

**INTEGRATED DATA AND ANALYSIS SYSTEM FOR
COMMERCIAL USED NUCLEAR FUEL SAFETY ASSESSMENTS**

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ABSTRACT

Uncertainties related to meeting packaging and transportation regulatory criteria are increasing as commercial used nuclear fuel (UNF) is being stored at reactor sites for longer time intervals than originally foreseen. As the storage times continue to increase issues associated with aging management and the potential consequences of the deleterious effects of aging will need to be assessed. The assessments demonstrate the continued efficacy of the storage system over extended storage (ES) periods, and also evaluate safety for subsequent transportation following ES. Licensed storage and transportation cask systems have well-defined assembly-loading criteria (e.g., specifications for “approved contents” in a storage cask system’s Certificate of Compliance). These specifications are typically used to define *limiting* loading conditions and characteristics for which the cask system’s safety analysis report has demonstrated compliance with the applicable regulatory requirements. In practice, due to the diversity in the discharged UNF available for loading (e.g., variations in UNF assembly burnup values, initial enrichments, discharge date, etc.), it is not possible to load a cask system with UNF assemblies that correspond exactly to the limiting licensing conditions. Hence, cask systems are loaded with assemblies that satisfy the limiting loading conditions with some amount of unquantified, uncredited margin. This reality in storage and transportation cask loading provides additional conservatism with respect to the regulatory safety requirements. These potentially large (depending on the specific loading conditions) safety margins may be quantified and potentially credited in the future to offset uncertainties in safety margins associated with ES and high-burnup fuel issues. To investigate this possibility, an integrated data and analysis capability is being developed to estimate safety margins in actual as-loaded storage and transportation casks. This paper describes how UNF inventory data, fuel assembly design data, site-specific cask loading data, and reactor operating data are coupled with fuel depletion, criticality safety, and thermal computational analysis capabilities to provide out-of-reactor nuclear safety evaluations in an autonomous manner. Comparisons with limiting loading specifications are provided to quantify the available margin present in a variety of cask systems being used at different nuclear sites.

INTRODUCTION

Commercial used nuclear fuel (UNF) in the United States is expected to remain in storage for considerably longer time periods than were originally intended (e.g., <40 years). Extended storage (ES) time and irradiation of nuclear fuel to high-burnup values (>45 GWd/t) results in increased uncertainties related to aging management of the structures, systems, and components important to safety during normal, off-normal, and accident conditions of ES and subsequent transportation. An integrated waste management system involves managing the waste from the time it is discharged from the reactor and designated as UNF to the time it is disposed of in a geologic repository. A set of possible pathways to developing the waste management system, as depicted in the *Strategy for the Management and Disposal of Used Nuclear Fuel and High-Level Radioactive Waste* [1], is presented in Figure 1. Because the UNF may be stored, transported, and handled multiple times before resting in a geologic repository, uncertainties associated with the physical characteristics of the fuel assemblies and canister systems will propagate and compound with time. However, these uncertainties need to be understood and addressed at each operational transition. To adequately implement aging management strategies in the future for shipping, handling, and ultimate disposal, considerations must be made to ensure that the fuel assembly data and other information needed to support UNF characterization activities are available and maintained.

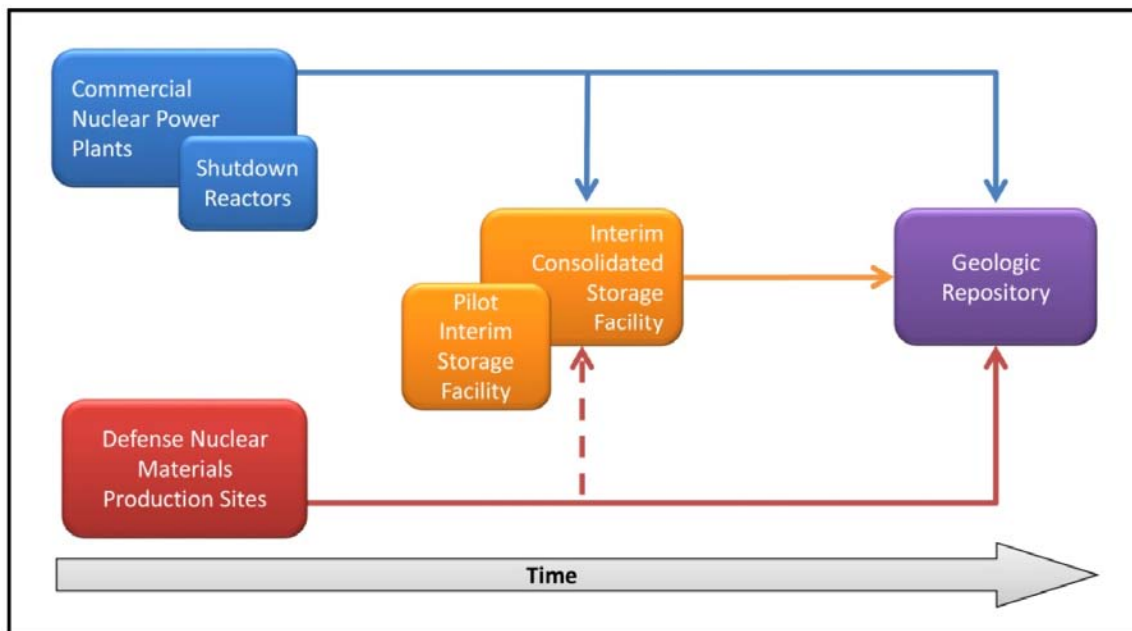


Figure 1. Possible waste management system pathways

To facilitate modeling and analysis capabilities for existing storage and transportation systems for used fuel management, a centralized, comprehensive, and integrated data and analysis tool is being assembled—UNF-Storage, Transportation & Disposal Analysis Resource and Data System (UNF-ST&DARDS). UNF-ST&DARDS is currently being developed to provide the foundation for tracking UNF from cradle to grave throughout the waste management system. Initial work is focused on building the system infrastructure and integrating existing data and analysis capabilities. The information generated by UNF-ST&DARDS allows realistic assessments of the current and future state of the UNF assemblies and canister systems from both a nuclear and mechanical performance perspective.

Performing actual as-loaded canister-specific evaluations is a unique capability that has been incorporated into UNF-ST&DARDS. Overly conservative analyses based on bounding generic canisters could lead to prematurely invoking compensatory measures within the waste management system, such as repackaging already packaged fuel, canning a significant fraction of UNF prior to storage, or requiring additional criticality control prior to transport and disposal (e.g., inserting control rod assemblies). For example, current thermal analysis methods typically overpredict the time-dependent temperature profiles by an amount that is not readily quantifiable in general, and would vary widely based on the individual characteristics of a given site. This would hinder efforts to accurately predict the potential for confinement breaches due to low-temperature degradation phenomena (e.g. deliquescence) and would tend to overpredict the number of fuel rods that may potentially fail during extended storage and/or transportation due to mechanical property changes (e.g., hydride reorientation). Computational power and software tools have progressed to the point that accurate and efficient evaluation of safety margins for specific UNF canisters, accounting for the actual as-loaded contents, is possible.

Initial development of UNF-ST&DARDS has been a collaboration between multiple national laboratories and several utilities. The system infrastructure consists of a UNF centralized database (which is designed to be fully comprehensive, with new data still being added), coupled with analysis tools for out-of-reactor nuclear safety analyses. Automation sequences have been developed and initiated to generate data that can be used to assess the state of specific populations of the UNF over time including UNF characterizations, neutronics analyses, and thermal analyses. Other technical areas such as dose, containment, and structural analyses are expected to be incorporated in the future. The centralized database currently stores data as a function of decay for ~150,000 UNF assemblies. Additionally, the system has been designed to meet robust QA requirements and maintains full data traceability within the database system.

The principal objectives of UNF-ST&DARDS is to provide a single controlled database to supply technical data for various waste management system analysis/evaluation tools as well as fuel cycle systems analyses, provide access to key technical data and analysis capabilities to characterize the UNF inventory, facilitate determinations of realistic safety margins and conditions of existing UNF in dry storage, and enable assessments of risks and uncertainties associated with the aging of discharged nuclear fuel and ramifications regarding transportability. This paper describes how UNF inventory data, fuel assembly design data, site-specific cask loading data, and reactor operating data are coupled with fuel depletion, criticality safety, and thermal analysis computational capabilities to provide out-of-reactor nuclear safety analyses/evaluations.

DATA COLLECTION

Data collection activities have been focused on UNF discharge data as well as UNF storage and transportation systems data. The most recent nuclear fuel discharge and storage data cover UNF discharged from commercial reactors as of December 31, 2002 [2]. These data, referred to as the RW-859 database, contain basic discharge information for 70,292 pressurized water reactor (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 US PWRs and BWRs as of December 31, 2002 [3]. The data collection authorization is under the auspices of the US Department of Energy (DOE) Office of the General Counsel, and the nuclear data survey has been designated as Form GC-859. Available spent fuel discharge data have not been updated since

2002, via the RW-859/GC-859 process [2], and as currently designed, the form does not include assembly-specific and reactor-cycle-specific information commonly used in detailed safety analyses (e.g., depletion parameter ranges used for UNF discharge characterization). Hence, additional effort is being applied to collect and consolidate useful and relevant data pertaining to UNF irradiation histories. This type of information would be necessary to support adequate demonstrations of the parameter bounds used to characterize the UNF.

Technical data contained within UNF-ST&DARDS includes UNF characteristics data, initial enrichments, burnup, assembly discharge dates, canister loading dates, canister/cask system data, and reactor cycle-specific data. Currently, there are four main types of data in the centralized database: (1) the RW-859 fuel assembly discharge information from the Energy Information Administration [2]; (2) fuel assembly design data; (3) reactor-specific operation data; and (4) cask design and loading data. The data is organized in relational structured query language (SQL) data tables within a MySQL database. Additional data sets related to individual facility data to support systems and routing analyses are expected to be added in the future.

Collection of additional data from the nuclear industry has been initiated with the help of the Nuclear Energy Institute (NEI). Reactor operating data, along with cask loading information for the Independent Spent Fuel Storage Installation (ISFSI) sites, have been provided by several nuclear utilities including the Tennessee Valley Authority and Duke Energy. ISFSI site data and some supplemental operations information have also been collected for the decommissioned reactors Connecticut Yankee (Haddam Neck), Maine Yankee, and Yankee Rowe. The data are currently being evaluated and incorporated into the centralized database. Additional data will continue to be incorporated as it becomes available.

ANALYSIS CAPABILITIES

The centralized database and the nuclear safety analysis automation tools have been developed simultaneously and consistently. Initial development capabilities have been focused on neutronics analyses and thermal analyses. Neutronics analyses are used to demonstrate key safety requirements [4, 5] and include both depletion and criticality calculations. Fundamentally, all analyses regarding UNF begin with understanding and simulating the nuclear material transformation process that the fresh fuel goes through to become UNF (i.e., characterizing the UNF is the least common denominator in nuclear related analyses). For example, a depletion calculation predicts 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. Thermal analyses are used to calculate component temperatures (e.g., peak clad temperature) and are also fundamental to understanding degradation mechanisms.

A collection of model templates for computer codes dedicated to out-of-reactor nuclear safety analyses (i.e., depletion/decay, criticality, and thermal analyses) has been developed for different reactor sites and storage and transportation system variants. Within UNF-ST&DARDS a template engine (or template processor) is used to combine site-specific input parameters from the centralized database with the model templates developed for the neutronics 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. The

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 (3) 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 [6], which is widely used for version control of files.

Technical data collection and its synthesis into appropriate formats are based on the well-established Standardized Computer Analysis for Licensing Evaluation (SCALE) code system [7] and the thermal-hydraulic analysis code COolant Boiling in Rod Arrays–Spent Fuel Storage (COBRA–SFS) [8] input requirements. The system has been built around the SCALE and COBRA-SFS codes, but the template building process is independent of code choice, and could be readily adapted for other neutronics or thermal-hydraulics codes.

Within UNF-ST&DARDS, the SCALE code system provides the computer codes and sequences for running depletion calculations. The TRITON two-dimensional (2D) depletion sequence [7] 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. This information can subsequently be used by ORIGEN-ARP [7] for rapid processing of problem-dependent cross sections. The TRITON 2D depletion calculation sequence employs CENTRM [7] for multi-group cross-section processing, NEWT [7] for 2D discrete-ordinates transport calculations, and ORIGEN-S [7] for depletion and decay calculations. The resultant nuclide concentrations and decay heat source terms are passed to the criticality and thermal analysis codes, respectively. The SCALE CSAS6 [7] criticality analysis sequence is used to perform criticality calculations 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} .

TRITON model templates have been developed for assembly types representative of the PWR Westinghouse (W) 14×14, 15×15, and 17×17, Babcock and Wilcox (B&W) 15×15, Combustion Engineering (CE) 14×14 and 16×16 assemblies, and custom assemblies for Yankee Rowe, Palisades, San Onofre, Haddam Neck, and Indian Point unit 1 reactors. Initial CSAS6 (KENO-VI) and COBRA-SFS model templates have been developed that are representative of the Trojan MPC-24E/EF, Rancho Seco Nuhoms-24PT, NAC UMS[®]-24 and UMS[®]-26, and Holtec MPC-32 storage canisters with appropriate representative assembly types for specific sites where these systems are deployed. Initial focus has been primarily based on vertical storage systems for PWR fuel, but models for horizontal storage systems as well as BWR fuel are currently in development. The model template database is continuously being updated as site-specific and assembly-specific data become available. A graphical depiction of the data and tool interface is presented in Figure 2.

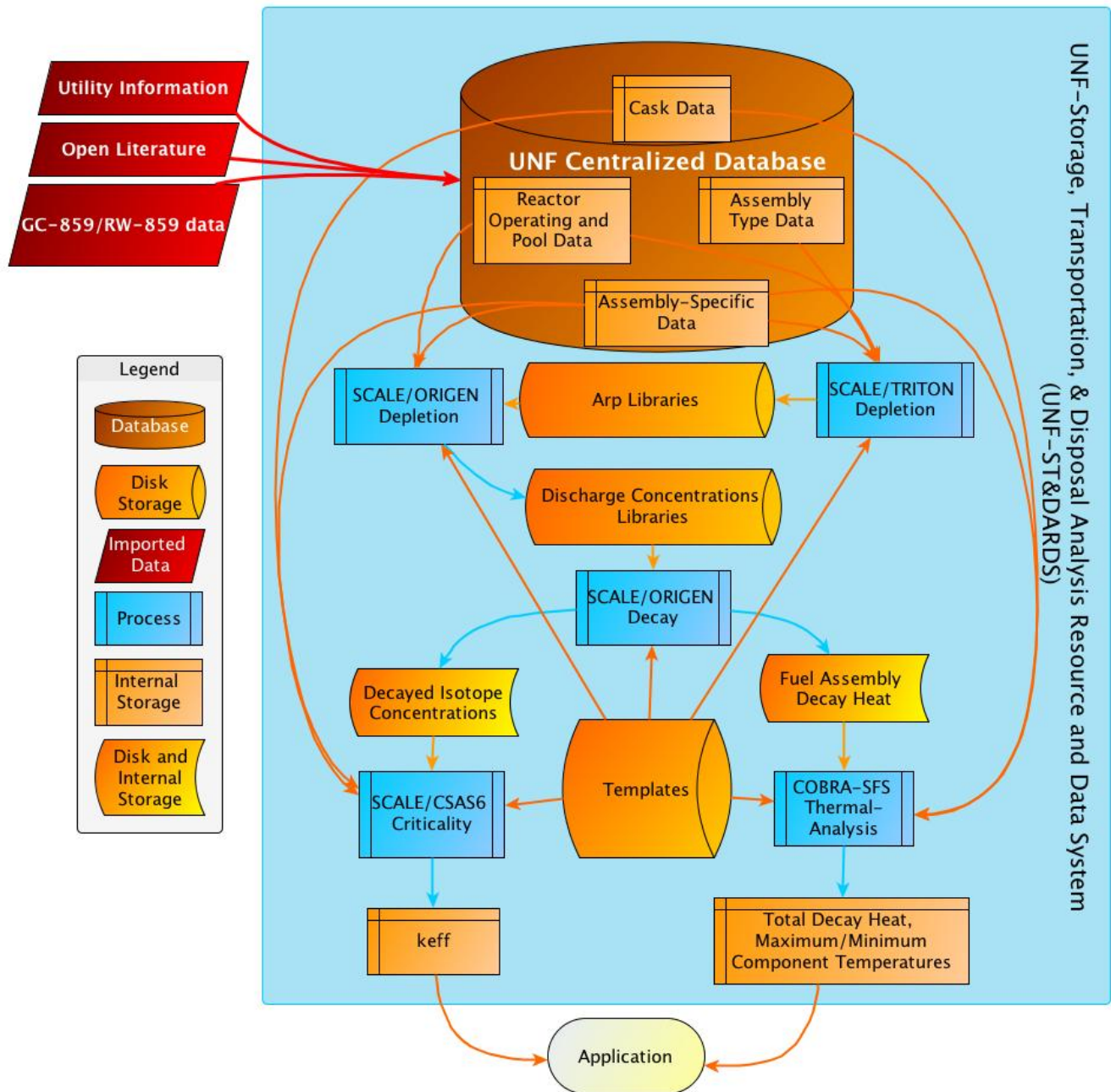


Figure 2. Data flow for analysis tools.

APPLICATION

An application of UNF-ST&DARDS can be executed through a graphical user interface (GUI) or via a command line. Upon execution, UNF-ST&DARDS creates JSON files that are used with the template engine and previously generated templates to create an input file that is then run by the appropriate code. The root template file is the main template for a given code's input file, and this file guides the template engine in assembling the various input parameter blocks and structures. The main template calls for the importation of various sets of sub-templates that build the functional units of the file. An example of a TRITON root template file stored within UNF-ST&DARDS, TDepl.tpl, is presented in Figure 3. The

“#” symbol is used to tell the template engine to execute a command. For example the “#import” tells the template engine to import the information from the “<assembly.type>.title.tmpl” template. The main template imports other templates based on different JSON objects such as <assembly.type>. Additionally, various logic flags signal whether a particular feature is present or not in a model (e.g., if the flag “bpra_present” is set to “true”, this tells the template engine to include any structures and materials related to a specified number of a specified type of burnable poison rod).

```

#import TemplateHeader.tmpl

=t-depl parm=(centrm,addnux=4,weight)
#import <assembly.type>.title.tmpl
<xslib>
'-----
' --- Rod array layout and naming ---
'-----
#import <assembly.type>.layout.comment.tmpl
'
' half assembly pitch is #eval fmt=%6.4f (0.5*<assembly.pitch>) as hap# cm
' fuel rod half pitch is #eval fmt=%6.4f (0.5*<fuel_pin.pitch>) as frhp# cm
'-----
' --- Alias Data ---
'-----
#import aliases/<assembly.type>.tmpl
'-----
' --- Composition Data ---
'-----
#import compositions/<assembly.type>.tmpl
'-----
' --- Cell Data ---
'-----
#import celldata/<assembly.type>.tmpl
'-----
' --- Depletion Data ---
'-----
#import depletion_data/<assembly.type>.tmpl
'-----
' --- Timetable Data -Tfuel, Cdens, Bconc etc ---
'-----
#import timetable_data/<assembly.type>.<reactor>.tmpl
'-----
' --- Burn Data ---
'-----
#import burn_data/<assembly.type>.<reactor>.tmpl
'-----
' --- Keep Data ---
'-----
#import keep_data/<assembly.type>.tmpl
'-----
' --- Model Data ---
'-----
#import model_data/<assembly.type>.tmpl
'-----
' --- Opus Data ---
'-----
#import <assembly.type>.opus_data.tmpl
End
'-----
' --- Save Data ---
'-----
#import <assembly.type>.save_data.tmpl

```

Figure 3. Example root template file.

Generation of the corresponding criticality or thermal model inputs is performed in a similar manner. Essentially, a full canister/cask model is assembled from a base canister/cask model that is filled with the fuel assemblies and burnup-dependent material data. The actual canister/cask-specific geometry,

assembly geometry data, and material data for the fuel assemblies and the fuel material compositions are provided for the selected analysis (e.g., criticality or thermal) by UNF-ST&DARDS. UNF-ST&DARDS obtains the decay data and writes this information to a JSON file. The file structure of the criticality template, along with the required JSON objects, is illustrated in Fig. 4.

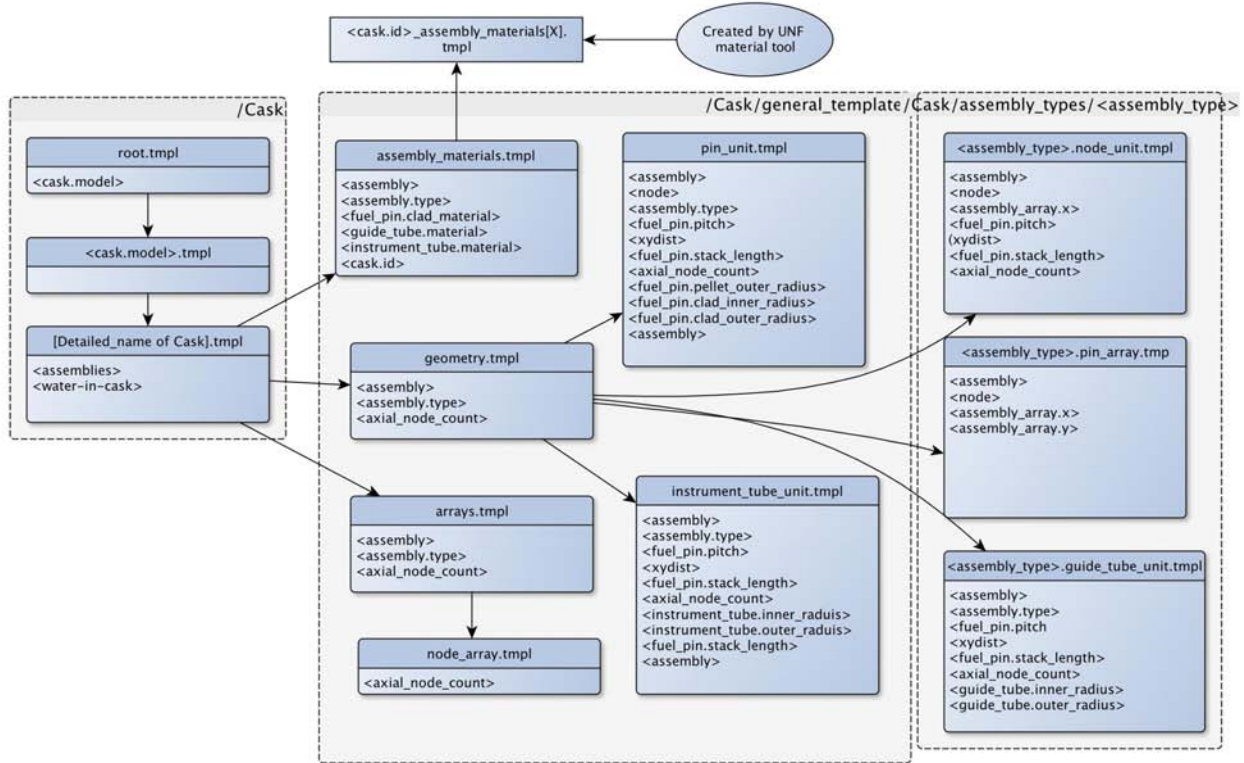


Fig. 4. File structure and associated JSON objects for the criticality calculations.

Explicit analyses (depletion, decay, criticality, and thermal) for all UNF assemblies and canisters/casks at a given site can be completed autonomously once UNF-ST&DARDS is executed. A process-flow description of the coupled data and analysis capabilities is as follows. Through the GUI or via the command line, a reactor unit or site is selected (e.g., Site A) with a date or dates identified for desired results. Next, UNF-ST&DARDS initiates the sequence of analyses for that site by selecting the appropriate templates and generating the input files from information about the UNF from the centralized database. Upon execution, depletion and decay calculations are automatically initiated in parallel for all UNF assemblies presently stored at the site for user-prescribed dates in time. Upon completion of the decay calculations, KENO-VI and COBRA-SFS input files are generated with the appropriate time-decayed UNF isotopic compositions and decay heat source term information, respectively. These files are executed automatically and in parallel for all the loaded storage casks for each date specified. Full output files are archived, but pertinent results such as peak and minimum clad temperatures, component temperatures, cask surface temperatures, total decay heat, and k_{eff} values are extracted and stored in the database for future use and additional data interrogation.

All data can be accessed through the MySQL database system via query lookups or through interactive features. Some of the results are graphically displayed by default through the GUI and can be observed from an assembly specific basis, a canister/cask specific basis, or collectively per site. The default

display options are being updated based on user needs. Examples of some of the interactive views from the GUI for analyzing results are shown in Figures 5–8. Figure 5 is a screen shot from the GUI showing a cross-sectional image of the cask and contents and associated loading information. Figure 6 illustrates clad temperature results for both peak and minimum clad temperature as a function of time, and Figure 7 shows a thermal map of the fuel rod temperatures that can be displayed both axially and as a function of time with slider bars. Because pertinent results are collected and retained within the database, they can be observed simultaneously on a per ISFSI basis, such as the realistic canister k_{eff} values illustrated in Figure 8 for Site B casks. Additional interactive features include the use of tooltips for further drill down capability. Examples include other UNF assembly data such as nuclide inventories and decay heat as a function of time.

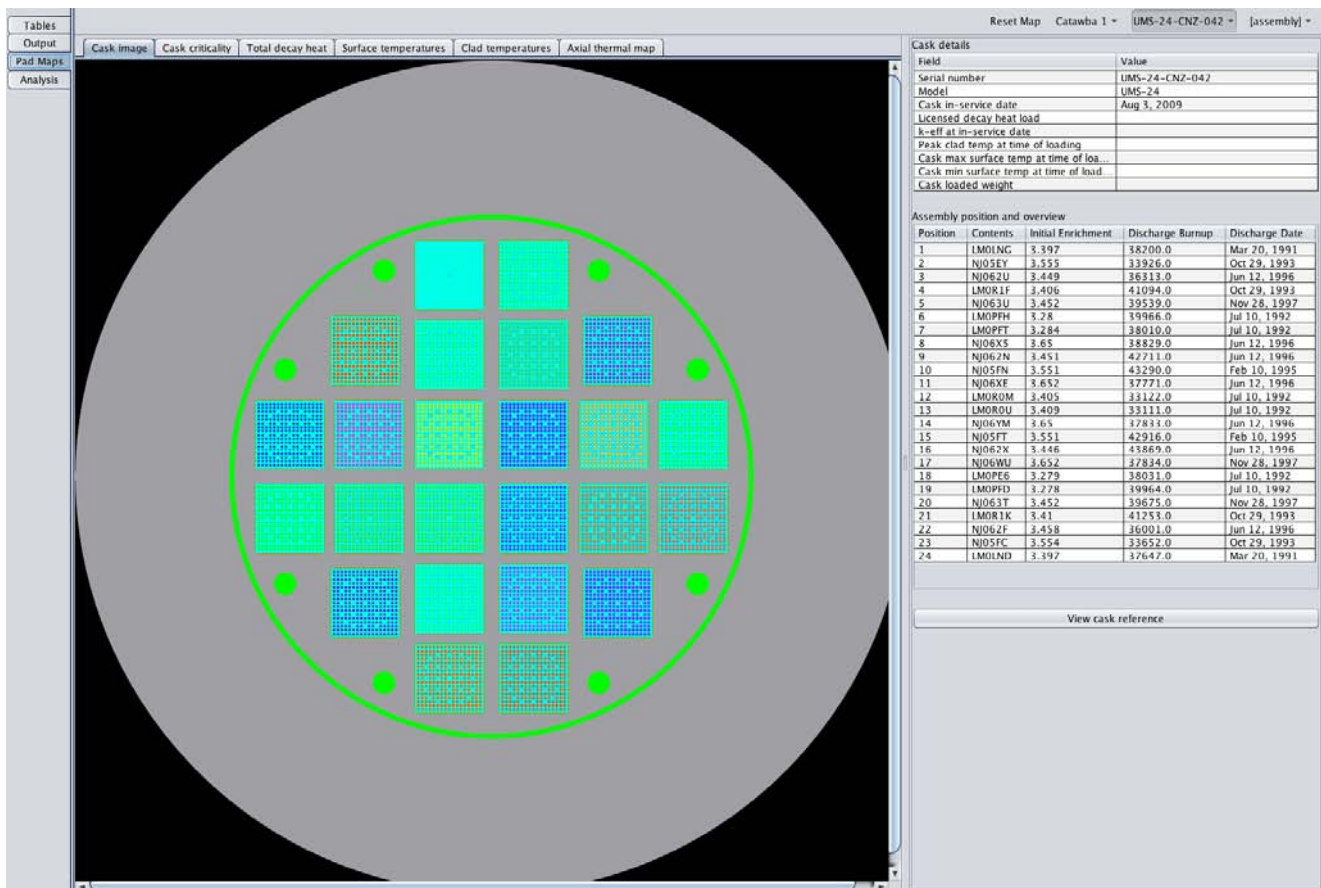


Figure 5. Screen shot of cask image display from UNF-ST&DARDS.

In addition to the default views, the data observed through the GUI can be exported as tables to other formats such as Microsoft Excel for additional processing and interrogation. An example application of this feature is shown in Figure 9, which presents the total decay heat for all casks stored at sites A and B at the time of this evaluation. This type of information can be used to facilitate identification of which canister/cask systems have cooled sufficiently to meet thermal requirements (e.g., transportation or disposal).

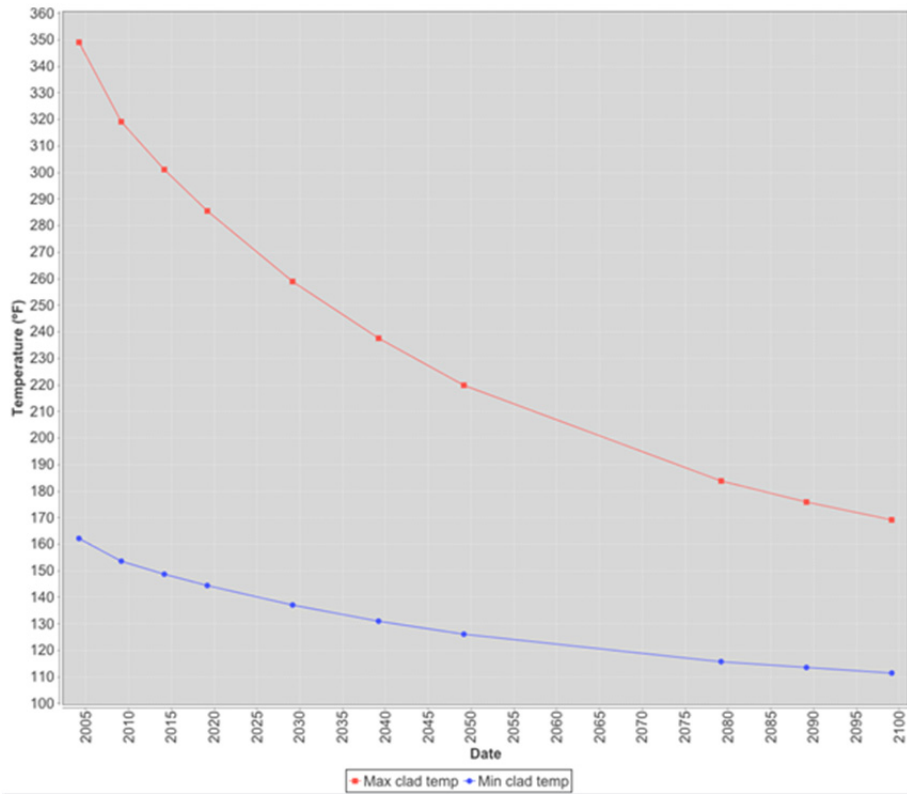


Figure 6. Example clad temperature data as a function of time for Site A Cask 1.

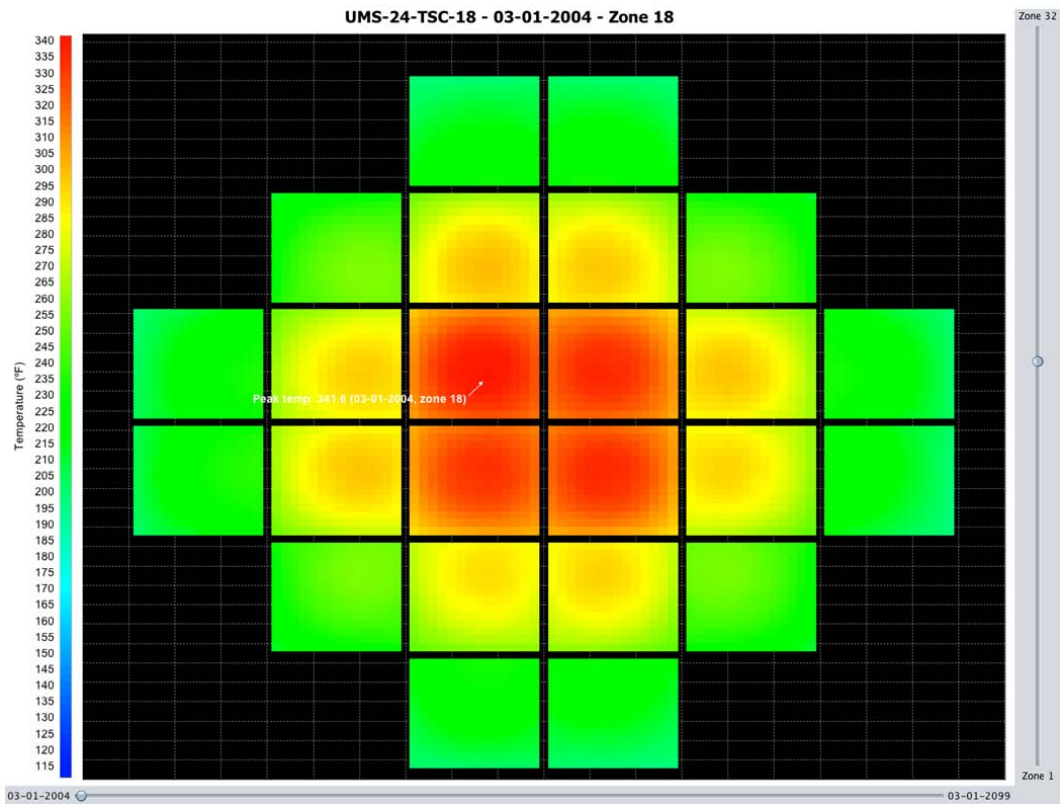


Figure 7. Fuel rod temperature map for specific time and axial location for Site A Cask 18.

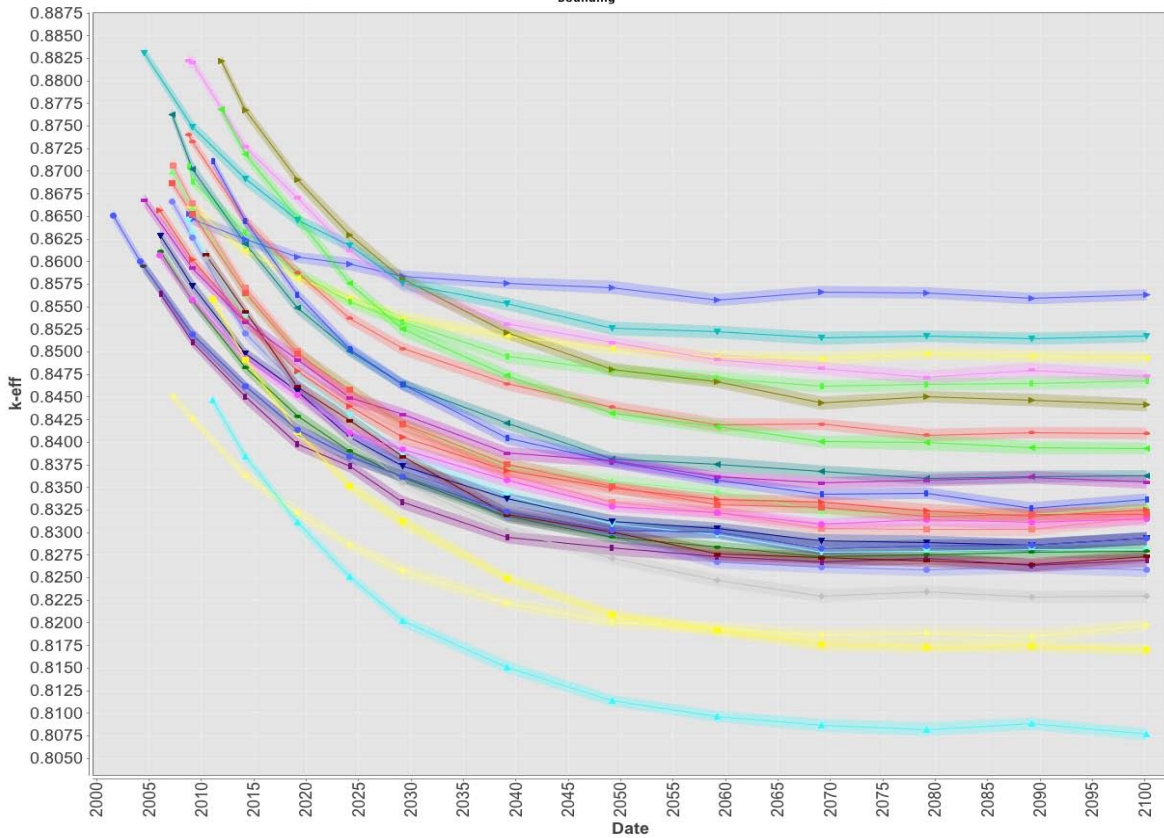


Figure 8. Example k_{eff} plot as a function of time for Site B casks (as of 2012).

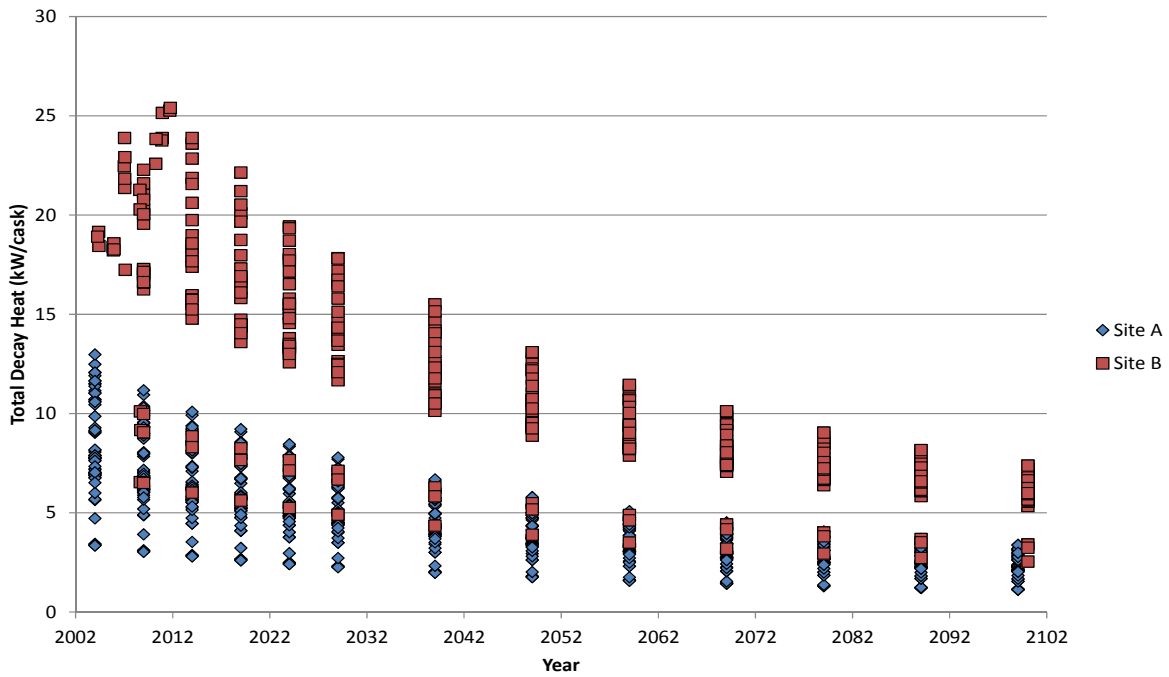


Figure 9. Example total decay heat plot as a function of time for all casks at Sites A and B.

All the assembly-specific information is retained within the database and can be extracted for further analysis using queries or advanced data mining tools such as Rapid Miner that can access data directly from the UNF-ST&DARDS database. An example application of this capability was to assess the remaining wt % ^{235}U present in the UNF inventory as a function of discharge burnup and initial wt % ^{235}U enrichment as illustrated in Figure 10, discretized by PWR and BWR fuel inventory. This information could be fed into a dynamic fuel cycle code that can simulate how the current U.S. fuel inventory might be used to transition from a once through fuel cycle scenario to an alternate fuel cycle scenario while using actual fuel inventory data.

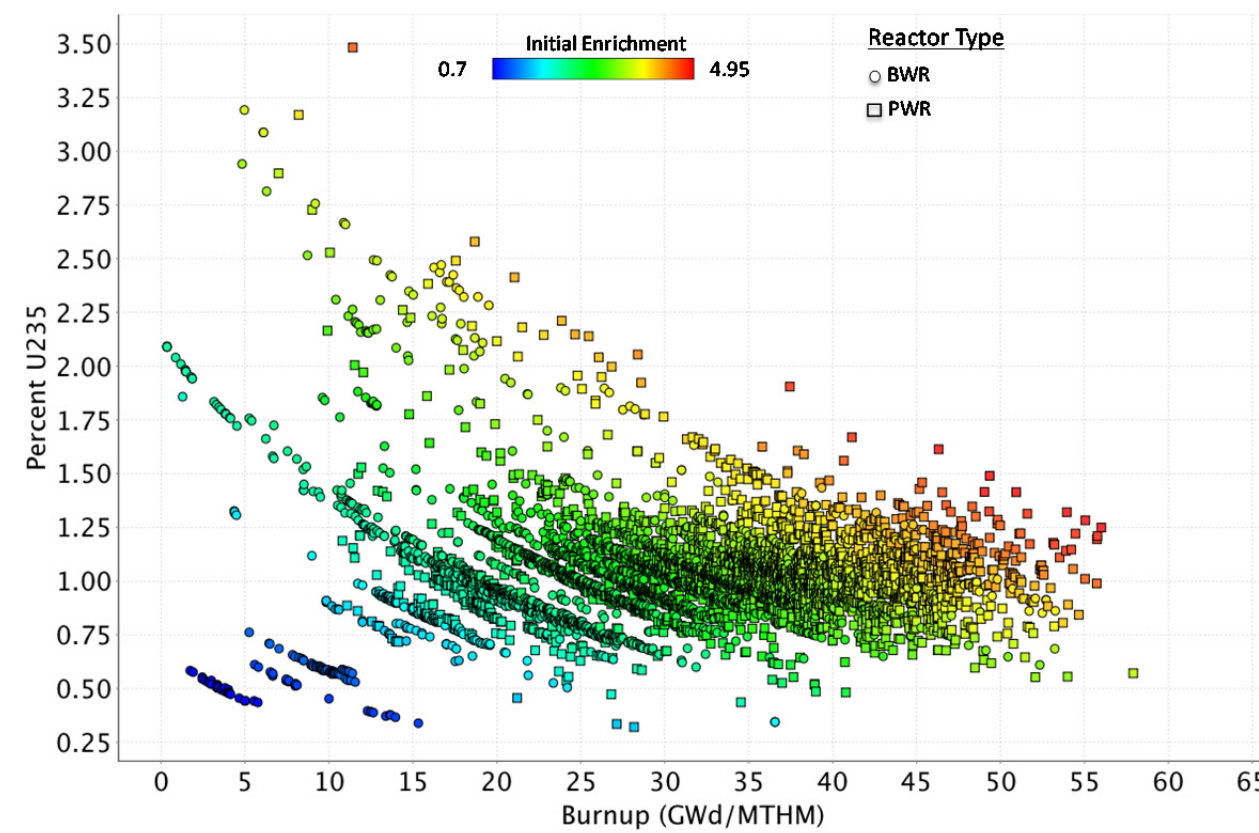


Figure 10. Depleted UNF ^{235}U concentrations per assembly in year 2014.

SUMMARY

The initial version of UNF-ST&DARDS is currently being developed to generate characteristics data for existing as-loaded casks to support the DOE Office of Nuclear Energy Fuel Cycle Technologies objectives, as well as establish an invaluable UNF archive for tracking the nuclear and mechanical properties of the nation's UNF throughout the waste management system. This capability can be used in understanding material corrosion rates and overall aging management of the nation's dry storage cask systems.

While the initial development activities of UNF-ST&DARDS have been focused on integrating neutronics and thermal calculation capabilities, the UNF characteristics that are generated provide the type of information also needed for fuel cycle decisions, safeguards, storage, transportation, disposal, and safety.

ACKNOWLEDGMENTS

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