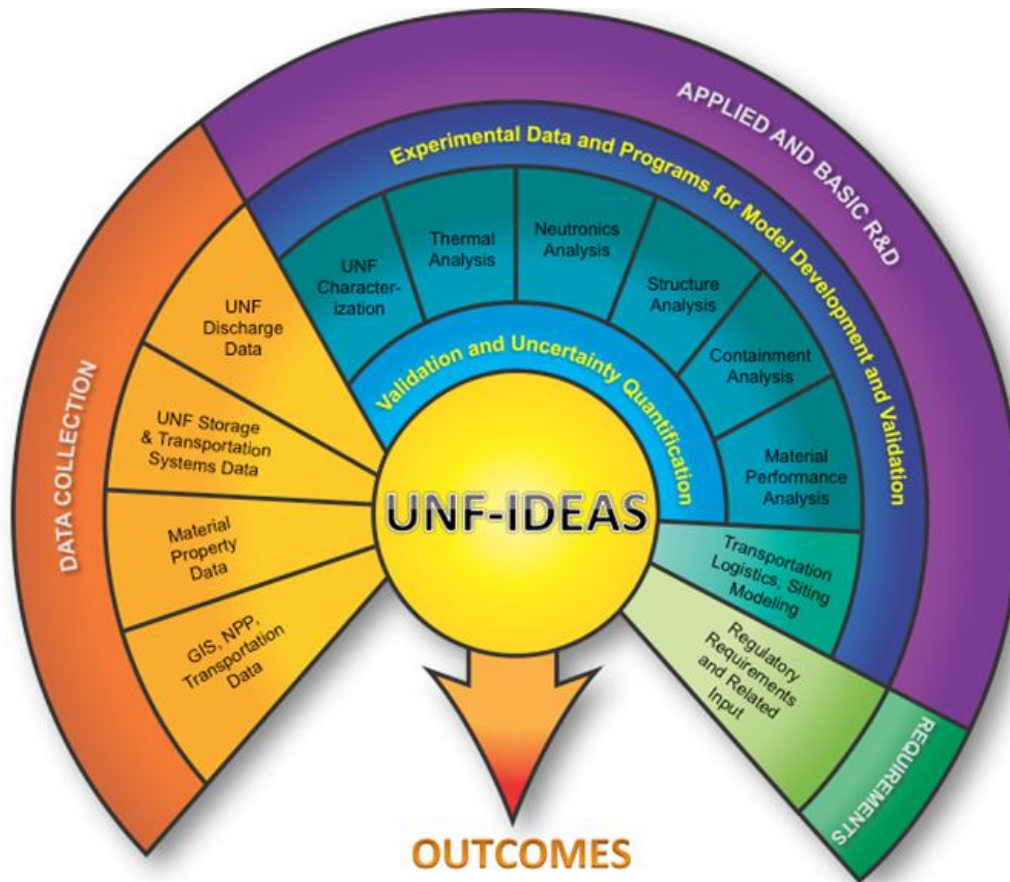
Used nuclear fuel (UNF) is expected to be stored at reactor sites for longer time intervals than originally foreseen. Extended storage over long periods of time may affect the integrity of important-to-safety structures, systems, and components (SSCs), thus potentially compromising the safety of fuel storage units. Current dry cask licensing experience has been based on the use of conservative modeling approximations and UNF assemblies with an average burnup up to 45 GWd/MTU to meet relatively short storage periods where temporal effects on material properties could be justified as relatively negligible. As documented in the *Gap Analysis to Support Extended Storage of Used Nuclear Fuel* [1], the ability of the SSCs to continue to meet safety functions over extended times and for subsequent transportation must be maintained and demonstrated. Uncertainties associated with the physical characteristics of the fuel assemblies at discharge will necessarily propagate and compound with increased storage times resulting in increases in UNF shipping, handling, and disposal costs. For most SSCs important to safety, additional data are required, often because there are limited data on new materials used in more modern fuel assemblies or dry storage cask systems, or because the effects of high burnup and extended storage are not fully known.

The key storage and transportation safety functions and gaps identified in Ref. [1] span many different technical disciplines. As indicated in *Used Nuclear Fuel Storage and Transportation Research, Development, and Demonstration Plan* [2], addressing these functions requires a number of different modeling and simulation (M&S) and experimental efforts. To address the technical issues associated with UNF storage, transportation, and disposal and to generate the technical data to support licensing and periodic relicensing activities in a timely and cost-effective manner, a centralized system is being developed that provides a predictive simulation capability and uncertainty quantification to enable extrapolation of results to extended storage timeframes. The centralized system is illustrated in Figure 1, and is known as the UNF Integrated Data, Experiments, and Analysis System (UNF-IDEAS). UNF-IDEAS will ensure that individual efforts are integrated and coordinated to accomplish the Department of Energy (DOE) Office of Nuclear Energy (NE) Fuel Cycle Technologies Nuclear Fuel Storage and Transportation (NFST) Planning Project and Used Fuel Disposition Campaign (UFDC) goals, identify and prioritize data and analysis needs based on impact to safety margins, inform future experimental demonstration programs to maximize return on investment, as well as establish an invaluable UNF archive.

The work documented in this report is focused on establishing the system infrastructure and integrating existing data and analysis capabilities forming the nucleus of UNF-IDEAS. The nucleus of UNF-IDEAS is referred to as the UNF M&S system throughout the remainder of this report and has been developed with the capability to completely automate depletion, criticality, and thermal analyses using fuel depletion conditions that are either bounding or nominal with respect to criticality/thermal analyses. In addition, the automation tool has been designed to perform either: (1) a fast-running but moderately-accurate depletion calculation using fuel assembly design and irradiation history data representative of generic assembly classes, or (2) a highly-accurate but slower-running depletion calculation using detailed fuel assembly-specific design and irradiation history data.



The current components of the UNF M&S system are hosted on an ORNL server (Jupiter) and results interrogation capability is provided through a separate application that will be transitioned to a web portal or other public access system.



**Figure 1. Illustration of UNF-IDEAS.**

A comprehensive, centralized UNF database and associated documentation are key components of the UNF M&S System. Currently, the initial version of the UNF M&S toolset consists of the following components:

- a centralized database containing technical information about discharged commercial UNF, as of December 2002, [3] fuel assembly design and operating parameters collected from publicly available documents such as *Characteristics of Spent Fuel, High-Level waste, and other Radioactive Wastes which may Require Long-Term Isolation* [4] and commercial reactor criticality data summary reports (e.g., Ref. [5]), cask loading patterns for use as inputs to the various safety analyses;
- established computer codes for depletion, criticality, and thermal calculations;
- a collection of fuel assembly and cask model templates for depletion, criticality, and thermal calculations;

- a collection of cross-section libraries representative of assembly types for fast depletion calculations;
- a computer code that has the capabilities to automate model development for depletion, criticality, and thermal calculations, execute the nuclear safety analysis codes, and provide the calculation results (e.g., nuclide concentration values, the effective neutron multiplication factor  $k_{eff}$  for a spent fuel storage cask, and temperature distribution for a spent fuel storage/transport cask).

## 2. UNF M&S System

The centralized database and the M&S automation tool are developed simultaneously in a consistent manner. The purpose of the M&S automation tool is to streamline nuclear safety evaluations for discharged commercial nuclear fuel assemblies using UNF technical data and model templates from an integrated UNF database. Initial development capabilities have been focused on neutronics analyses and thermal analyses. A collection of model templates for computer codes dedicated to out-of-reactor nuclear safety analyses (i.e., depletion, criticality, and thermal analyses) is being developed for each of the commercial reactor sites. Technical data collection and its synthesis into appropriate formats are based on the well-established Standardized Computer Analysis for Licensing Evaluation (SCALE) code system [6] and the thermal-hydraulic analysis code COolant Boiling in Rod Arrays–Spent Fuel Storage (COBRA–SFS) [7] input requirements. The schematic of the UNF M&S System is illustrated in Figure 2.

As illustrated in Figure 2, model templates for depletion, criticality, and thermal analyses utilize fuel assembly and storage cask information from the UNF database. Depletion calculations predict nuclide concentrations in irradiated fuel and associated radiation and decay heat source terms, which are used as part of the input to subsequent criticality and thermal calculations, respectively. The resultant outputs are rolled back into the database for subsequent use and processing to support various data analyses that can be applied to inform decision making across the UNF management system. The executable and supporting data files for SCALE and COBRA–SFS are integrated into the UNF M&S System.

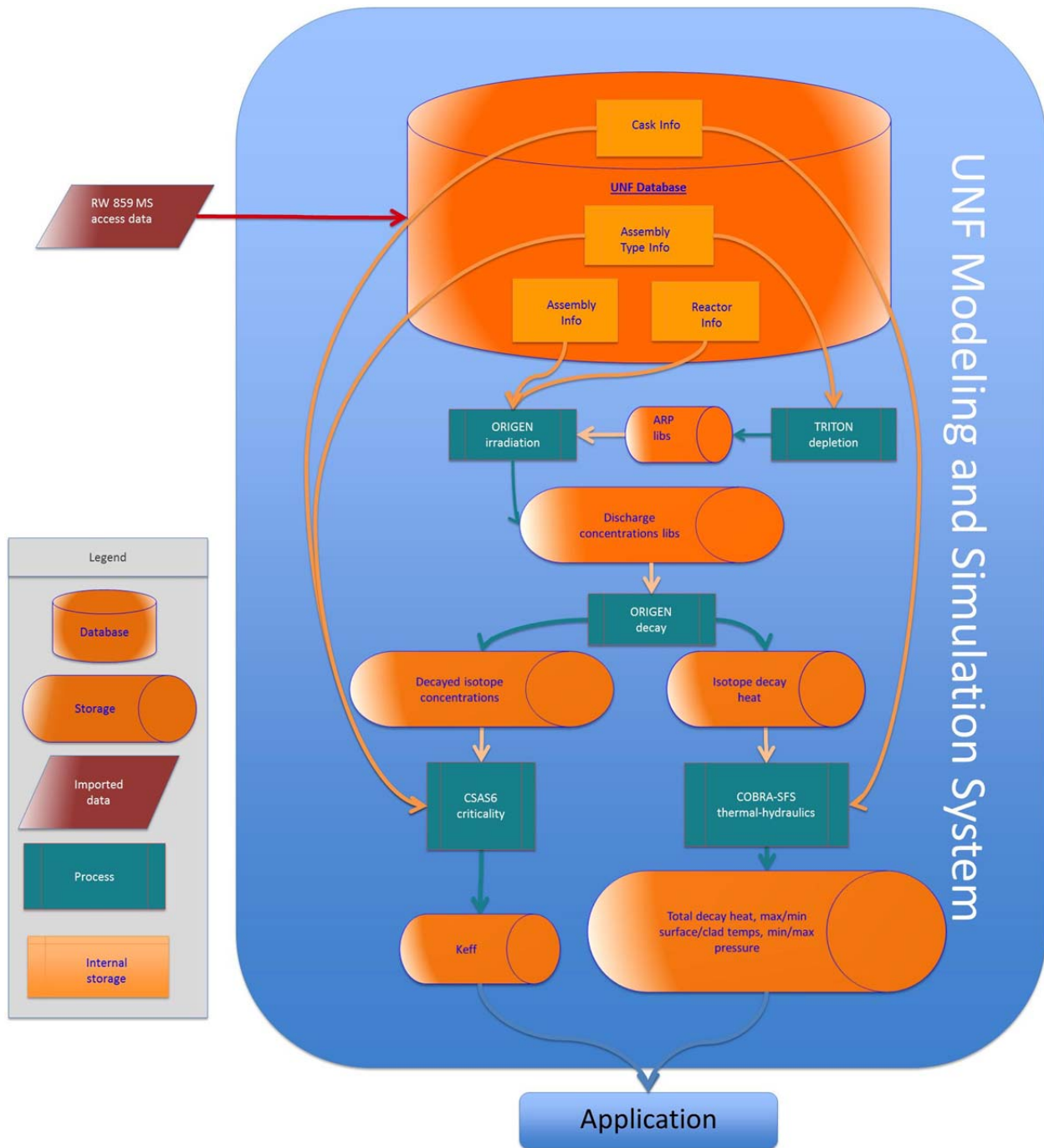


Figure 2. Schematic of UNF Modeling and Simulation System

## 2.1 UNF Database

The UNF database is an electronic database that functions within the UNF M&S System. It is continuously updated as new information becomes available and new analyses are completed. The

purpose of the database is to supply all the technical data identified as input parameters to the various safety analyses including cask loading patterns, assembly design characteristics, initial enrichment, final burnup, initial uranium content, discharge date, and reactor- and cycle-specific data. It also serves as a repository for all computational analysis results that can be used for various analyses of actual UNF and cask characteristics. There are four primary types of M&S tool input data in the UNF database: (1) data originating from the RW/GC-859 database, currently consisting of the RW-859 fuel assembly discharge information from Ref. [3]; (2) fuel assembly design data (e.g., technical data collected from Ref. [8]); (3) reactor-specific operation data; and (4) cask design and loading data. M&S tool output data is also stored within the UNF database once it has completed processing.

The centralized database is organized in Structured Query Language (SQL) relational database tables that store the various data. Appropriate relationships among the variables in the SQL data tables have been implemented so that all the relevant parameters are automatically made available for use in a safety analysis, based on the analysis type, reactor identifier, assembly type, and cask type. Technical data source traceability is being documented in PDF files, which were included in the database and linked to the corresponding SQL data tables.

### **2.1.1 Cask Data**

As of January 2011, 90 facilities have placed used fuel in dry storage [9] using a variety of casks with different loading capacities. Cask data consists of cask design data (i.e., cask geometry configuration, materials of construction, and design dimensions), which typically is provided in safety analysis reports for spent fuel dry storage systems, and cask loading data (i.e., cask loading patterns and component loading), which is specific to a storage facility and is not readily available. Currently within the database the cask design information is built into the KENO-VI and COBRA model templates and is not viewable unless reading the input files. General cask information including general dimensions, gross weight, and design basis licensed information is being collected for inclusion in the UNF database for general information purposes and will be available in a subsequent update to the UNF database. The only cask loading pattern information that is available as of December 2012 within the database is for Maine Yankee. Loading information for Brown's Ferry, Sequoyah, Catawba, and McGuire nuclear plants as well as for the ISFSIs at the sites of the decommissioned reactors Connecticut Yankee and Yankee Rowe will be incorporated in FY 2013.

### **2.1.2 RW-859 Data**

The most recent nuclear fuel discharge and storage data covers UNF discharged from commercial reactors as of December 31, 2002 [3]. These data, referred to as the RW-859 database, contain basic discharge information for 70,292 PWR UNF assemblies and 93,351 boiling water reactor (BWR) assemblies. The UNF assemblies in the RW-859 database are categorized into assembly classes based on assembly outside dimensions, which are further subdivided by assembly type for a total of 134 individual fuel assembly types discharged from both U.S. PWRs and BWRs as of December 31, 2002 [10]. Currently, the data collection authorization is under the auspices of the U.S. DOE Office of the General Counsel and the nuclear data survey has been redesignated as Form GC-859. This data has been provided as a Microsoft Access database. The information from the database has been imported into the the UNF database to work within the UNF M&S System as illustrated in Figure 2.

UNF discharge data available in the RW-859 database for use in the UNF M&S System include:

- reactor and fuel assembly identifiers;
- assembly type;
- initial  $^{235}\text{U}$  enrichment;
- initial uranium content;
- assembly discharge burnup;
- reactor cycle corresponding to assembly discharge; and
- reactor cycle start and end dates.

Fuel assembly initial enrichment, final burnup, and discharge date are essential parameters for determining nuclide concentrations and associated source terms. However, these parameters are insufficient for modeling purposes because a depletion calculation model requires far more input parameters (e.g., fuel pin dimensions, fuel temperature and specific power, moderator density and temperature, etc.). Therefore, technical data beyond that available in the RW-859 database, including basic fuel assembly and reactor cycle-specific data, has been collected to facilitate model development. These data sets are described in the following subsections.

### 2.1.3 Fuel Assembly Data

Currently, the UNF database contains basic design data for representative fuel assembly types collected from publicly available sources (e.g., Ref. [5]). Assembly design data include:

- assembly array size, rod pitch, and assembly pitch;
- number of guide tubes/water rods and their assembly locations;
- fuel pellet and clad dimensions;
- assembly reactivity control components;
- design dimensions for assembly guide tube, instrument tube, water rod, or assembly channel;
- design dimensions for burnable poison and control rods; and
- construction materials.

It is expected that the current data will be supplemented in the future as additional detailed assembly-specific information becomes available.

### 2.1.4 Reactor Data

Limited cycle-specific data for selected reactors is available within the database. Most was primarily taken from commercial reactor criticality data summary reports (e.g. Refs. [5], [11] [12]). These data include:

- cycle specific burnup;
- soluble boron concentration as a function of time;
- control rod insertion history;
- batch loadings;
- axial burnup profiles; and
- moderator temperature.

Additional reactor cycle-specific data is expected to be provided by the nuclear industry for operational or decommissioned U.S. commercial nuclear reactors and uploaded into the database. Currently, reactor operating data from Maine Yankee is available in the database. Other data is currently being processed for upload into the database and will be available in a future update. This data includes operating history information for the Sequoyah Nuclear Plant, Units 1 and 2, Watts Bar Nuclear Plant Unit 1, Connecticut Yankee, Yankee Rowe, V.C. Summer, and the Duke Energy plants to name a few.

### 2.1.5 Surrogate Data

Some of the depletion modeling parameters are not directly available and need to be derived from the available technical data. These modeling parameters are referred to as surrogate data. An example of such a modeling parameter is assembly average specific power. This parameter is assembly- and irradiation-cycle specific and is typically calculated as the assembly burnup for an irradiation cycle divided by the cycle length. However, the current RW-859 database does not provide end-of-cycle assembly burnup values for use in specific power calculations. Only assembly final burnup and the assembly discharge cycle are available from the database. Therefore, an assumption has been made concerning the number of cycles in which a fuel assembly has been irradiated. It has been assumed that an assembly with a final burnup smaller than 30 GWd/MTU has been irradiated for two consecutive cycles and an assembly with a final burnup greater than 30 GWd/MTU has been irradiated for three consecutive cycles. This assumption is used to calculate irradiation time and specific power for assembly-specific depletion calculations. The impact of this assumption on the cask  $k_{eff}$  values is considered to be small based on the results of previous parametric studies (Refs. [13] and [14]), however the impact on source terms and thermal analyses could be more significant but would be dependent on the decay time.

### 2.1.6 ARP Cross-section Libraries

Due to the large number of discharged fuel assemblies and axially varying burnup, a fast-running depletion calculation method using pre-generated problem-specific cross-section libraries is used to enable the numerous depletion calculations required for analysis purposes. For comparison, an ORIGEN depletion calculation using pre-generated cross sections requires less than a minute of computer time per assembly, whereas a detailed TRITON depletion calculation for the same assembly may require up to two days of computer time using a single processor. The fast-running method is slightly less accurate than the highly-accurate but slower-running TRITON depletion calculation method. As more detailed assembly-specific technical information is incorporated into the database, detailed TRITON depletion analyses can be completed as needed. The results of the detailed depletion analyses will also be retained within the database and used for specific assembly characterization.

As previously described, the RW-859 data base provides the commercial UNF inventory as of 2002. The UNF assemblies are categorized into assembly classes which are further subdivided by assembly type for a total of 134 individual fuel types. The majority of the fuel types within a given class have similar



characteristics that can be represented by a fuel type within that class. For example, the CE Fort Calhoun assembly types XFC14A, XFC14C, and XFC14W, and the generic CE 14×14 assembly type (CE1414C) differ primarily with respect to assembly length. These assembly types have the same pellet diameter, rod diameter, rod pitch, and clad material, that is, the two-dimensional representations of these assemblies are identical and can be represented by the CE1414C assembly type. Therefore, ARP cross-section libraries are generated for representative assemblies within assembly classes or specific reactors as described in Table 1 through Table 4.

ARP cross-section library interpolation parameters are fuel initial enrichment, fuel burnup, and moderator density. The initial enrichment and moderator density values and the burnup range to be used in the ARP cross-section library generation process are provided in Table 5. Two sets of ARP cross-section libraries were generated, one set using nominal (i.e., average) operating parameters and the other set using operating parameters that are bounding with respect to criticality analyses. Depletion parameters for nominal analyses are calculated as the average values of reactor-specific operating data available in the centralized database. Bounding depletion parameters for criticality analyses are parameters that increase discharged fuel reactivity. For bounding criticality analyses, decreased moderator density than typical values, higher fuel and moderator temperatures than typical values, burnable absorber rod insertion, and a constant soluble boron concentration (e.g., 1000 ppm) throughout the irradiation time period for PWR assemblies (see Table 6) increase discharge fuel reactivity (Refs. [13] and [14]). These parameters harden the neutron spectrum, which in effect reduces the utilization of initial  $^{235}\text{U}$  fissile material and generates higher actinide nuclide concentrations. The burnup profiles presented in Table 7, which have been previously demonstrated to be bounding with respect to criticality (Refs. [15] and [16]), are used to calculate nuclide concentrations for bounding criticality analyses. A nominal burnup profile is based on average burnup values for fuel axial zones provided in an axial burnup profile database (e.g., Ref. [17]). For thermal analyses, a pointed axial burnup profile is more conservative than a flat axial burnup profile.

**Table 1. ARP libraries for PWR generic assembly classes**

Generic assembly class	Array size	Version	Assembly type	Representative assembly type
B&W 15×15	15×15	B&W Mark B	B1515B	B1515B4
	15×15	B&W Mark B10	B1515B10	
	15×15	B&W Mark B3	B1515B3	
	15×15	B&W Mark B4	B1515B4	
	15×15	B&W Mark B4Z	B1515B4Z	
	15×15	B&W Mark B5	B1515B5	
	15×15	B&W Mark B5Z	B1515B5Z	
	15×15	B&W Mark B6	B1515B6	
	15×15	B&W Mark B7	B1515B7	
	15×15	B&W Mark B8	B1515B8	
	15×15	B&W Mark B9	B1515B9	
	15×15	B&W Mark BGD	B1515BGD	
	15×15	B&W Mark BZ	B1515BZ	
	15×15	W	B1515W	
	CE 14×14	14×14	ANF	
14×14		CE	C1414C <sup>a</sup>	
14×14		W	C1414W	
14×14		CE	XFC14A <sup>a</sup>	
14×14		CE	XFC14C <sup>a</sup>	
14×14		CE	XFC14W <sup>a</sup>	
CE 16×16 <sup>b</sup>	16×16	CE	C1616CSD	CE1616CSD
	16×16	CE System 80	C8016C	
	16×16	CE	XSL16C	
W 14×14	14×14	ANF	W1414A	W1414WL
	14×14	ANF Top Rod	W1414ATR	
	14×14	B&W	W1414B	
	14×14	W LOPAR	W1414WL	
	14×14	W OFA	W1414WO	
	14×14	W Std	W1414W	
W 15×15	15×15	ANF	W1515A	W1515WL
	15×15	ANF HT	W1515AHT	
	15×15	ANF Part Length	W1515APL	
	15×15	W LOPAR	W1515WL	
	15×15	W OFA	W1515WO	
	15×15	W Standard	W1515W	
	15×15	W Vantage 5	W1515WV5	
W 17×17	17×17	ANF	W1717A	W1717WL
	17×17	W	W1717WRF	
	17×17	W	W1717WVJ	
	17×17	W LOPAR	W1717WL	
	17×17	W Vantage 5H	W1717WVH	
	17×17	South Texas <sup>c</sup>	WST17W	
	17×17	B&W Mark B	B1717B	
	17×17	W OFA	W1717WO	
	17×17	W Pressurized	W1717WP	
	17×17	W Vantage	W1717WV	
	17×17	W Vantage +	W1717WV+	
	17×17	W Vantage 5	W1717WV5	
	17×17	W Vantage 5	W1717WV5	

<sup>a</sup>CE14×14 assembly types with different lengths, but same pellet diameter, rod diameter and pitch, and clad material [8].

<sup>b</sup>CE16×16 assembly types with different assembly lengths and number of non-fueled rods, but same pellet diameter, rod diameter and pitch, and clad material [8].

<sup>c</sup>The W17×17 South Texas and LOPAR assembly types have same pellet diameter, rod diameter and pitch, and clad material, but different lengths [8].

Table 2. ARP libraries for BWR generic assembly classes

Generic assembly class	Array size	Version	Assembly type	Representative assembly type	
GE BWR/2,3	7×7	ANF	G2307A	G4607G3B	
	7×7	GE-2a	G2307G2A		
	7×7	GE-2b	G2307G2B		
	7×7	GE-3	G2307G3		
	8×8	8×8	ANF	G2308A	G4607G4B
		8×8	ANF Pressurized	G2308AP	
		8×8	GE-10	G2308G10	
		8×8	GE-4	G2308G4	
		8×8	GE-5	G2308G5	
		8×8	GE-7	G2308G7	
		8×8	GE-8a	G2308G8A	
		8×8	GE-8b	G2308G8B	
		8×8	GE-9	G2308G9	
		8×8	GE-Barrier	G2308GB	
	8×8	GE-Pressurized	G2308GP		
	9×9	9×9	ANF	G2309A	G4609A
9×9		ANF IX	G2309AIX		
9×9		GE-11	G2309G11		
9×9			9X9IXQFA		
GE BWR/4-6	7×7	GE-2	G4607G2	G4607G3B	
	7×7	GE-3a	G4607G3A		
	7×7	GE-3b	G4607G3B		
	8×8	8×8	ANF-Pressurized	G4608AP	G4608G4B
		8×8	GE-10	G4608G10	
		8×8	GE-11	G4608G11	
		8×8	GE-12	G4608G12	
		8×8	GE-4a	G4608G4A	
		8×8	GE-4b	G4608G4B	
		8×8	GE-5 (Retrofit Fuel)	G4608G5	
		8×8	GE-8	G4608G8	
		8×8	GE-9	G4608G9	
		8×8	GE-Barrier	G4608GB	
	8×8	GE-Pressurized	G4608GP		
	8×8	WE	G4608W		
	9×9	9×9	ANF	G4609A	G4609A
		9×9	ANF 9-5	G4609A5	
		9×9	ANF 9X	G4609A9X	
		9×9	ANF IX	G4609AIX	
		9×9	ANF X+	G4609AX+	
		9×9	GE-11	G4609G11	
		9×9	GE-13	G4609G13	
	10×10	10×10	ANF	G4610A	G4610G14
		10×10	ANF IX	G4610AIX	
10×10		CE	G4610C		
10×10		GE-12	G4610G12		
10×10		GE-14	G4610G14		
10×10		ATRIUM10	ATRIUM10		

**Table 3. Representative assembly types for reactor-specific PWR ARP libraries**

Reactor-specific assembly class	Array size	Version	Assembly type	Representative assembly type
Palisades	15×15	ANF CE	XPA15A XPA15C	XPA15C
Yankee Rowe	15×16	ANF CE UNC W	XYR16A XYR16C XYR16U XYR18W	XYR16C
San Onofre-1	14×14	W W D W M	XSO14W XSO14WD XSO14WM	XSO14W
Haddam Neck	15×15	B&W SS B&W Zir Gulf SS Gulf Zir NUM SS NUM Zir W W Zir	XHN15B XHN15BZ XHN15HS XHN15HZ XHN15MS XHN15MZ XHN15W XHN15WZ	XHN15B
Indian Point-1	13×13	W	XIP14W	XIP14W

**Table 4. Representative assembly types for reactor-specific BWR ARP libraries**

Reactor-specific assembly class	Array size	Version	Assembly type	Representative assembly type
Dresden-1	6×6 6×6 7×7 8×8 6×6 6×6 6×6 6×6	ANF GE GE SA-1 GE PF Fuels GE Tpe III-B GE Type III-F GE Type V	XDR06A XDR06G XDR07GS XDR08G XDR06G3B XDR06G3F XDR06G5	XDR06G5
Humboldt Bay	6×6 6×6 7×7	6×6 ANF GE GE Type II	XHB06A XHB06G XHB07G2	
LaCrosse <sup>a</sup>	10×10 10×10	AC ANF	XLC10L XLC10A	XLC10A
Big Rock Point	9×9 11×11 7×7 8×8 8×8 11×11 11×11	ANF ANF GE GE GE GE NFS	XBR09A XBR11A XBR07G XBR08G XBR09G XBR11G XBR11N	XBR11A

<sup>a</sup>LaCrosse was an Allis Chalmers (AC) reactor; fuel rod cladding material is stainless steel 348H.

**Table 5. Range of <sup>235</sup>U initial enrichment, fuel final burnup, and moderator density values for ORIGEN/ARP libraries**

Parameter	Bounding operating conditions	Nominal operating conditions
Initial enrichment values (wt % <sup>235</sup> U)	1.0; 1.5; 2.0; 3.0; 4.0; 5.0; 6.0	1.0; 1.5; 2.0; 3.0; 4.0; 5.0; 6.0
Burnup range for a PWR ARP library (GWD/MTU)	0 - 90	0 - 90
Burnup range for a BWR ARP library (GWD/MTU)	0 - 72	0 - 72
PWR moderator density values (g/cm <sup>3</sup> )	See Table 6	0.60; 0.75; 0.80
BWR moderator density values (g/cm <sup>3</sup> )	See Table 6	0.10; 0.30; 0.50; 0.65; 0.80

**Table 6. Bounding depletion modeling parameters for ORIGEN/ARP libraries**

Parameter/Reactor type	B&W PWR <sup>a</sup>	W PWR <sup>b</sup>	CE PWR <sup>c</sup>	GE BWR <sup>d</sup>
Fuel rod mixture <sup>e</sup>	UO <sub>2</sub>	UO <sub>2</sub>	UO <sub>2</sub>	UO <sub>2</sub>
Fuel density (g/cm <sup>3</sup> ) <sup>f</sup>	10.741	10.741	10.741	10.741
Specific Power (MW/MTU) <sup>g</sup>	30	30	30	22.38
Fuel temperature (K) <sup>g</sup>	1144.1	1157	1171.6	1200
Moderator temperature (K) <sup>g</sup>	588.7	598.2 <sup>h</sup>	598.55	560.7
Moderator density (g/cm <sup>3</sup> ) <sup>g</sup>	0.6905	0.6668 <sup>h</sup>	0.6656 <sup>i</sup>	0.3 <sup>j</sup>
Soluble boron concentration (ppm) <sup>g</sup>	1000	1000	1000	N/A
Burnable absorber exposure <sup>k</sup>	All assembly guide tubes contain burnable poison rods fully inserted throughout irradiation time	All assembly guide tubes contain pyrex rods fully inserted throughout irradiation time	None	Full-length control blade insertion
Type of absorber	Al <sub>2</sub> O <sub>3</sub> -B <sub>4</sub> C	SiO <sub>2</sub> -B <sub>2</sub> O <sub>3</sub>	N/A	B <sub>4</sub> C
B <sub>4</sub> C wt %	3.5 <sup>l</sup>	12.5 <sup>m</sup>	N/A	70 <sup>n,o</sup>
Axial burnup profile	See Table 7	See Table 7	See Table 7	Uniform

<sup>a</sup>Ref. [18].<sup>b</sup>Ref. [5] except for specific power and soluble boron concentration which are the same as for B&W.<sup>c</sup>Ref. [19], assembly AH1, except for specific power and soluble boron concentration which are the same as for B&W.<sup>d</sup>Ref. [20].<sup>e</sup>NUREG/CR-6760 (Ref. [21]) has demonstrated that use of UO<sub>2</sub> rods in place of integral burnable absorber rods made of either UO<sub>2</sub>-Gd<sub>2</sub>O<sub>3</sub>, UO<sub>2</sub>-Er<sub>2</sub>O<sub>3</sub>, or Al<sub>2</sub>O<sub>3</sub>-B<sub>4</sub>C generates nuclide concentration values that are bounding for criticality analyses.<sup>f</sup>Value given as 98% UO<sub>2</sub> theoretical density.<sup>g</sup>For bounding conditions, this parameter is constant throughout the irradiation time.<sup>h</sup>Based on 155 bar operating pressure and 325 °C outlet temperature for the McGuire nuclear power plant.<sup>i</sup>Based on the 598.55 K moderator temperature and 154.94 bar operating pressure for the Saint Lucie 2 nuclear power plant.<sup>j</sup>For both the in-channel and by-pass flow moderator regions.<sup>k</sup>NUREG/CR-6761 (Ref. [22]) has demonstrated that use of burnable poison rods in the PWR depletion simulations is conservative with respect to criticality. Similarly for the BWR fuel [20].<sup>l</sup>B<sub>4</sub>C weight percent in Al<sub>2</sub>O<sub>3</sub>-B<sub>4</sub>C.<sup>m</sup>B<sub>2</sub>O<sub>3</sub> weight percent in SiO<sub>2</sub>-B<sub>2</sub>O<sub>3</sub>.<sup>n</sup>Ref. [23].<sup>o</sup>Percent of B<sub>4</sub>C theoretical density (2.52 g/cm<sup>3</sup>, Ref. [6]).

Table 7. PWR bounding axial burnup profiles [15]

Axial zone no.	Fraction of active fuel height	Burnup < 18 GWd/MTU	18 ≤ Burnup < 30 GWd/MTU	Burnup ≥ 30 GWd/MTU
		1	2	3
1	0.0278	0.649	0.668	0.652
2	0.0833	1.044	1.034	0.967
3	0.1389	1.208	1.150	1.074
4	0.1944	1.215	1.094	1.103
5	0.2500	1.214	1.053	1.108
6	0.3056	1.208	1.048	1.106
7	0.3611	1.197	1.064	1.102
8	0.4167	1.189	1.095	1.097
9	0.4722	1.188	1.121	1.094
10	0.5278	1.192	1.135	1.094
11	0.5833	1.195	1.140	1.095
12	0.6389	1.190	1.138	1.096
13	0.6944	1.156	1.130	1.095
14	0.7500	1.022	1.106	1.086
15	0.8056	0.756	1.049	1.059
16	0.8611	0.614	0.933	0.971
17	0.9167	0.481	0.669	0.738
18	0.9722	0.284	0.373	0.462

## 2.2 M&S Toolset

The M&S toolset development has been focused on thermal and neutronics analyses to demonstrate the integrated capabilities of the UNF M&S System. The M&S toolset consists of thermal analysis tools, and neutronics analysis tools which are used for fuel assembly depletion, decay, and criticality analyses.

As a result of the large number of spent fuel assemblies and cask loading patterns that may require detailed modeling of fuel depletion, a fast, reliable, and quality-assurable method of input model creation has been developed. Assembly and cask model templates are currently being developed for depletion, criticality, and thermal calculations. The fuel assembly and cask model templates as well as input parameters from the combined UNF database are used by a Java-based template engine to develop complete input files for depletion, criticality, and thermal calculations. Model templates contain three basic components: (1) input data blocks that do not vary as a function of fuel assembly characteristics (e.g., description of cask dimensions and construction materials for criticality or thermal calculations); (2) input parameters that vary as a function of assembly characteristics (e.g., fuel pin dimensions in an assembly model for depletion calculations or nuclide concentrations in a cask model for criticality calculations); and sub-templates to be imported (e.g., templates describing fuel pin arrays for depletion or criticality calculations). Model template development, update, and review are conducted using the Mercurial distributed source control management tool, which is widely used for version control of files.

A template engine (or template processor) is used to combine UNF technical data with the model templates developed for depletion, criticality, and thermal calculations to produce complete input files for those calculations. A template engine is a string substitution program designed to take advantage of repeated structures in text files. The template engine takes the input parameters data structures represented by a JavaScript Object Notation (JSON) data structure and the root template file. With these two components, the template engine conducts attribute replacement and sub-template imports. Template



engine also performs evaluations for an input parameter and inserts the evaluated value in the appropriate place within a model template. These evaluations are performed using simple mathematical expressions that define relationships between input parameters and other parameters with available data in the UNF database.

### 2.2.1 Neutronics Analysis Tools

UNF characterization begins with neutronics analyses to predict nuclide concentrations in irradiated fuel and associated radiation and decay heat source terms, which are used as part of the input to subsequent criticality and thermal calculations, respectively. The code system selected for neutronics analyses is the SCALE code system [6].

SCALE is a system of computer codes for depletion, decay, criticality, and shielding analyses. This computer code system has been developed by Oak Ridge National Laboratory and distributed for more than 30 years through the Radiation Safety Information Computational Center and the Nuclear Energy Agency Data Bank under license agreement. SCALE has been used for safety analysis and design by regulators, licensees, and research institutions around the world. This code is accepted by the U.S. Nuclear Regulatory Commission for criticality safety applications [24]. SCALE 6.1 is the most recent release version of the SCALE code system. The SCALE computer codes/sequences used by UNF M&S System are described further.

The SCALE code system provides the computer codes/sequences for running depletion calculations. Within SCALE, the TRITON two-dimensional (2-D) depletion sequence [6] (Sect. T01) is used to perform either: 1) assembly-specific detailed depletion calculations that provide actinide and fission product nuclide concentrations in discharged nuclear fuel assemblies, or 2) depletion calculations that generate cross-section libraries for generic assembly/reactor specific classes and a range of fuel operating conditions, which subsequently can be used by ORIGEN-ARP [6] (Sect. D1) for rapid processing of problem-dependent cross-sections. The TRITON 2-D depletion calculation sequence employs CENTRM [6] (Sect. F18) for multi-group cross-section processing, NEWT [6] (Sect. F21) for 2-D discrete ordinates transport calculations, and ORIGEN-S [6] (Sect. F07) for depletion and decay calculations. Once ARP libraries or TRITON depletion results are generated they are processed with ORIGEN to provide discharge concentrations which can be subsequently decayed to provide time-dependent isotopic compositions and decay heat source terms. The resultant nuclide concentrations and decay heat source terms are passed to the criticality and thermal analysis codes, respectively. Criticality calculations are performed with the SCALE CSAS6 [6] (Sect. C6) analysis sequence for a loaded fuel cask using the KENO-VI Monte Carlo code with the continuous energy ENDF/B-VII cross section library to determine the effective neutron multiplication factor,  $k_{eff}$ .

#### 2.2.1.1 TRITON Depletion Model Templates

TRITON models are stored in a compact form as a set of templates, for each type of fuel assembly, representative of the PWR Westinghouse (W) 14×14, 15×15, 17×17, Babcock and Wilcox 15×15, Combustion Engineering 14×14 and 16x16 assemblies, and custom assemblies for Yankee Rowe, Palisades, San Onofre, Haddam Neck and Indian Point unit 1 reactors. The assembly-specific parameters supplied include fuel pin, guide tube, and removable absorber rod patterns, dimensions, materials, and temperatures, fuel and removable absorber initial enrichments, moderator temperature and density, cycle-dependent specific power and irradiation time, and soluble boron concentration.

### 2.2.1.2 CSAS6/KENO-VI Criticality Model Templates

CSAS6 models are stored in a compact form as a set of templates for each type of cask, which permits an automated method of input file assembly with verified dimensions and conditions stored in a single location. Initial CSAS6 (KENO-VI) model templates have been developed that are representative of the Trojan MPC-24E/EF, Rancho Seco Nuhoms-24PT, the Maine Yankee NAC UMS-24, and Sequoyah MPC-32 storage casks with appropriate representative assembly types for those specific sites. The assembly-specific parameters supplied include assembly pattern description, which depends on the assembly type, and nuclide concentrations in fuel mixtures, which depend on assembly characteristics such as final burnup, initial enrichment, axial burnup profile, and decay time. The cask models include a very large number of fuel mixtures because each fuel assembly and each axial burnup zone in the model has a unique fuel composition. For example, the cask model for the MPC24E/EF cask has a total of 432 different fuel mixtures, which is determined as the product between the number of fuel assemblies in the cask (i.e., 24 fuel assemblies) and the number of axial burnup zones modeled (e.g., 18 axial zones for the PWR active fuel region). The ENDF/B-VII continuous-energy cross-section library is used for the CSAS6 criticality calculations.

While the current criticality analyses provide reasonable estimates of cask system  $k_{eff}$  values, due to the wide variability in radial and axial burnup distribution across the cask, coupled with flux trap regions for some casks, many of these systems are considered high-dominant ratio systems. High-dominance ratio systems represent a particularly challenging issue when performing Monte Carlo criticality simulations, and can result in slow flux convergence either requiring very long run times or other source biasing techniques to increase convergence. The current templates have been set up to run for relatively long run times to address this issue. Because the UNF M&S System runs in an automated fashion and each cask is different, the results generated are good for scoping studies, but confirmation of flux convergence would be required for licensing justification. A discussion on the dominance ratio effects and results observed are provided in Appendix A.

## 2.2.2 Thermal Analysis Tool

COolant Boiling in Rod Arrays–Spent Fuel Storage (COBRA–SFS) is a thermal-hydraulic code used to perform calculation of flow and temperature distributions in spent fuel storage systems under a wide range of flow conditions, including mixed and natural convection. The COBRA software series was originally designed for thermal-hydraulic analysis of nuclear fuel rod bundles in reactor cores. COBRA–SFS uses the same subchannel formulation, but has been extensively modified and improved for application to single phase analysis of spent fuel storage and transportation systems with radiative, convective, and conductive heat transfer. Several features specific to UNF storage analyses are incorporated in COBRA–SFS, including the capability to model a detailed radiation heat transfer model, which includes individual fuel rods and boundary conditions that simulate radiation and natural convection heat transfer from storage system surfaces, and calculate three-dimensional conduction heat transfer through fuel basket and cask body. Within the UNF M&S System, COBRA–SFS is used to determine the spatial distribution of the temperature within the cask.

### 2.2.2.1 COBRA-SFS Thermal Model Templates

COBRA-SFS model templates are being developed for the representative cask systems currently in use. The initial focus has been on vertical storage systems including the HI-STORM-100 MPC-24E and MPC-32 design variants, as well as the NAC UMS-24 class 1 and class 2 design variants. Models for horizontal storage systems are also currently in development. The model template database will be further improved as more site-specific and assembly-specific data becomes available. Current capabilities available are for the Maine Yankee site.

## 2.3 Modeling and Simulation Automation Tool

The M&S automation tool controls the interfaces and results processing within the UNF M&S System. User interaction is accomplished through a graphical user interface that provides the option for the type of analysis to be performed and can graphically display the results of the various analyses.

The M&S automation tool has the following capabilities:

- (1) ARP cross-section library generation for representative assembly types. The ARP cross-section libraries are used in fast-running depletion calculations with ORIGEN.
- (2) Depletion analysis to provide UNF nuclide inventories. Nuclide inventory information is needed for burnup credit criticality safety analyses, for developing nuclear reprocessing and safeguards technologies, and for radiological dose assessments. Options are implemented for a highly-accurate depletion calculation with TRITON (which is appropriate if detailed fuel assembly-specific design and irradiation history data are available), and a fast-running depletion calculation with ORIGEN using ARP cross sections generated for fuel assemblies representative of generic assembly classes. In addition, the fast-running depletion calculation path provides the option for using ARP cross-section libraries generated with either nominal (i.e., average) or bounding irradiation history parameters with respect to criticality.
- (3) CSAS6 nuclear criticality safety evaluations for spent fuel in transport and dry storage casks to demonstrate compliance with regulatory requirements in 10 CFR Part 71 and Part 72. A total of 28 actinide and fission product nuclides are considered in the fuel compositions for burnup credit criticality safety analyses, as recommended in Interim Staff Guidance – 8, Revision 3, *Burnup Credit in the Criticality Safety Analyses of PWR Spent Fuel in Transportation and Storage Casks* [25].
- (4) COBRA-SFS thermal analysis for spent fuel in storage/transport casks to demonstrate compliance with regulatory requirements in 10 CFR Part 71 and Part 72.

### 2.3.1 Graphical User Interface

The graphical user interface (GUI) provides options for the user to select the type of evaluation (e.g., criticality analysis) and the type of analysis (e.g., analysis using bounding depletion parameters respect to criticality) to be performed, and to update the existing set of ARP cross-section libraries, as illustrated in Figure 3.

Analysis Type	Evaluation	ARP Library Update
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
<input checked="" type="checkbox"/> Bounding	<input type="checkbox"/> UNF Isotopes	<input type="checkbox"/> Update existing
<input type="checkbox"/> Nominal	<input checked="" type="checkbox"/> Cask	<input type="checkbox"/> Create new
<input type="checkbox"/> Detailed	<input type="checkbox"/> Cask Loading	
<input type="text" value="Date for Evaluation"/>	<input type="text" value="Site ID"/> ▼	<input type="text" value="Name"/>
<input type="button" value="Run"/>	<input type="text" value="Cask ID"/> ▼	

Figure 3. Analysis options provided by GUI.

Additional GUI features are available for displaying different sets of results, some of these re illustrated in Section 3. Options are also available to dump user selected results and information to a CSV or SQLITE file.

### 2.3.2 Automated Processes

Component interaction and process flow for the various calculations are depicted in the flow charts shown in this section.

#### 2.3.2.1 ARP Cross-Section Library Generation

ARP cross-section libraries are generated for fuel assembly types that are representative of generic assembly classes and for reactor-specific assembly types (see Table 1 through Table 4). These libraries reside in the UNF database once generated or are generated and retained within the UNF database for use in fast-running depletion calculations with ORIGEN. The process flow charts for ARP cross-section library generation using bounding and nominal operating parameters are illustrated in Figure 4 (a) and (b), respectively. To generate ARP cross-section libraries for a representative assembly type, a TRITON input file is generated for each fuel initial enrichment and moderator density value identified in Table 5.

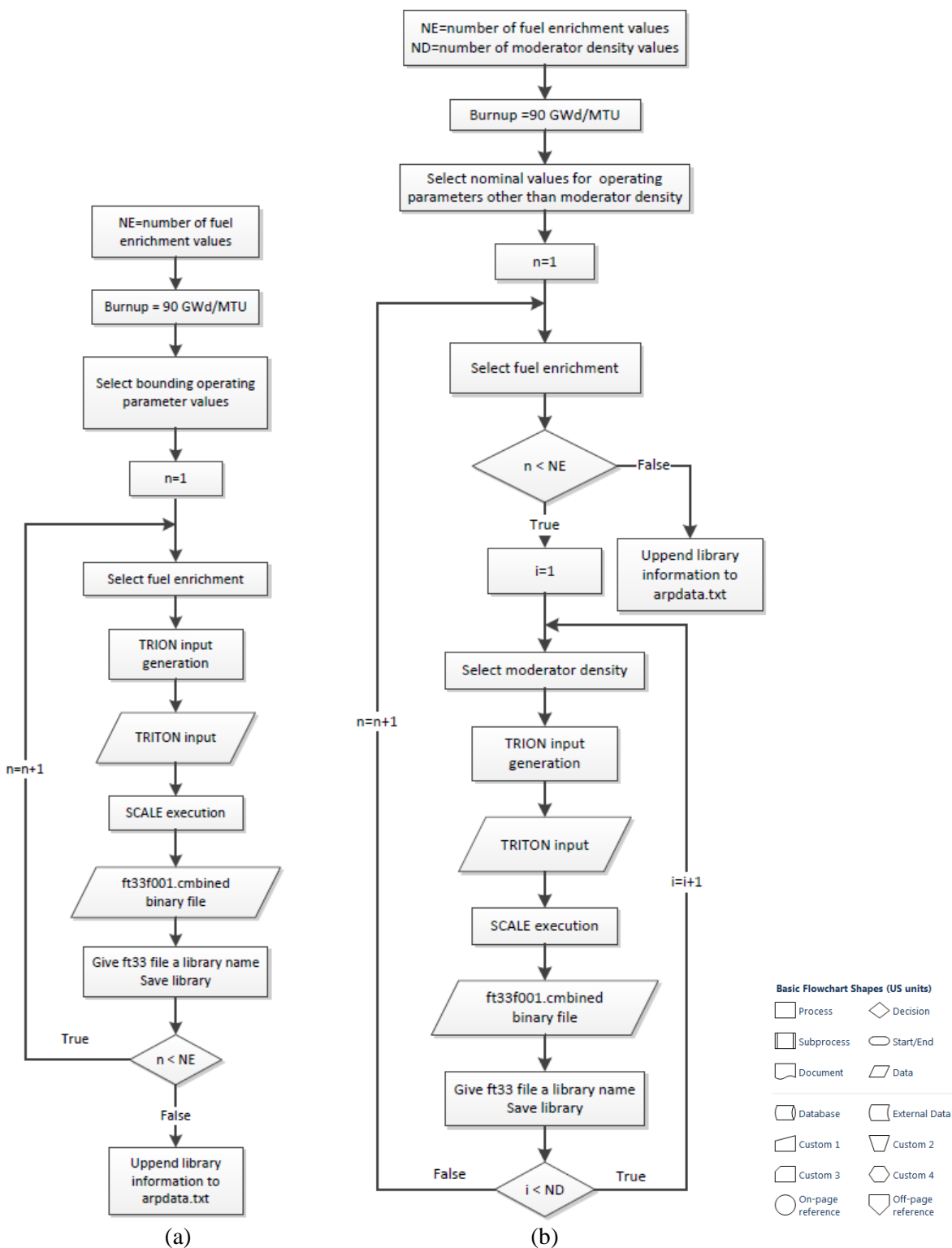


Figure 4. Flow chart illustrating generation of ARP cross-section libraries using (a) bounding operating parameters; (b) nominal operating parameters.

### 2.3.2.2 Cask Nuclear Safety Analyses

The process flow for cask thermal and criticality safety analyses is depicted in Figure 5. This process includes three sub-processes denoted as sub-process A, B, and C, which are dedicated to calculating nuclide concentration and the decay source term as a function of fuel assembly and axial burnup zone, CSAS6 input file generation; and COBRA-SFS input file generation, respectively. The automatically generated CSAS6 and COBRA-SFS output files are retained within the UNF database.

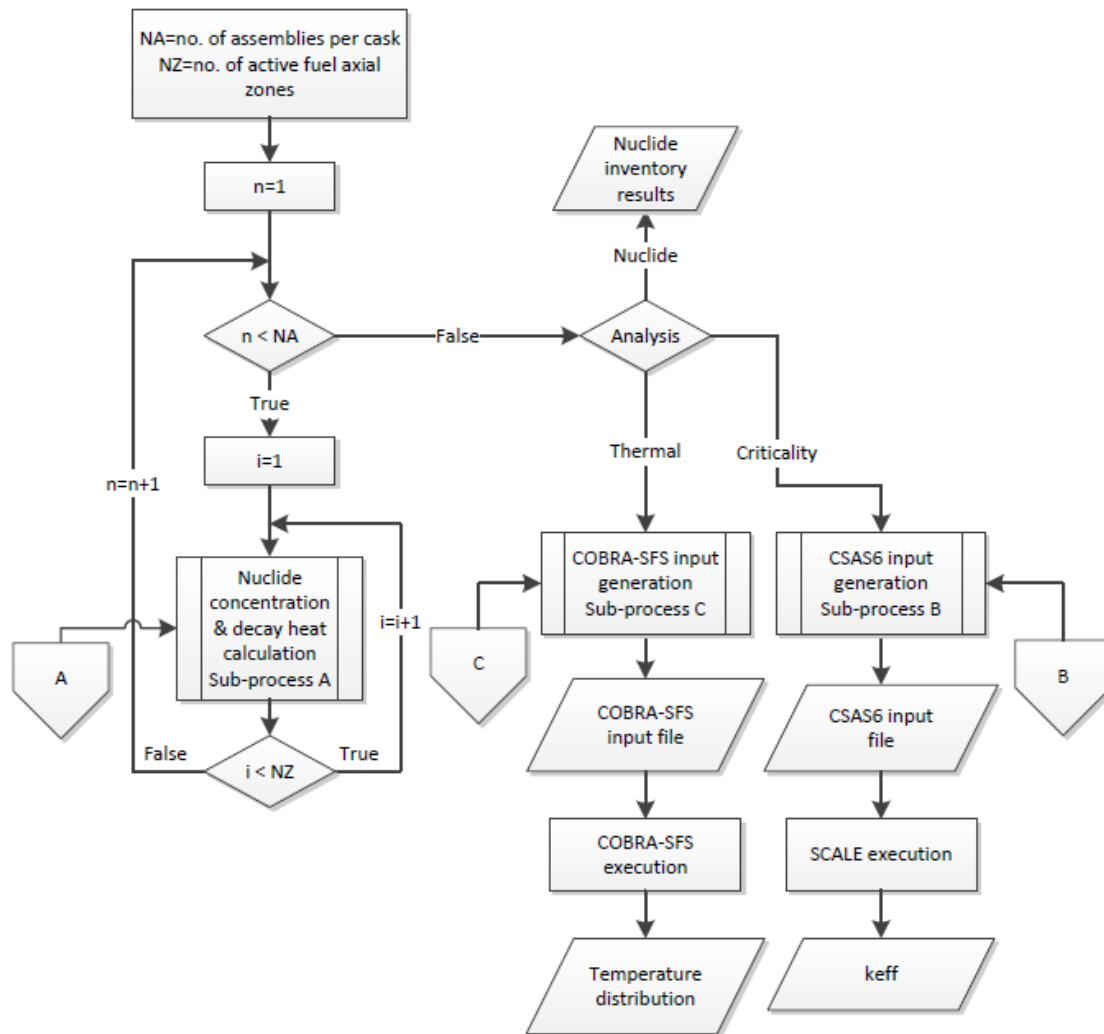
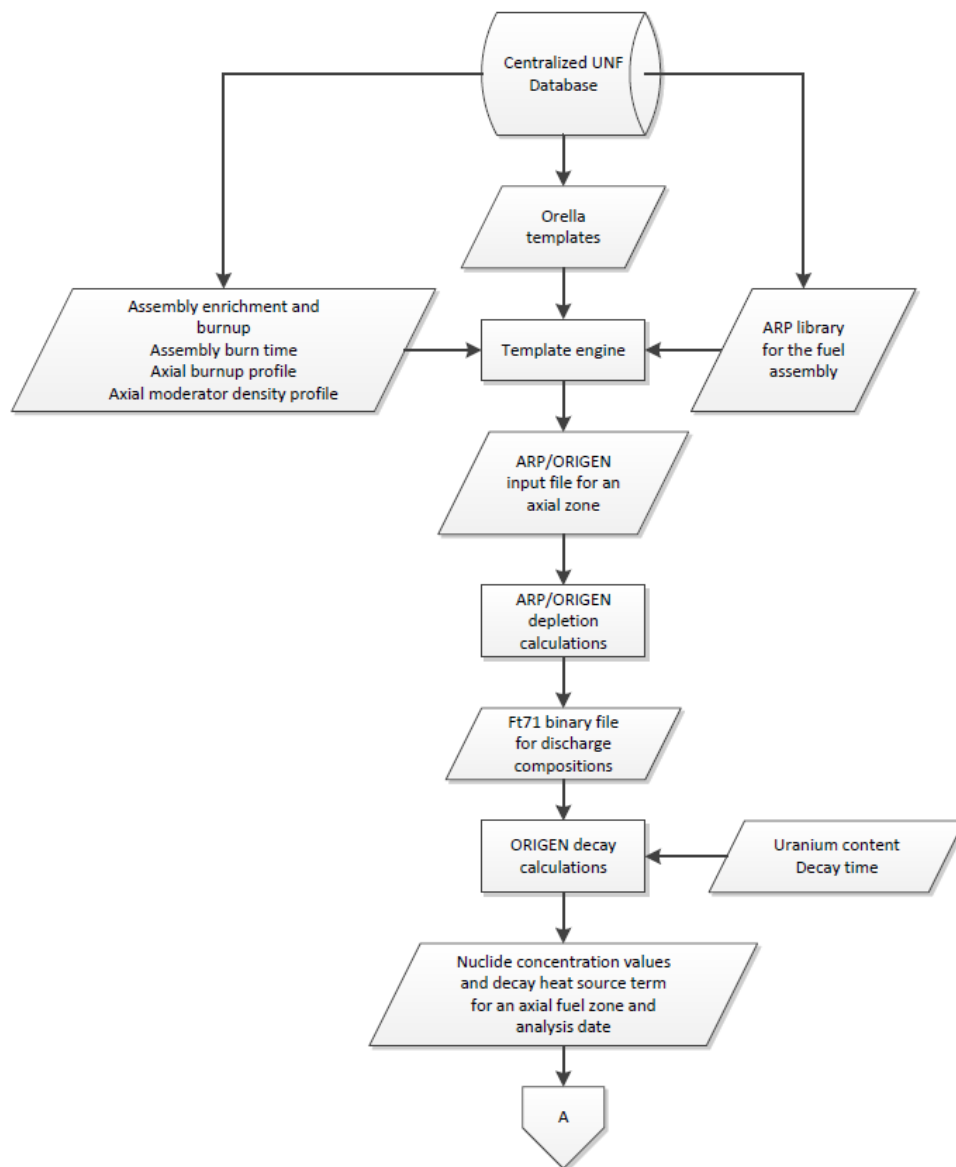


Figure 5. Flow chart illustrating cask safety analysis processes.

### 2.3.2.3 Nuclide Concentration and Decay Heat Source Term Calculation

Nuclide concentration values and associated decay source terms for use in criticality and thermal calculations, respectively, are calculated as a function of fuel assembly and axial burnup zone, as described in Figure 6.





**Figure 6. Flow chart illustrating the processes for nuclide concentration and decay heat source term calculations.**

For an assembly type, the Orella template engine within the M&S automation tool uses the Orella templates, the ARP library corresponding to the assembly type, and a set of input parameters to generate a complete Orella input file. The assembly-dependent Orella input parameters include assembly enrichment and burnup, assembly burn time, the burnup axial profile, and the axial moderator density profile. Orella generates a series of input files for ARP/ORIGEN depletion calculations. The result of the ARP/ORIGEN calculations is a binary file containing discharge fuel compositions, which is retained within the UNF database. The binary file is then used to calculate the nuclide concentrations and fuel decay heat source term corresponding to the decay time of interest. These calculations are automatically performed according to an established calculation sequence resulting in nuclide concentration and decay heat values being passed to the next sub-processes dedicated to CSAS6 and COBRA-SFS input file generation.

### 2.3.2.4 CSAS6 Input File Generation

The flow chart for generating a CSAS6 input file for criticality calculations is illustrated in Figure 7. The template engine assembles a CSAS6 input file using the CSAS6 model templates for the evaluated cask, the assembly- and axial burnup zone-dependent nuclide concentration values previously determined with ORIGEN, and the JSON with parameter values selected for the evaluated fuel assemblies.

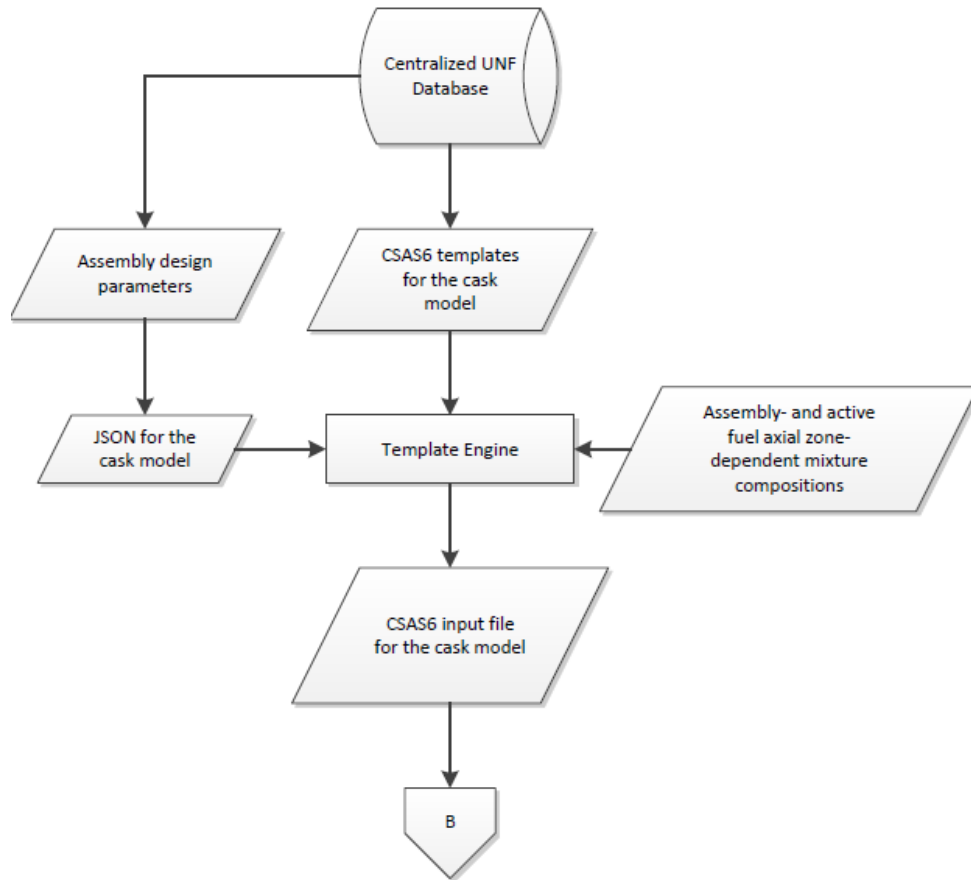


Figure 7. Flow chart illustrating the generation of a CSAS6 input file for cask criticality calculations.

### 2.3.2.5 COBRA-SFS Input File Generation

The flow chart for generating a COBRA-SFS input file for thermal calculations is illustrated in Figure 8. The template engine assembles a COBRA-SFS input file using the COBRA-SFS model templates for the evaluated cask, the decay heat values previously determined with ORIGEN, and the JSON with parameter values selected for the evaluated fuel assemblies.

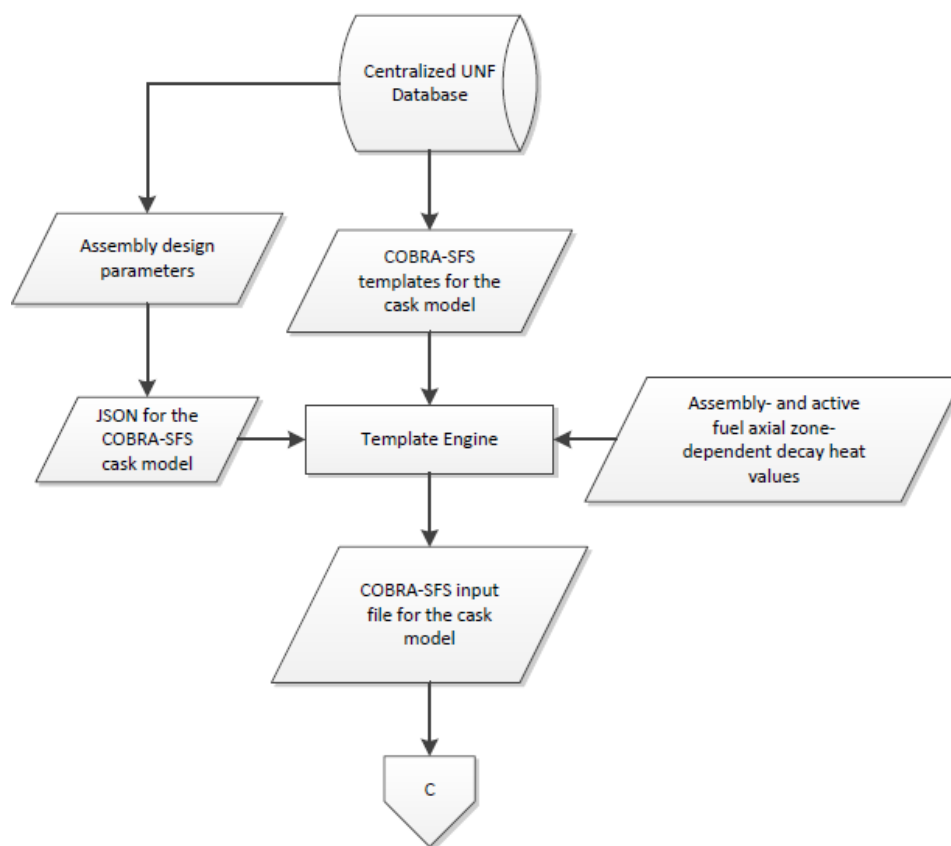


Figure 8. Flow chart illustrating generation of a COBRA-SFS input file for cask thermal calculations.

### 3. SUMMARY

This report documents completion of the the initial version of the M&S toolset and the beta version of the UNF database. The UNF database and the M&S toolset are being developed simultaneously in a consistent manner and make up the UNF M&S System. Technical data collection and its synthesis into appropriate formats are based on the SCALE and COBRA-SFS input requirements for depletion, criticality, and thermal analysis, whereas model templates for the computer codes utilize fuel assembly and storage cask information from the UNF database. Currently, the UNF database contains data from the RW-859 database, basic fuel assembly data such as assembly design parameters for representative assembly types, reactor- and cycle-specific data, and cask data, which are organized in relational SQL data tables.

The current version of the UNF M&S System has the capability to automate generation of PWR ARP cross-section libraries, calculation of discharge assembly nuclide concentrations based on the UNF characteristics provided by the RW-859 database, generation of CSAS6 and COBRA-SFS input files, and automated results extraction capabilities. The UNF M&S System was executed to provide depletion and discharge data for the assemblies in the 2002 discharge inventory. To date ~76,000 unique fuel assembly discharge isotopic compositions are available. Note that these are preliminary results and full testing of the complete system and verification of results is on-going at the time of this writing.

To provide a demonstration of the coupled data and analysis capabilities, the UNF M&S System has been applied to the Maine Yankee ISFSI. Maine Yankee consists of 64 dry storage casks, four being greater than class-C (GTCC) containers, six being NAC UMS-24 class-2 canisters to hold fuel assemblies with control element assemblies inserted in the guide tubes, and the rest comprised of NAC-UMS 24 class-1 canisters. The UNF inventory consists of 1,432 complete fuel assemblies, two partially consolidated assemblies, and two partially full failed fuel containers.

The Maine Yankee assemblies were decayed out to 2099, and individual cask criticality and thermal analysis models were executed as a function of time with the decayed isotopic compositions and corresponding decay heat source terms starting from the cask service date (2004). A visual depiction of some of the interactive capabilities is illustrated in

Figure 9. For example, a cask can be selected from the satellite photo to view specifics about. Cask content information for cask serial number TSC-024 is presented in Figure 10. Results and information that are readily available for individual cask systems include peak and minimum clad temperatures, component temperatures, cask surface temperatures, total decay heat,  $k_{eff}$  values, energy of average lethargy of neutron causing fission, system mass, among others. Figure 11 shows peak and minimum clad temperatures with cask TSC-024 as a function of time, Figure 12 shows  $k_{eff}$  as a function of time for cask TSC-058, and Figure 13 shows additional drill down capability to view individual fuel assembly isotopic concentrations as a function of time. This capability is available for both assemblies that have been loaded into casks and assemblies that still reside in wet storage.

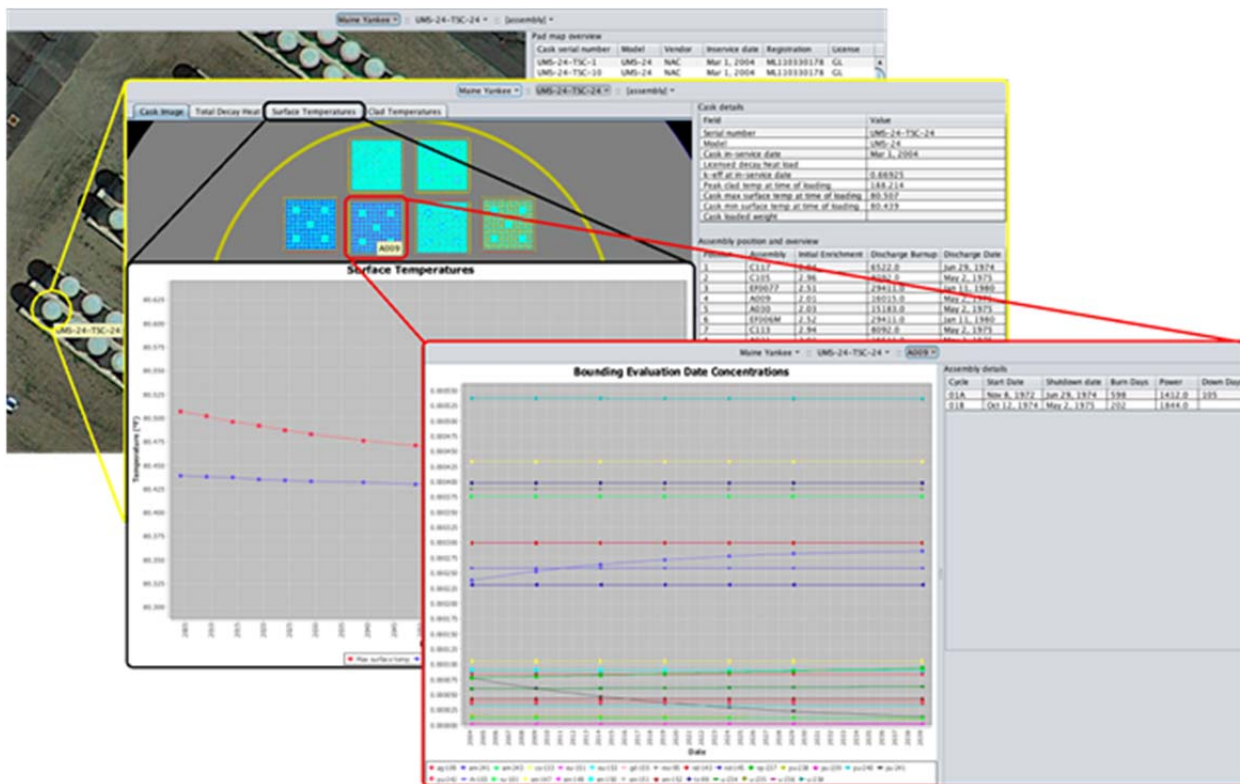


Figure 9. Screen capture illustrating interactive UNF capabilities.

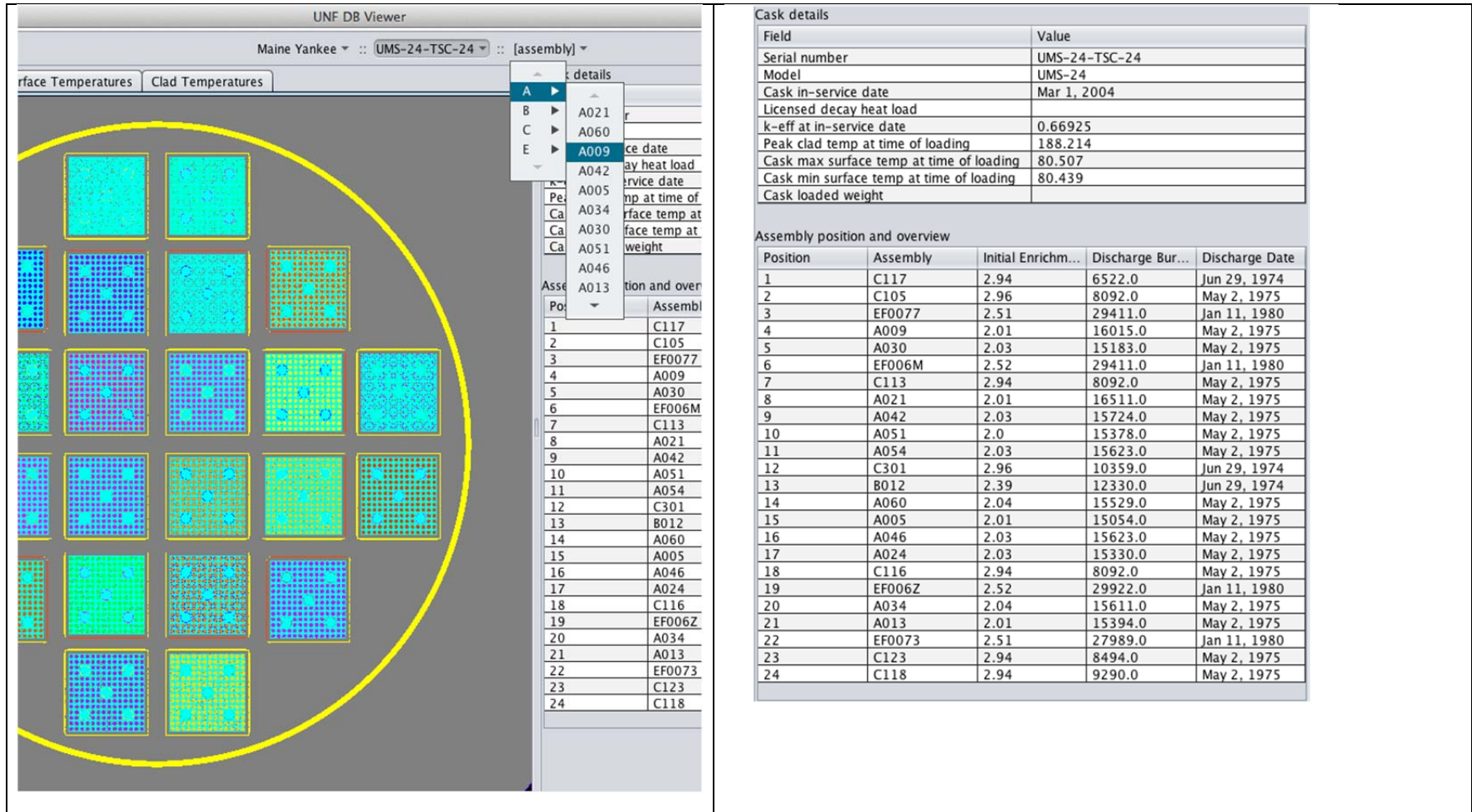


Figure 10. Example view of cask contents

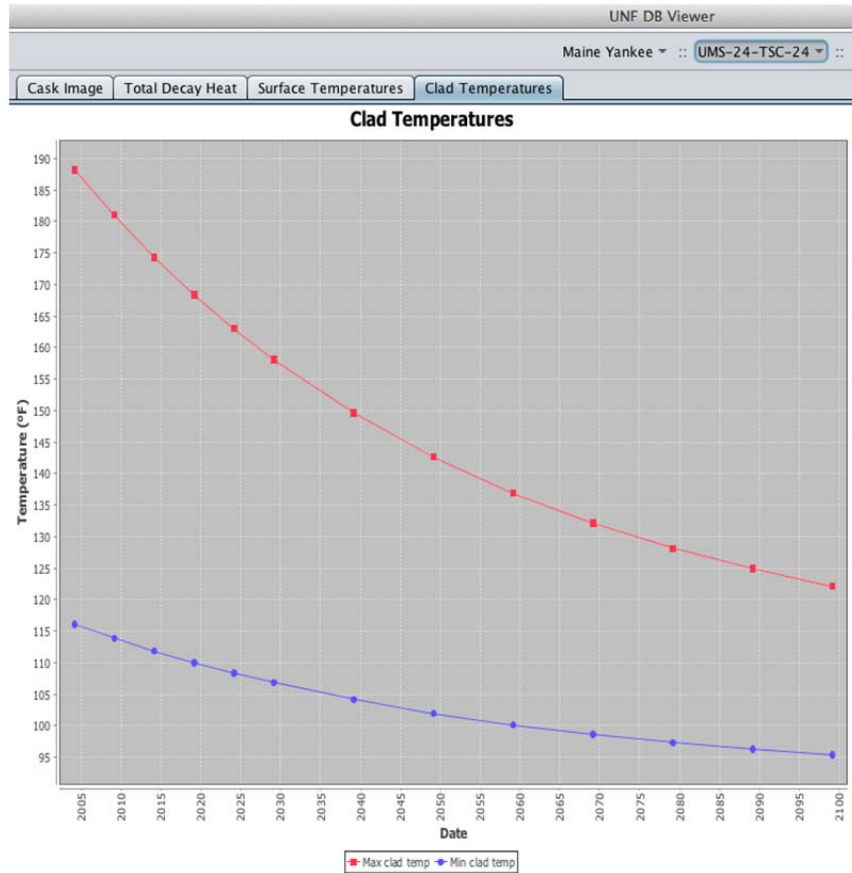


Figure 11. Example of cask clad temperature data as a function of time for Maine Yankee cask TSC-024

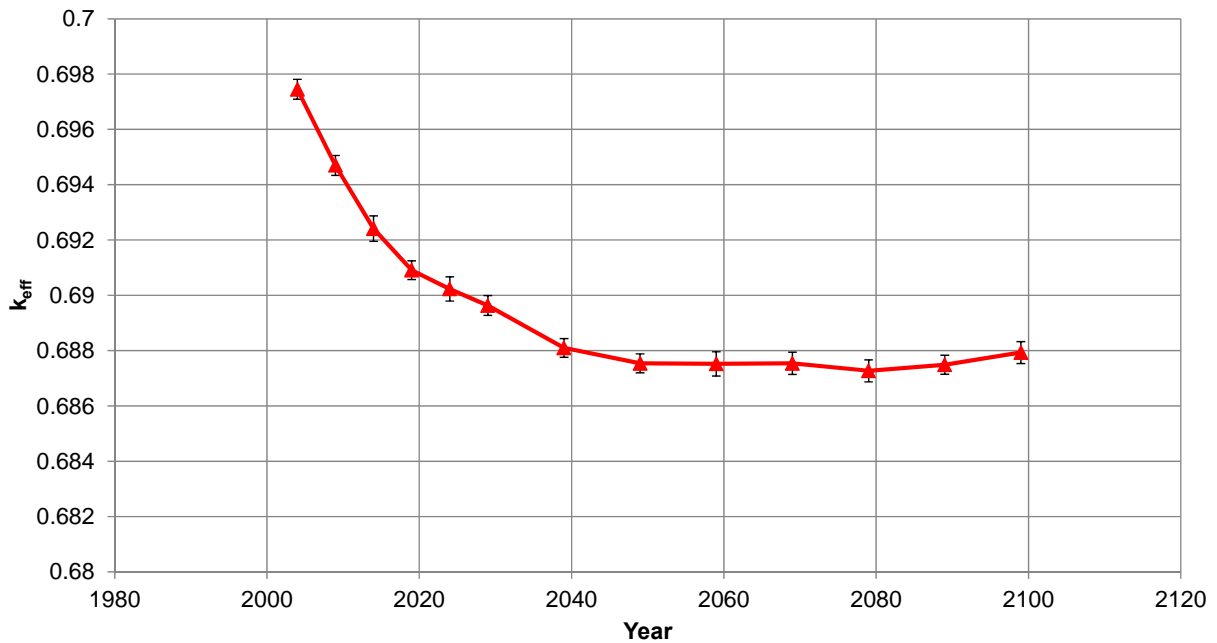


Figure 12. Example  $k_{eff}$  plot as a function of time for Maine Yankee cask TSC-058



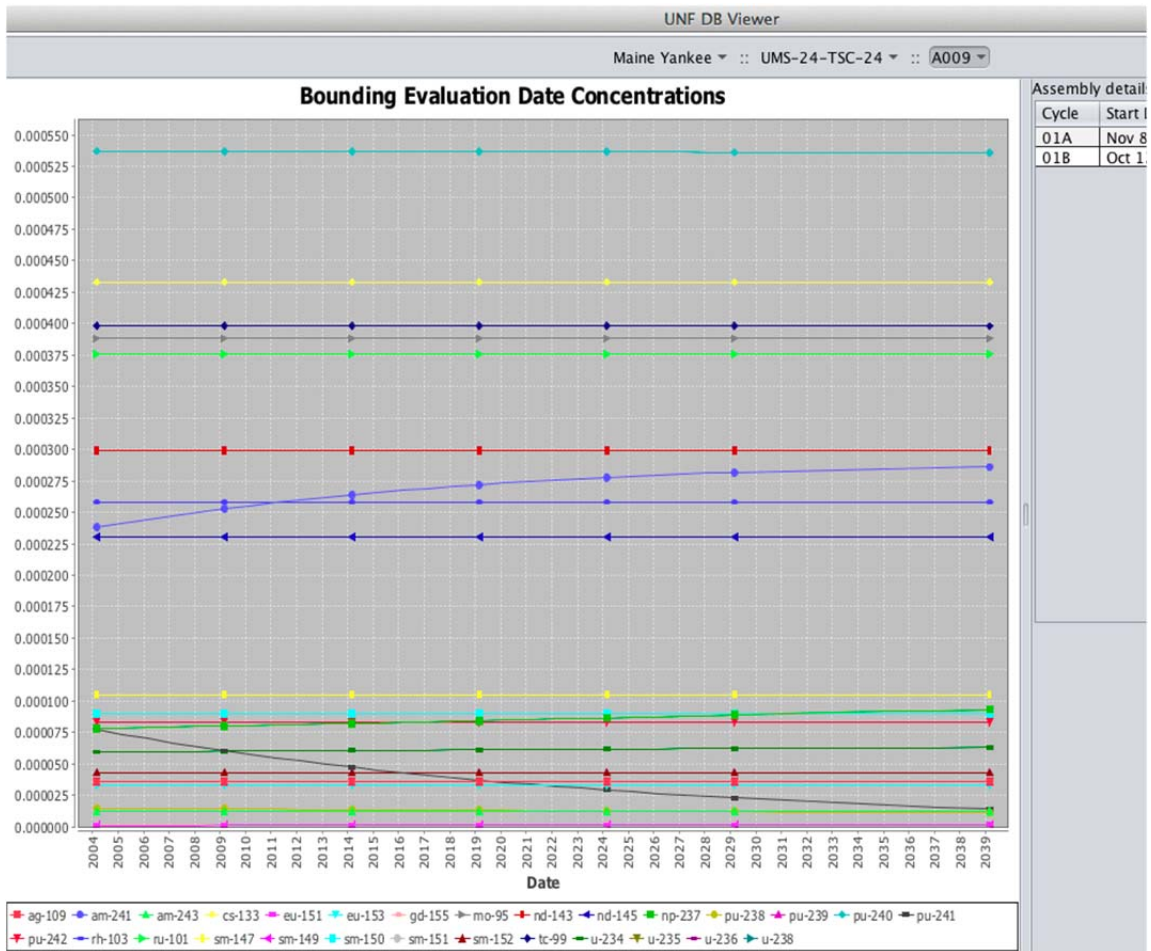


Figure 13. Example view of fuel assembly isotopic compositions for assembly A009 within cask TSC-024



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# APPENDIX A: DISCUSSION ON DOMINANT RATIO SYSTEMS

# Eigenvalue Convergence of High Dominant Ratio Systems

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December 2012

The transport equation as an eigenvalue problem can be solved using the power iteration method. This method is employed for example in the KENO-VI code of SCALE. It can be proved<sup>1</sup> that the multiplication constant with this method at iteration  $(n + 1)$ ,  $k_{eff}^{(n+1)}$ , converges to the largest eigenvalue  $k_0$  as:

$$k_{eff}^{(n+1)} = k_0[1 - \rho^n(1 - \rho)f + \dots]$$

where  $\rho$  is the dominance ratio, i.e., the ratio of the first two eigenvalues of the transport problem.

Analyzing the apparent error<sup>2</sup>,  $a_n \equiv k_{eff}^{(n+1)} - k_{eff}^{(n)}$  and the real error,  $r_n \equiv k_{eff}^{(n+1)} - k_0$ , it results that their ratio behaves asymptotically as:

$$\left| \frac{a_n}{r_n} \right| \sim \frac{1 - s\rho}{\rho}$$

This means that if the dominant ratio is close to one, the apparent error can be much smaller than the real error. Put another way, this means that although the  $k_{eff}$  curve as a function of iteration number might look fairly flat, it still might be too far from the converged, true value. In the above formulae, the factors  $f$  and  $s$  account for the initial flux (fission density) guess and they are smaller if this guess is better chosen.

A used fuel storage cask can be considered to be one such high-dominance-ratio system. This is especially the case when the fuel assemblies stored in the cask are separated by large distances filled with water.

To analyze the convergence properties of such a system, we looked at the Maine Yankee TSC-24 storage cask. This cask is loaded with 24 CE14x14 fuel assemblies, depleted to burnups ranging from  $\sim 6$  GWd/MTU to  $\sim 30$  GWd/MTU. The initial fuel enrichment for these assemblies varied between 2 wt%  $^{235}\text{U}/\text{U}$  and 2.96 wt%  $^{235}\text{U}/\text{U}$ . A plot of the fission density distribution is shown in Figure 1. Assemblies C117 and C105 in locations 1 and 2 show the highest density of fissions. It is also obvious from the Y-Z plot the used fuel storage trend of the fission density distribution to peak at the top of the cask. This is due to the axial fuel burnup profile used in the depletion calculations that makes the fuel assembly less burned at its top.

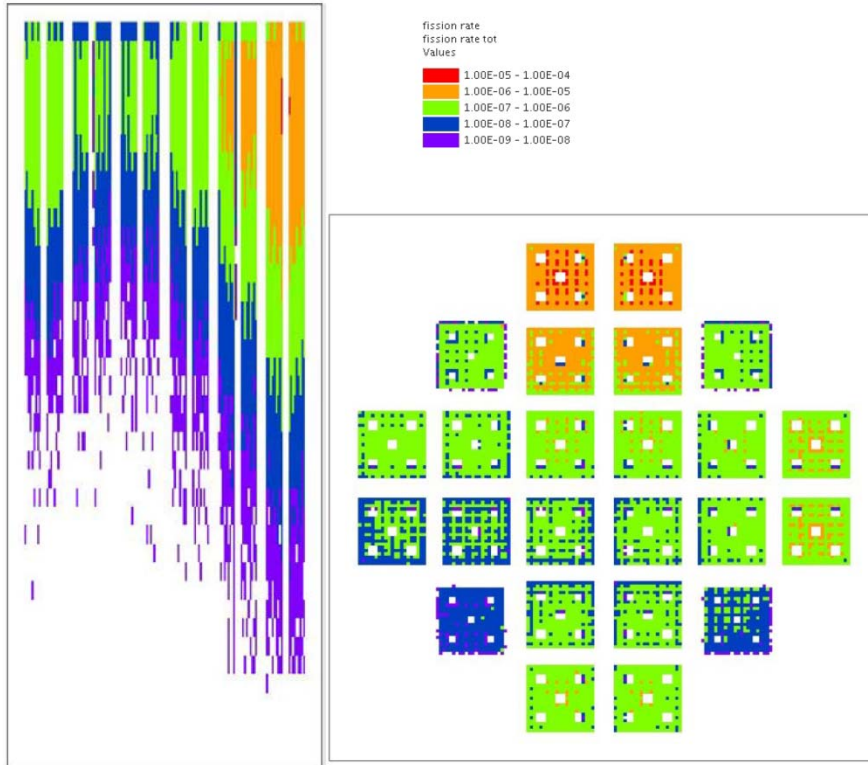


Figure 1. Fission density distribution in the Y-Z plane at x=12 cm (left) and X-Y plane at z=365 cm in the Maine Yankee TSC-24 fuel cask in year 2004.

A review of the best practices in criticality problems suggest<sup>1</sup> that “For the initial source guess in a criticality calculation, choose a uniform distribution in all fissionable regions of the problem. If only a one or a few source points are used, more cycles will be needed to assure convergence. For applications where only  $k_{eff}$  is sought, examine plots of  $k_{eff}$  vs. cycle to determine the proper number of cycles to discard before beginning the  $k_{eff}$  tally.”

A flat distribution in KENO-VI corresponds to the start option 0. Following the above recommendation, we started therefore by examining the convergence behavior of the eigenvalue for this problem using the flat start source option. From the user’s point of view, it is of interest to see which combination of skipped generations (nsk) and number of particles per generation (npg) converges the fastest. The plot in figure 2 suggest that the best option from the convergence speed perspective is to use fewer particles per generation and more generations for the same total number of particles simulated. As seen, at the end of the same runtime (or, more exactly the same total number of particles simulated, 33 million in this case), using more than 50,000 particles per cycle produce a final result which might be too far from the true value. One question in this case is what would happen if, for cases with larger batches, more generations are skipped (in Figure 2, the active generations start after the discontinuity)? The allure of the plots does not suggest that a significant improvement would take place in the convergence, within the same timeframe. It can, however, be remarked the smoother behavior of the curves for larger batches cases.

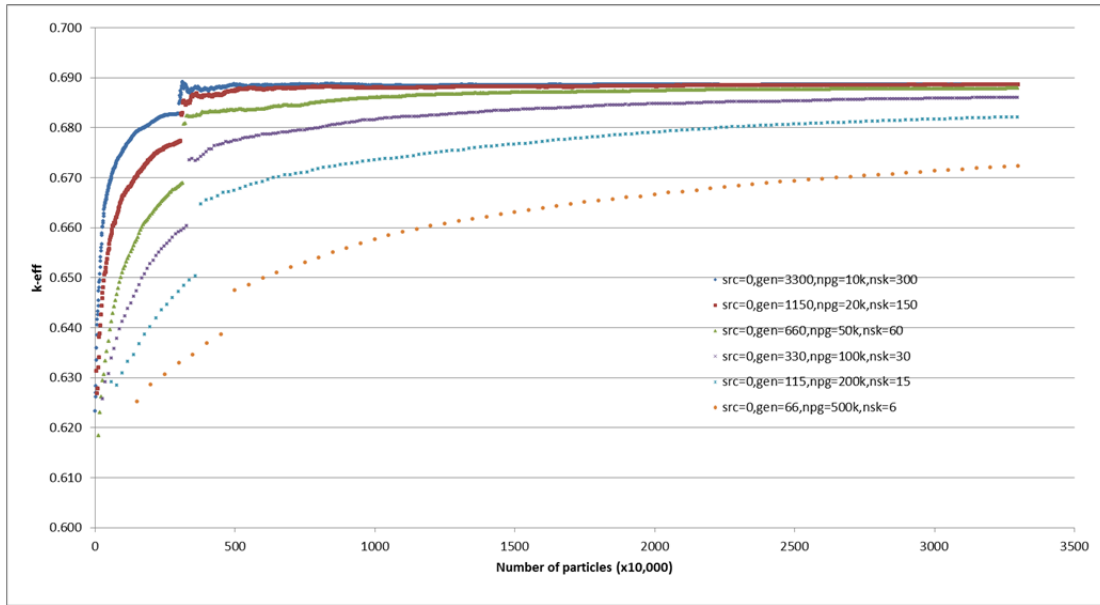


Figure 2. Convergence as a function of runtime for different number of particles per generation

The next options that we analyzed were the start source options. Several start source options are available in KENO-VI. Among them, option 7 that uses an axial distribution  $(1 - \cos(z))^2$ , with flat distribution of fission points in x-y plane, option 8 with user input axial distribution (flat in x-y) and option 6 with arbitrary user input points.

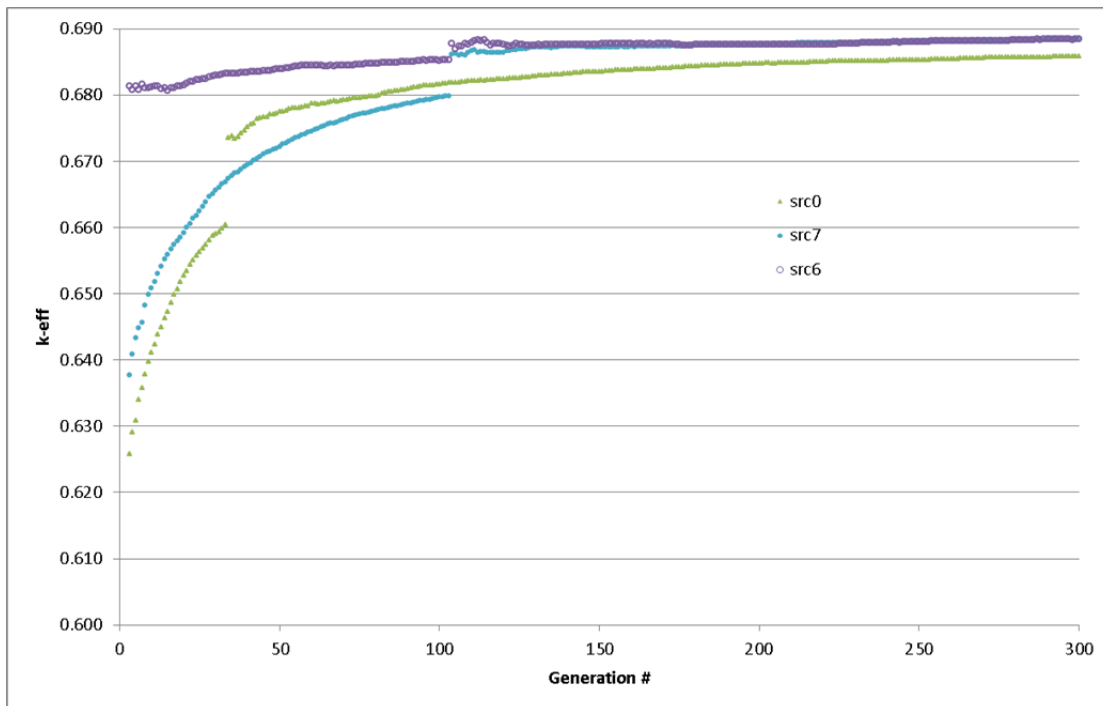


Figure 3. Convergence for different source guess options

Figure 3 compares the approach to convergence with three different source guess options, each running 100k particles per generation. As noticed in this figure, a better initial guess makes for a better start for

the active generations. The figure shows that source option 7 performs better during the non-active generations than a flat source option 0. A user defined source guess that defines the start points to account for the specific conditions in the individual fuel assemblies (fuel enrichment, burnup, and position in the cask) performs further better.

The better start, however, does not seem to necessarily guarantee a faster final convergence, as shown in Figure 4. This figure shows a comparison between the same options 7 and 6 as in Figure 3, but to the end of the calculations (1100 total generations) with a zoom in on the ordinate axis. Source option 0 was excluded from comparison, because it used fewer non-active generations and its later behavior might be due to this, at least in part. For the cases shown in Figure 4, 100 generations were skipped.

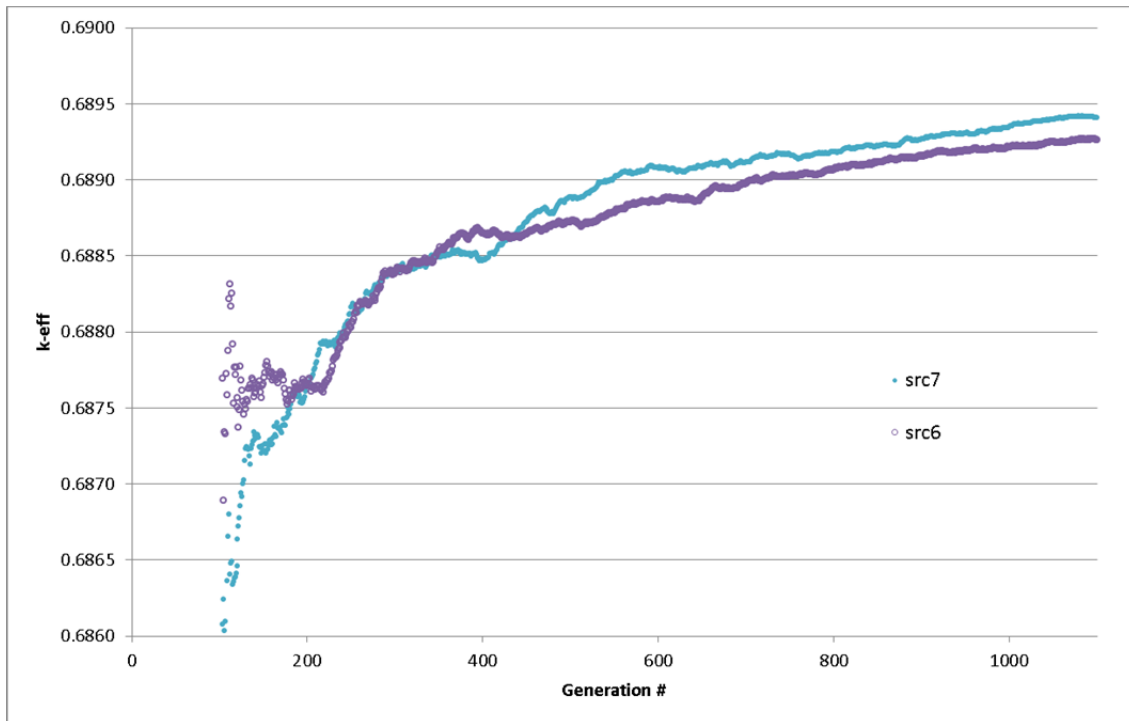


Figure 4. Better initial guess might not necessarily guarantee faster convergence

The final point that we can make from the analysis of the TSC-24 cask refers to the slow convergence of the criticality problem for this cask, discussed theoretically at the beginning of this study. For this purpose, a comparison of different runtimes was conducted for the TSC-24 criticality evolution with the decay (cooling) time of the fuel assemblies.

Figure 5 shows a comparison of the calculated eigenvalue at different decay times with three number of particles (runtimes), from 35 million to 110 million particles, with 100k particles per generation in each case. As one can notice, if the longest runtime is considered as reference, the plot shows that the 35 million case is not converged, within the statistics (in all cases 95% confidence error bars are shown).

In addition to the number of particles comparison the plot in Figure 5 also shows that source options 7 and 6 produce fairly similar results for the same runtime (35 million particles).



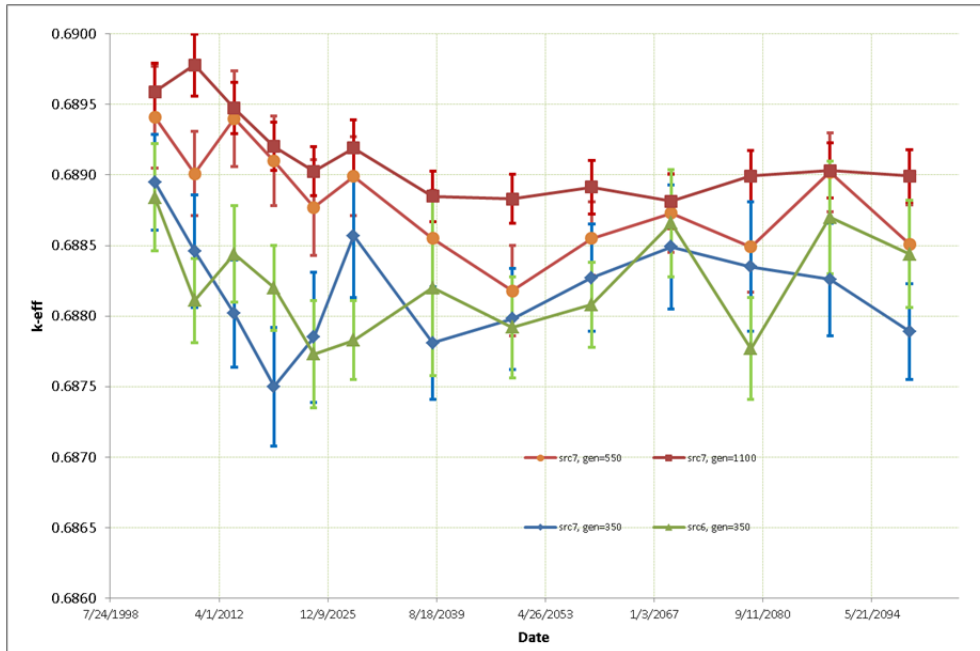


Figure 5. Time evolution of the criticality for TSC-24 for different runtimes

As a conclusion, the analysis presented shows that choosing an optimal combination of source guess, number of particles skipped, number of generations run, number of particles per generation is not straightforward and should be carefully weighted to achieve reliable results. For this purpose, convergence diagnostics in the transport code is desirable. This can be even more useful when automatic calculations are performed, that make difficult or impossible a user's analysis of the convergence behavior.

Also, the long runtimes needed to achieve convergence indicate that implementation of advanced acceleration methods in the Monte Carlo transport code is also highly desirable.

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## APPENDIX B: UNF M&S SYSTEM STATUS

The following tables provide a status listing of the contents within the UNF database and the processed results from the UNF M&S System. Table B-1 identifies the different reactors by ID number and name. The columns are as follows:

First contact –	Indicates if direct contact has been initiated with the utility to acquire additional operations information
Agreement to participate	Indicates if the site has agreed to participate
<b>Reactor Data</b>	<b>Identifies specific reactor data needs, x indicates data in-house</b>
Cycle specific burnup	
Soluble boron	
Rod insertion history	
Moderator Temp	
Axial profile data	
<b>Assembly Data</b>	<b>Identifies specific assembly design information needs, x indicates data in-house</b>
Geometric configuration	
Materials of Construction	
Design dimensions	
Control Components	
<b>Cask Data</b>	<b>Identifies specific cask design information needs, x indicates data in-house</b>
Geometry	
Materials of Construction	
Design Dimension	
Cask Loading Patterns	
Component Loading	
<b>Models</b>	<b>Identifies if specific site template models are available, x indicates templates complete</b>
Triton/Arp	
Criticality	
Thermal	
<b>Discharge isotopics</b>	<b>Identifies is discharge isotopics have been generated, x indicates yes</b>
Bounding	
Nominal	

Tables B-2 and B-3 identify status of PWR and BWR assembly type depletion status, respectively, and which ARP libraries are available. Table B-4 provides status on an individual site basis for how many assemblies have been processed and have unique discharge compositions available.

Table B-1. Status of information collected for the different sites

ID	Reactor	First contact	Agreement to participate	Reactor Data										Assembly Data				Cask Data				Discharge isotopics	Bounding	Nominal		
				Cycle specific burnup	Soluble boron	Rod insertion history	Moderator Temp	Axial profile data	Geometric configuration	Materials of Construction	Design dimensions	Control Components	Geometry	Materials of Construction	Design Dimension	Cask Loading Patterns	Component Loading	Triton/Arp	Criticality	Thermal						
101	Farley - Unit 1																							0.00	0.00	
102	Farley - Unit 2																								0.00	0.00
301	Palo Verde - Unit 1																								0.00	0.00
302	Palo Verde - Unit 2																								0.00	0.00
303	Palo Verde - Unit 3																								0.00	0.00
401	Arkansas Nuclear One - Unit 1																								0.00	0.00
402	Arkansas Nuclear One - Unit 2																								0.00	0.00
501	Calvert Cliffs - Unit 1	X	X																						0.00	0.00
502	Calvert Cliffs - Unit 2	X	X																						0.00	0.00
601	Pilgrim - Unit 1																								0.00	0.00
701	Brunswick - Unit 1																								0.00	0.00
702	Brunswick - Unit 2																								0.00	0.00
703	Shearon Harris 1																								100.00	0.00
705	H. B. Robinson																								0.00	0.00
901	Perry - Unit 1																								100.00	0.00
1001	Braidwood - Unit 1																								100.00	0.00
1002	Braidwood - Unit 2																								100.00	0.00
1003	Byron - Unit 1																								100.00	0.00
1004	Byron - Unit 2																								100.00	0.00
1005	Dresden - Unit 1 (D)																								0.00	0.00
1006	Dresden - Unit 2																								0.00	0.00
1007	Dresden - Unit 3																								0.00	0.00
1008	LaSalle County - Unit 1																								100.00	0.00
1009	LaSalle County - Unit 2																								100.00	0.00
1010	Quad Cities - Unit 1																								23.06	0.00
1011	Quad Cities - Unit 2																								25.55	0.00
1012	Zion - Unit 1																								0.00	0.00
1013	Zion - Unit 2																								0.00	0.00
1101	Indian Point - Unit 1																								0.00	0.00
1102	Indian Point - Unit 2																								0.00	0.00
1201	Big Rock Point																								0.00	0.00
1204	Palisades																								0.00	0.00
1301	Lacrosse																								0.00	0.00
1402	Enrico Fermi 2																								0.00	0.00
1501	Catawba - Unit 1	X	X																						0.00	0.00
1502	Catawba - Unit 2	X	X																						0.00	0.00
1504	McGuire - Unit 1	X	X																						0.00	0.00
1505	McGuire - Unit 2	X	X																						0.00	0.00
1506	Oconee - Unit 1	X	X																						0.00	0.00
1507	Oconee - Unit 2	X	X																						0.00	0.00
1508	Oconee - Unit 3	X	X																						0.00	0.00
1601	Beaver Valley - Unit 1																								0.00	0.00
1602	Beaver Valley - Unit 2																								0.00	0.00
1701	Crystal River 3																								0.00	0.00
1801	St Lucie - Unit 1																								34.55	0.00
1802	St Lucie - Unit 2																								48.95	0.00
1803	Turkey Point - Unit 3																								0.00	0.00
1804	Turkey Point - Unit 4																								0.00	0.00
1901	Three Mile Island - Unit 1																								31.63	0.00
1903	Oyster Creek																								31.00	0.00
2001	Hatch - Unit 1																								100.00	0.00
2002	Hatch - Unit 2																								100.00	0.00
2003	Vogtle - Unit 1																								66.78	0.00
2004	Vogtle - Unit 2																								100.00	0.00
2101	River Bend																								100.00	0.00
2201	South Texas Project - Unit 1																								89.63	0.00
2202	South Texas Project - Unit 2																								100.00	0.00
2301	Clinton - Unit 1																								100.00	0.00
2401	Duane Arnold																								33.05	0.00
2501	Wolf Creek																								100.00	0.00
2701	Waterford 3																								100.00	0.00
2801	Maine Yankee	X	X			X																			100.00	0.00
2901	Grand Gulf																								100.00	0.00
3001	Cooper Station																								100.00	0.00
3101	Nine Mile Point - Unit 1																								13.95	0.00
3102	Nine Mile Point - Unit 2																								100.00	0.00
3201	Millstone - Unit 1																								28.33	0.00
3202	Millstone - Unit 2																								100.00	0.00
3203	Millstone - Unit 3																								90.37	0.00
3301	Monticello																								1.83	0.00
3302	Prairie Island - Unit 1																								0.00	0.00
3303	Prairie Island - Unit 2																								0.00	0.00



Table B-2. Status of PWR assembly class depletion information

Assembly Class	Assembly code	Geometric data	Materials of Construction	Design dimensions	Control Components	Bounding ARP Libraries	Nominal Arp Libraries
B&W 15x15	B1515B						
B&W 15x15	B1515B10						
B&W 15x15	B1515B3						
B&W 15x15	B1515B4						
B&W 15x15	B1515B4Z						
B&W 15x15	B1515B5						
B&W 15x15	B1515B5Z						
B&W 15x15	B1515B6						
B&W 15x15	B1515B7						
B&W 15x15	B1515B8						
B&W 15x15	B1515B9						
B&W 15x15	B1515BGD						
B&W 15x15	B1515BZ						
B&W 15x15	B1515W						
CE 14x14	C1414A						
CE 14x14	C1414C						
CE 14x14	C1414W						
CE 14x14	XFC14A						
CE 14x14	XFC14C						
CE 14x14	XFC14W						
CE 16x16 <sup>b</sup>	C1616CSD						
CE 16x16 <sup>b</sup>	C8016C						
CE 16x16 <sup>b</sup>	XSL16C						
W 14x14	W1414A						
W 14x14	W1414ATR						
W 14x14	W1414B						
W 14x14	W1414WL						
W 14x14	W1414WO						
W 14x14	W1414W						
W 15x15	W1515A						
W 15x15	W1515AHT						
W 15x15	W1515APL						
W 15x15	W1515WL						
W 15x15	W1515WO						

W 15x15	W1515W						
W 15x15	W1515WV5						
W 17x17	W1717A						
W 17x17	W1717B						
W 17x17	W1717WRF						
W 17x17	W1717WVJ						
W 17x17	W1717WL						
W 17x17	W1717WVH						
W 17x17	WST17W						
W 17x17	B1717B						
W 17x17	W1717WO						
W 17x17	W1717WP						
W 17x17	W1717WV						
W 17x17	W1717WV+						
W 17x17	W1717WV5						
<b>Reactor-specific assembly class</b>							
Palisades	XPA15A						
Palisades	XPA15C						
Yankee Rowe	XYR16A						
Yankee Rowe	XYR16C						
Yankee Rowe	XYR16U						
Yankee Rowe	XYR18W						
San Onofre-1	XSO14W						
San Onofre-1	XSO14WD						
San Onofre-1	XSO14WM						
Haddam Neck	XHN15B						
Haddam Neck	XHN15BZ						
Haddam Neck	XHN15HS						
Haddam Neck	XHN15HZ						
Haddam Neck	XHN15MS						
Haddam Neck	XHN15MZ						
Haddam Neck	XHN15W						
Haddam Neck	XHN15WZ						
Indian Point-1	XIP14W						

Table B-3. Status of BWR assembly class depletion information

Assembly Class	Assembly code	Geometric data	Materials of Construction	Design dimensions	Control Components	Bounding ARP Libraries	Nominal Arp Libraries
GE BWR/2,3	G2307A						
GE BWR/2,3	G2307G2A						
GE BWR/2,3	G2307G2B						
GE BWR/2,3	G2307G3						
GE BWR/2,3	G2308A						
GE BWR/2,3	G2308AP						
GE BWR/2,3	G2308G10						
GE BWR/2,3	G2308G4						
GE BWR/2,3	G2308G5						
GE BWR/2,3	G2308G7						
GE BWR/2,3	G2308G8A						
GE BWR/2,3	G2308G8B						
GE BWR/2,3	G2308G9						
GE BWR/2,3	G2308GB						
GE BWR/2,3	G2308GP						
GE BWR/2,3	G2309A						
GE BWR/2,3	G2309AIX						
GE BWR/2,3	G2309G11						
GE BWR/2,3	9X9IXQFA						
GE BWR/4-6	G4607G2						
GE BWR/4-6	G4607G3A						
GE BWR/4-6	G4607G3B						
GE BWR/4-6	G4608AP						
GE BWR/4-6	G4608G10						
GE BWR/4-6	G4608G11						
GE BWR/4-6	G4608G12						
GE BWR/4-6	G4608G4A						
GE BWR/4-6	G4608G4B						
GE BWR/4-6	G4608G5						
GE BWR/4-6	G4608G8						
GE BWR/4-6	G4608G9						
GE BWR/4-6	G4608GB						
GE BWR/4-6	G4608GP						
GE BWR/4-6	G4608W						
GE BWR/4-6	G4609A						



GE BWR/4-6	G4609A5						
GE BWR/4-6	G4609A9X						
GE BWR/4-6	G4609AIX						
GE BWR/4-6	G4609AX+						
GE BWR/4-6	G4609G11						
GE BWR/4-6	G4609G13						
GE BWR/4-6	G4610A						
GE BWR/4-6	G4610AIX						
GE BWR/4-6	G4610C						
GE BWR/4-6	G4610G12						
GE BWR/4-6	G4610G14						
GE BWR/4-6	ATRIUM10						
<b>Reactor-specific assembly class</b>							
Dresden-1	XDR06A						
Dresden-1	XDR06G						
Dresden-1	XDR07GS						
Dresden-1	XDR08G						
Dresden-1	XDR06G3B						
Dresden-1	XDR06G3F						
Dresden-1	XDR06G5						
Dresden-1	XDR06U						
Humboldt Bay	XHB06A						
Humboldt Bay	XHB06G						
Humboldt Bay	XHB07G2						
LaCrosse <sup>a</sup>	XLC10L						
LaCrosse <sup>a</sup>	XLC10A						
Big Rock Point	XBR09A						
Big Rock Point	XBR11A						
Big Rock Point	XBR07G						
Big Rock Point	XBR08G						
Big Rock Point	XBR09G						
Big Rock Point	XBR11G						
Big Rock Point	XBR11N						

Table B-4. Status of reactor discharge concentrations available

ID	Reactor	Discharge isotopics - Assembly Count	Bounding	Bounding Progress	Nominal	Nominal Progress
101	Farley - Unit 1	1050	0	0.00	0	0.00
102	Farley - Unit 2	961	0	0.00	0	0.00
301	Palo Verde - Unit 1	948	0	0.00	0	0.00
302	Palo Verde - Unit 2	948	0	0.00	0	0.00
303	Palo Verde - Unit 3	851	0	0.00	0	0.00
401	Arkansas Nuclear One - Unit 1	1043	0	0.00	0	0.00
402	Arkansas Nuclear One - Unit 2	1026	0	0.00	0	0.00
501	Calvert Cliffs - Unit 1	1242	0	0.00	0	0.00
502	Calvert Cliffs - Unit 2	1068	0	0.00	0	0.00
601	Pilgrim - Unit 1	2274	0	0.00	0	0.00
701	Brunswick - Unit 1	2360	0	0.00	0	0.00
702	Brunswick - Unit 2	2356	0	0.00	0	0.00
703	Shearon Harris 1	577	577	100.00	0	0.00
705	H. B. Robinson	1149	0	0.00	0	0.00
901	Perry - Unit 1	2088	2088	100.00	0	0.00
1001	Braidwood - Unit 1	726	726	100.00	0	0.00
1002	Braidwood - Unit 2	759	759	100.00	0	0.00
1003	Byron - Unit 1	932	932	100.00	0	0.00
1004	Byron - Unit 2	854	854	100.00	0	0.00
1005	Dresden - Unit 1 (D)	892	0	0.00	0	0.00
1006	Dresden - Unit 2	3741	0	0.00	0	0.00

1007	Dresden - Unit 3	2976	0	0.00	0	0.00
1008	LaSalle County - Unit 1	2194	2194	100.00	0	0.00
1009	LaSalle County - Unit 2	1912	1912	100.00	0	0.00
1010	Quad Cities - Unit 1	3161	729	23.06	0	0.00
1011	Quad Cities - Unit 2	2955	755	25.55	0	0.00
1012	Zion - Unit 1	1143	0	0.00	0	0.00
1013	Zion - Unit 2	1083	0	0.00	0	0.00
1101	Indian Point - Unit 1	160	0	0.00	0	0.00
1102	Indian Point - Unit 2	1078	0	0.00	0	0.00
1201	Big Rock Point	527	0	0.00	0	0.00
1204	Palisades	1081	0	0.00	0	0.00
1301	Lacrosse	334	0	0.00	0	0.00
1402	Enrico Fermi 2	1708	0	0.00	0	0.00
1501	Catawba - Unit 1	944	0	0.00	0	0.00
1502	Catawba - Unit 2	836	0	0.00	0	0.00
1504	McGuire - Unit 1	1072	0	0.00	0	0.00
1505	McGuire - Unit 2	1020	0	0.00	0	0.00
1506	Oconee - Unit 1	1186	0	0.00	0	0.00
1507	Oconee - Unit 2	1156	0	0.00	0	0.00
1508	Oconee - Unit 3	1103	0	0.00	0	0.00
1601	Beaver Valley - Unit 1	876	0	0.00	0	0.00
1602	Beaver Valley - Unit 2	580	0	0.00	0	0.00
1701	Crystal River 3	824	0	0.00	0	0.00
1801	St Lucie - Unit 1	1369	473	34.55	0	0.00
1802	St Lucie - Unit 2	909	445	48.95	0	0.00
1803	Turkey Point - Unit 3	941	0	0.00	0	0.00
1804	Turkey Point - Unit 4	939	0	0.00	0	0.00
1901	Three Mile Island - Unit 1	898	284	31.63	0	0.00
1903	Oyster Creek	2800	868	31.00	0	0.00
2001	Hatch - Unit 1	3079	3079	100.00	0	0.00
2002	Hatch - Unit 2	2756	2756	100.00	0	0.00
2003	Vogtle - Unit 1	900	601	66.78	0	0.00
2004	Vogtle - Unit 2	739	739	100.00	0	0.00
2101	River Bend	2148	2148	100.00	0	0.00

2201	South Texas Project - Unit 1	627	562	89.63	0	0.00
2202	South Texas Project - Unit 2	627	627	100.00	0	0.00
2301	Clinton - Unit 1	1580	1580	100.00	0	0.00
2401	Duane Arnold	1912	632	33.05	0	0.00
2501	Wolf Creek	925	925	100.00	0	0.00
2701	Waterford 3	960	960	100.00	0	0.00
2801	Maine Yankee	1434	1434	100.00	0	0.00
2901	Grand Gulf	3160	3160	100.00	0	0.00
3001	Cooper Station	2593	2593	100.00	0	0.00
3101	Nine Mile Point - Unit 1	2524	352	13.95	0	0.00
3102	Nine Mile Point - Unit 2	1932	1932	100.00	0	0.00
3201	Millstone - Unit 1	2884	817	28.33	0	0.00
3202	Millstone - Unit 2	1020	1020	100.00	0	0.00
3203	Millstone - Unit 3	654	591	90.37	0	0.00
3301	Monticello	2400	44	1.83	0	0.00
3302	Prairie Island - Unit 1	909	0	0.00	0	0.00
3303	Prairie Island - Unit 2	906	0	0.00	0	0.00
3401	Fort Calhoun	839	299	35.64	0	0.00
3501	Diablo Canyon - Unit 1	908	908	100.00	0	0.00
3502	Diablo Canyon - Unit 2	828	828	100.00	0	0.00
3503	Humboldt Bay	390	0	0.00	0	0.00
3601	Susquehanna - Unit 1	2956	2956	100.00	0	0.00
3602	Susquehanna - Unit 2	2584	2584	100.00	0	0.00
3701	Limerick - Unit 1	2335	2331	99.83	0	0.00
3702	Limerick - Unit 2	2266	2248	99.21	0	0.00
3704	Peach Bottom - Unit 2	3594	3592	99.94	0	0.00
3705	Peach Bottom - Unit 3	3333	3332	99.97	0	0.00
3801	Trojan	780	780	100.00	0	0.00
3901	Fitzpatrick	2664	0	0.00	0	0.00
3902	Indian Point - Unit 3	833	0	0.00	0	0.00
4201	Hope Creek	2376	0	0.00	0	0.00
4202	Salem - Unit 1	992	0	0.00	0	0.00
4203	Salem - Unit 2	812	0	0.00	0	0.00
4401	Ginna	1007	0	0.00	0	0.00
4501	Rancho Seco	493	0	0.00	0	0.00

4601	V.C. Summer	812	0	0.00	0	0.00
4701	San Onofre - Unit 1	665	0	0.00	0	0.00
4702	San Onofre - Unit 2	1096	505	46.08	0	0.00
4703	San Onofre - Unit 3	999	516	51.65	0	0.00
4803	Browns Ferry - Unit 1	1584	1584	100.00	0	0.00
4804	Browns Ferry - Unit 2	2952	2952	100.00	0	0.00
4805	Browns Ferry - Unit 3	2160	2160	100.00	0	0.00
4808	Sequoyah - Unit 1	815	0	0.00	0	0.00
4809	Sequoyah - Unit 2	884	488	55.20	0	0.00
4810	Watts Bar - Unit 1	297	0	0.00	0	0.00
4901	Comanche Peak - Unit 1	744	0	0.00	0	0.00
4902	Comanche Peak - Unit 2	529	529	100.00	0	0.00
5001	Davis-Besse	821	821	100.00	0	0.00
5101	Callaway	1118	1118	100.00	0	0.00
5201	North Anna - Unit 1	926	926	100.00	0	0.00
5202	North Anna - Unit 2	964	964	100.00	0	0.00
5203	Surry - Unit 1	1015	0	0.00	0	0.00
5204	Surry - Unit 2	998	52	5.21	0	0.00
5302	Columbia	2244	2244	100.00	0	0.00
5401	Point Beach - Unit 1	920	0	0.00	0	0.00
5402	Point Beach - Unit 2	802	0	0.00	0	0.00
5501	Kewaunee	904	0	0.00	0	0.00
5601	Yankee Rowe	533	0	0.00	0	0.00
5701	Haddam Neck	1102	0	0.00	0	0.00
5801	Cook - Unit 1	1238	0	0.00	0	0.00
5802	Cook - Unit 2	960	304	31.67	0	0.00
5901	Seabrook	624	559	89.58	0	0.00
6001	Vermont Yankee	2671	708	26.51	0	0.00
TOTALS		163646	76436	46.71	0	0.00