SCALE 6: COMPREHENSIVE NUCLEAR SAFETY ANALYSIS CODE SYSTEM

REACTOR SAFETY

KEYWORDS: *reactor physics, sensitivity/uncertainty, criticality safety*

S. M. BOWMAN*

Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831-6170

Received August 3, 2010
Accepted for Publication October 11, 2010

Version 6 of the Standardized Computer Analyses for Licensing Evaluation (SCALE) computer software system developed at Oak Ridge National Laboratory, released in February 2009, contains significant new capabilities and data for nuclear safety analysis and marks an important update for this software package, which is used worldwide. This paper highlights the capabilities of the SCALE system, including continuous-energy flux calculations for processing multigroup problem-dependent cross sections, ENDF/B-VII continuous-energy and multigroup nuclear cross-section data, continuous-energy Monte Carlo criticality safety calculations, Monte Carlo radiation shielding analyses with automated three-dimensional variance reduction techniques, one- and three-dimensional sensitivity and uncertainty analyses for criticality safety evaluations, two- and three-dimensional lattice physics depletion analyses, fast and accurate source terms and decay heat calculations, automated burnup credit analyses with loading curve search, and integrated three-dimensional criticality accident alarm system analyses using coupled Monte Carlo criticality and shielding calculations.

I. INTRODUCTION

The Standardized Computer Analyses for Licensing Evaluation[1] (SCALE) computer software system developed at Oak Ridge National Laboratory (ORNL) is widely used and is accepted around the world for nuclear safety analyses. SCALE runs on Linux, UNIX, Windows, and Macintosh computers. Version 6 of SCALE, released in February 2009, contains significant improvements and additions to its codes and data. This paper highlights the diverse and comprehensive capabilities of SCALE to perform analyses for the following types of applications:

1. cross-section processing
2. criticality safety
3. sensitivity/uncertainty
4. spent nuclear fuel characterization
5. radiation source terms
6. reactor lattice physics
7. radiation shielding
8. nuclear safeguards.

*E-mail: bowmansm@ornl.gov

II. MODULAR SYSTEM

SCALE is a modular system designed to integrate the calculation capabilities of individual computer programs into easy-to-use automated sequences. The programs that perform the calculations are referred to as "functional modules." The automated sequences are controlled by other programs, referred to as "control modules," that read the user input, prepare input files for each functional module, call each module in sequence via the SCALE driver program, and automate the passing of data from one module to the next in the calculation sequence. Lists of the most frequently used functional and control modules are given in Tables I and II, respectively.

An illustration of an automated sequence using the TRITON control module is shown in Fig. 1. In this illustration, the SCALE driver reads the input and calls TRITON, which creates the input files for the Bondarenko AMPX Interpolator (BONAMI), Continuous Energy Transport Module[2] (CENTRM), and Pointwise Multigroup Converter (PMC) functional modules to perform problem-dependent resonance self-shielding of the multigroup cross sections and to create a problem-dependent library that is passed to the New Transport Algorithm[3] (NEWT) module to perform a two-dimensional (2-D)

TABLE I

Widely Used SCALE Functional Modules

Module	Function
BONAMI	Resonance self-shielding of cross sections with Bondarenko factors
CENTRM/PMC	1-D continuous energy discrete ordinates code for resonance processing
Denovo	3-D discrete ordinates code used for variance reduction in shielding analyses
KENO	3-D Monte Carlo code for calculation of neutron multiplication factor (k_{eff})
Monaco	3-D Monte Carlo code with combinatorial and array geometry features used to perform radiation shielding analysis
NEWT	2-D flexible mesh discrete ordinates code for lattice physics and criticality safety
ORIGEN	General purpose point-depletion and decay code to calculate isotopic, decay heat, radiation source terms, and curie levels
XSDRN	General 1-D discrete ordinates code for Zone weighting of cross sections Eigenvalue calculations for neutron multiplication Fixed-source calculation for shielding analysis Adjoint calculation for determining importance functions

TABLE II

SCALE Control Modules

Control Modules	Analysis Functions	Key Functional Modules
CSAS5, CSAS6	3-D Monte Carlo k_{eff} calculation	KENO V.a, KENO-VI
MAVRIC	3-D Monte Carlo shielding sequence with automated 3-D variance reduction	Monaco, Denovo
ORIGEN-ARP	Point depletion/decay with reactor-specific cross sections	ARP, ORIGEN
SAS1	1-D discrete ordinates shielding sequence	XSDRN
STARBUCS	3-D burnup credit analysis	ORIGEN-ARP, KENO
TRITON	Multimaterial depletion with 2-D discrete ordinates or 3-D Monte Carlo	NEWT, KENO, ORIGEN
TSUNAMI-1D, -3D	1-D and 3-D sensitivity/uncertainty for criticality safety	XSDRN, KENO

lattice transport effective neutron multiplication factor (k_{eff}) calculation. Once NEWT has completed the calculation, it passes the neutron flux and cross-section data to COUPLE, which collapses the cross sections to one group for use in the Oak Ridge Isotope Generation[4] (ORIGEN) depletion and decay module. The updated nuclide concentrations are then passed back to the resonance self-shielding modules to prepare problem-dependent cross sections for the NEWT calculation at the next depletion step. The cycle is repeated until all depletion steps are completed. Finally, the ORIGEN Post-processing Utility for SCALE (OPUS) is invoked to produce the final output edits requested by the user.

III. SCALE STANDARD COMPOSITION LIBRARY

The SCALE Standard Composition Library provides users with a simple and straightforward method of specifying material mixtures and concentrations for a given problem. The library consists of more than 700 compounds, alloys, mixtures, and nuclides commonly used within criticality, shielding, and lattice physics problems. The data include the associated physical densities and natural isotopic distributions, if applicable. The compositions in the library describe various predefined isotopes, elements, compounds, alloys, and other materials that can be used to define the material mixtures for a given problem. Each composition is identified by an easily recognizable name such as "H2O," "UO2," or "BORON." Additionally, there are four fissile solutions available for which the user can specify the heavy metal, acid, and water components (UO_2F_2, $UO_2[NO_3]_2$, $Pu[NO_3]_4$, and $Th[NO_3]_4$).

The library contains actual theoretical densities at naturally occurring or nominal conditions. These densities may be modified or overridden by the user. In addition, for multiple-isotope nuclides such as boron, the

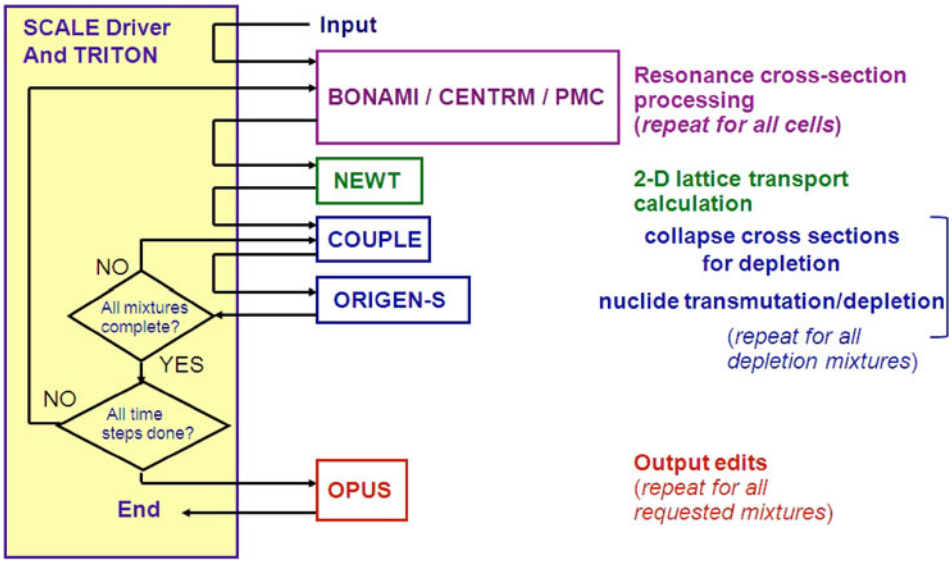

Fig. 1. SCALE flowchart for TRITON control module.

naturally occurring isotopic distribution of the element is assumed by default but may be overridden by the user. The temperature of each material is used to calculate resonance data, Bondarenko data, and thermal scattering data.

SCALE calculates the atomic number densities for each nuclide in each material by combining data in the Standard Composition Library with user input data for each material, which includes a standardized alphanumeric name, a mixture number, and other optional data such as density, density multiplier (that can represent weight fraction or percent theoretical density), temperature, and isotopic distribution. For multigroup calculations, the user also specifies one-dimensional (1-D) unit cell descriptions defining the materials, dimensions, and boundary conditions of the geometry that will be used in the resonance self-shielding calculations necessary for multigroup cross-section processing.

IV. MULTIGROUP CROSS-SECTION PROCESSING

In SCALE 6, the user may perform resonance self-shielding of multigroup cross sections for multiple unit cells. Each unit cell specification contains the cell type (infinite homogeneous medium, multiregion, lattice cell, or doubly heterogeneous), cell geometry type, and appropriate material and geometry data. Each unit cell is modeled using the CENTRM resolved resonance processor module.[5] CENTRM is a 1-D discrete ordinates code that uses a pointwise continuous-energy cross-section library to produce a set of pointwise continuous-energy fluxes at discrete spatial intervals for each unit cell. Using these fluxes, the PMC module collapses the pointwise continuous-energy cross sections into multigroup cross sections for each nuclide in each material in the unit cell. CENTRM can be used to explicitly model fuel or absorber materials in subdivided regions, such as concentric rings in a fuel pin, to more precisely model the spatial effect on the flux and cross sections. Other modules in SCALE 6 can then use these multigroup cross sections to calculate quantities such as k_{eff}, fluxes, and doses.

CENTRM/PMC can also process discrete-level inelastic cross-section data. The pointwise thermal flux solution in CENTRM can utilize bound thermal scattering kernels based on Evaluated Nuclear Data File (ENDF)/B $S(\alpha,\beta)$ data. Downscattering from inelastic continuum data and thermal upscattering into the pointwise range are optionally available by a multigroup treatment. Because CENTRM/PMC calculates a problem-dependent flux profile, it provides a rigorous cross-section treatment that explicitly handles effects from overlapping resonances, fissile material in the fuel and surrounding moderator, anisotropic scattering, and inelastic-level scattering.

Another feature of CENTRM is the capability to treat nonuniform arrays of absorber bodies. Users can input Dancoff factors computed by Monte Carlo techniques with the MCDancoff module in SCALE 6, and the SCALE Material Information Processor Library will determine Dancoff-equivalent unit cells for CENTRM calculations.

A resonance self-shielding option in SCALE can address doubly heterogeneous cells[6,7] (e.g., pebble bed or prismatic fuel, where small micrograins of fuel and moderator matrix are contained in larger spheres or rods) by applying sequential CENTRM/PMC resonance calculations for the low- and high-level heterogeneities. This method computes pointwise disadvantage factors to obtain

cell-homogenized cross sections from the low-level unit cell to use in the high-level unit cell resonance-shielding computation.

SCALE includes both continuous-energy and multigroup ENDF/B-VI and VII cross-section libraries. The multigroup libraries include a 238-group general purpose criticality safety library, a fine-group coupled shielding library with 200 neutron and 47 gamma energy groups, and a broad-group coupled shielding library with 27 neutron and 19 gamma groups.

V. KENO MONTE CARLO CRITICALITY SAFETY MODULES

The KENO three-dimensional (3-D) Monte Carlo criticality safety codes[8] in SCALE have been used worldwide for three decades. The two versions available in SCALE 6, KENO-V.a and KENO-VI, can perform continuous-energy or multigroup calculations.

KENO-V.a has been part of SCALE for 25 years. Its simplified geometry system makes it very easy to use and more computationally efficient than other Monte Carlo criticality safety codes. The geometry models consist of units that are constructed by nesting partial or whole spheres, cylinders, and rectangular cuboids oriented along *x*-, *y*-, and *z*-axes. These units can be combined in rectangular arrays or inserted in other units using a feature known as "holes." These geometric limitations enable very fast particle tracking while still permitting users to construct very complex geometry models.

The criticality search capabilities in the Criticality Safety Analysis Sequence No. 5 (CSAS5)/KENO-V.a sequence have been expanded to allow each unit cell to be explicitly identified with either a unit or a material that is to be modified in KENO-V.a. A search case can alter the material densities, the pitch of the cells in a lattice, or simple geometry boundaries. Because multiple unit cells are now allowed, a critical search can be performed on lattices containing more than one fuel type. As the geometry or material in KENO V.a is modified, the unit cell is similarly modified, thus ensuring that the cross sections for the material are appropriately processed. Cell-weighted materials may now be included in the searches, updating the geometry, material, and cross sections as the search progresses.

KENO-VI was introduced 15 years ago in SCALE to provide users with a more general geometry system, known as the SCALE Generalized Geometry Package (SGGP). KENO-VI is capable of modeling more than 15 bodies, including cones, hexprisms, planes, rhomboids, and wedges. The code allows intersection of bodies, truncation of bodies with planes, and rotation of bodies to any angle. In addition to rectangular arrays, KENO-VI provides the following array types: dodecahedral (a 3-D stack of dodecahedrons) and three hexagonal array types, as shown in Fig. 2.

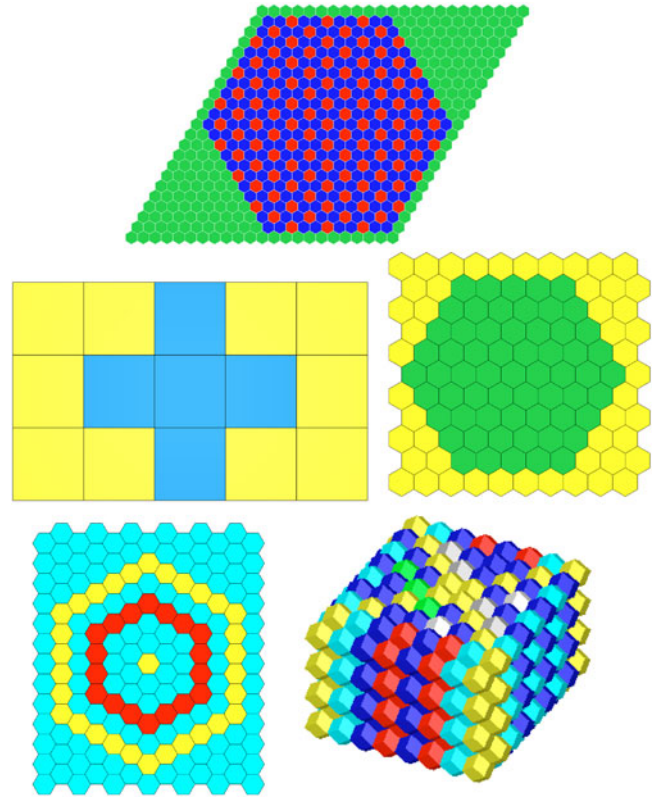

Fig. 2. KENO-VI array types: hexagonal, rectangular, standard hex, rotated hex, and dodecahedral.

The added complexity of the KENO-VI generalized geometry results in longer running times compared with KENO-V.a. In general, a KENO-V.a model that has been converted to KENO-VI will require approximately four times the amount of computer run time in KENO-VI than it did in KENO V.a. The KENO-VI run times are comparable to other generalized geometry Monte Carlo codes.

Both versions of KENO include the capability to generate 2-D color plots through slices of the geometry model. A sample *x*-*y* plot of a KENO cask model is shown in Fig. 3. Extensive verification and validation of both versions have been performed using a wide variety of criticality safety experiments.[8]

VI. HTML OUTPUT FOR KENO

An advanced Hypertext Markup Language (HTML)-formatted output interface for KENO has been developed as part of recent upgrades to SCALE. The use of HTML as an alternative output interface for SCALE codes provides the user with a convenient and familiar means of navigating and visualizing data. HTML output can be viewed in any modern web browser that is freely distributed or preinstalled on many computer systems. HTML

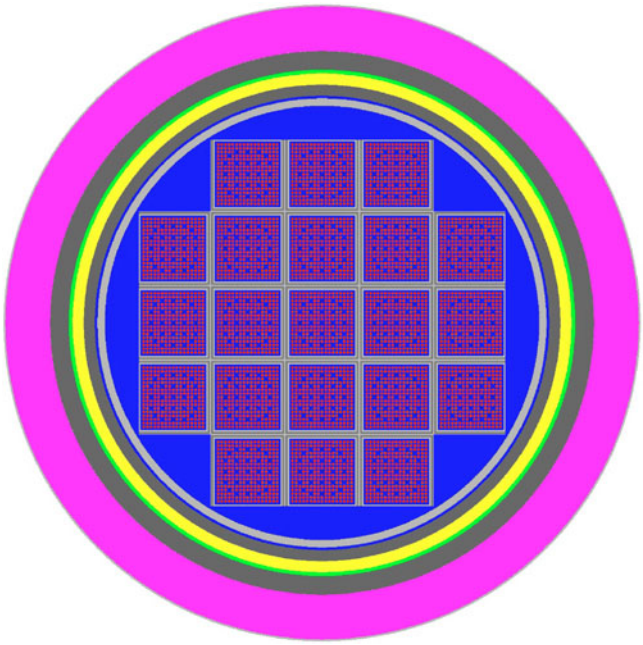

Fig. 3. Two-dimensional plot of KENO fuel cask model.

presents a wide variety of formatting options for varying fonts, colors, and data tables. More advanced technologies such as Java applets and JavaScript are readily incorporated into the output for advanced navigation and data visualization. In addition to easily navigated and color-coded tables of data, interactive plotting capabilities are available so that the user may view data in colorful, interactive, and customizable plots. Data available for plotting within the HTML interface include k_{eff} by generation (Fig. 4), the distribution of k_{eff} values (Fig. 5), flux spectra by region (Fig. 6), and fission and absorption rates by region (Fig. 7). Future development plans call for adding HTML output to other SCALE modules.

VII. KENO CONTINUOUS-ENERGY CROSS-SECTION DATA

The KENO continuous-energy calculational capability introduced in SCALE 6 required the development of ENDF/B-VI and ENDF/B-VII continuous-energy cross-section libraries. The independence of the KENO continuous-energy data from other continuous-energy Monte Carlo codes and data is ensured by developing a

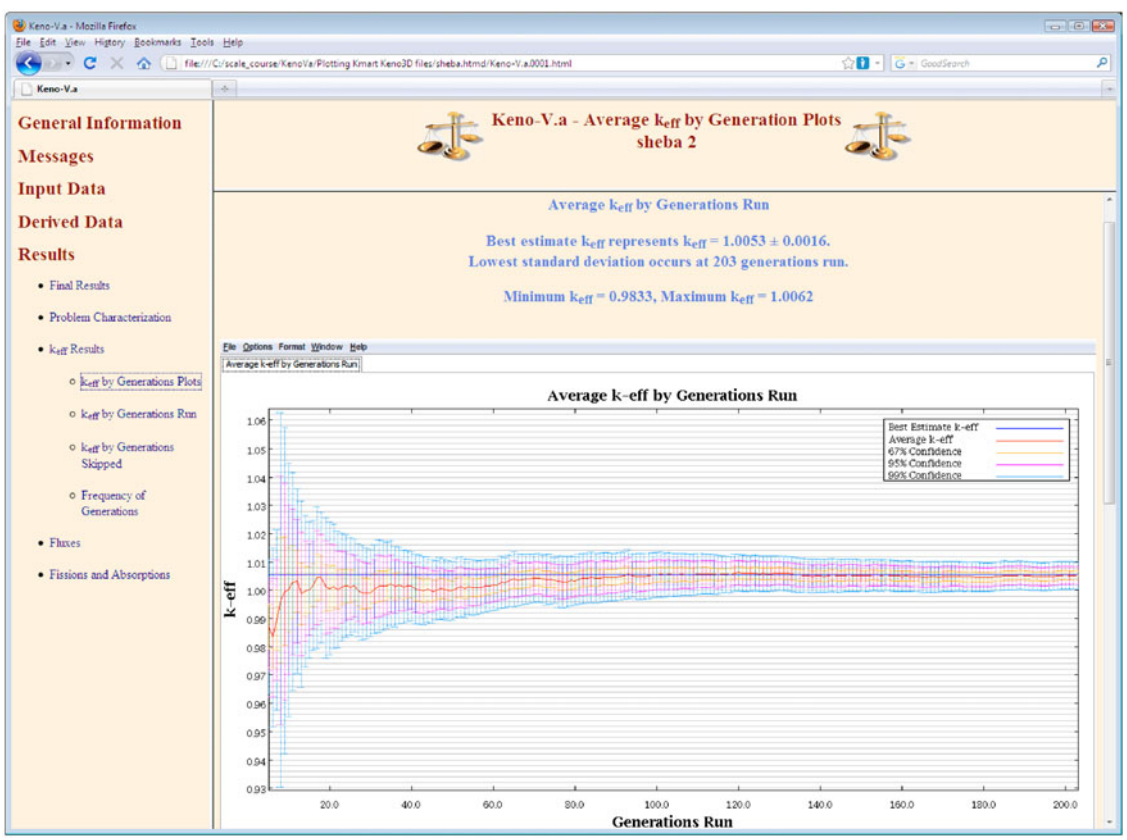

Fig. 4. KENO V.a HTML output showing plot of average k_{eff} by generations run.

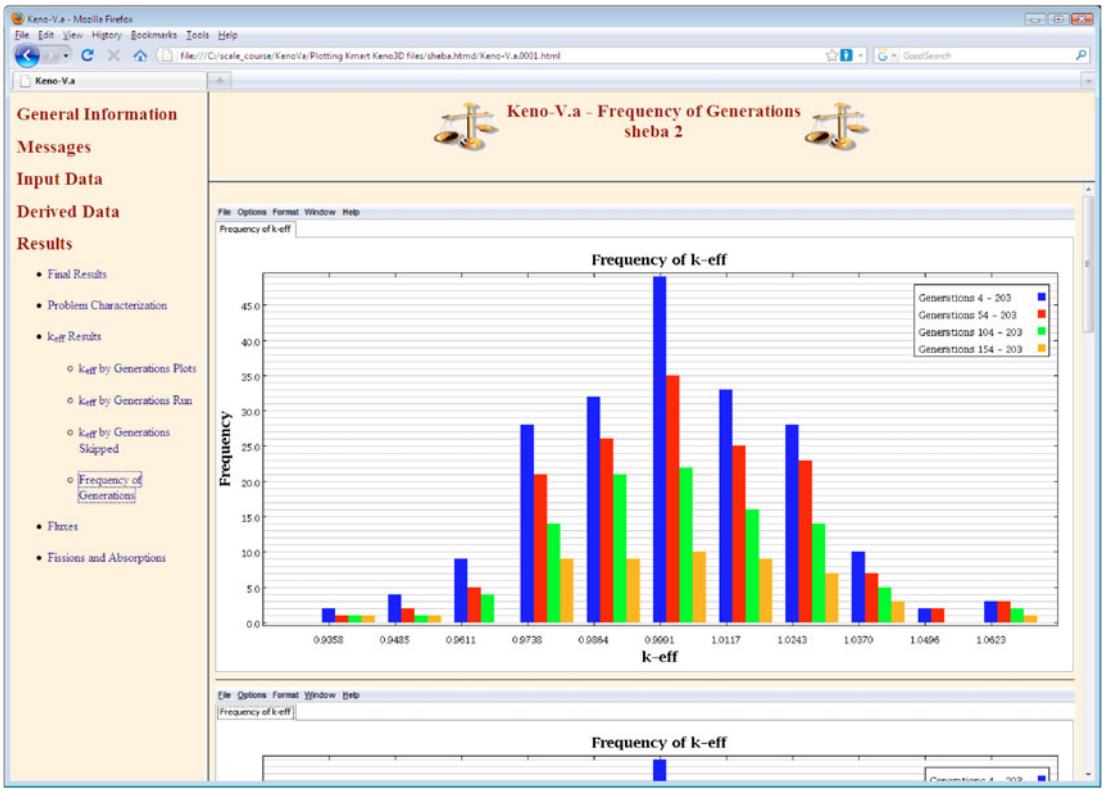

Fig. 5. KENO V.a HTML output showing plot of frequency of k_{eff}.

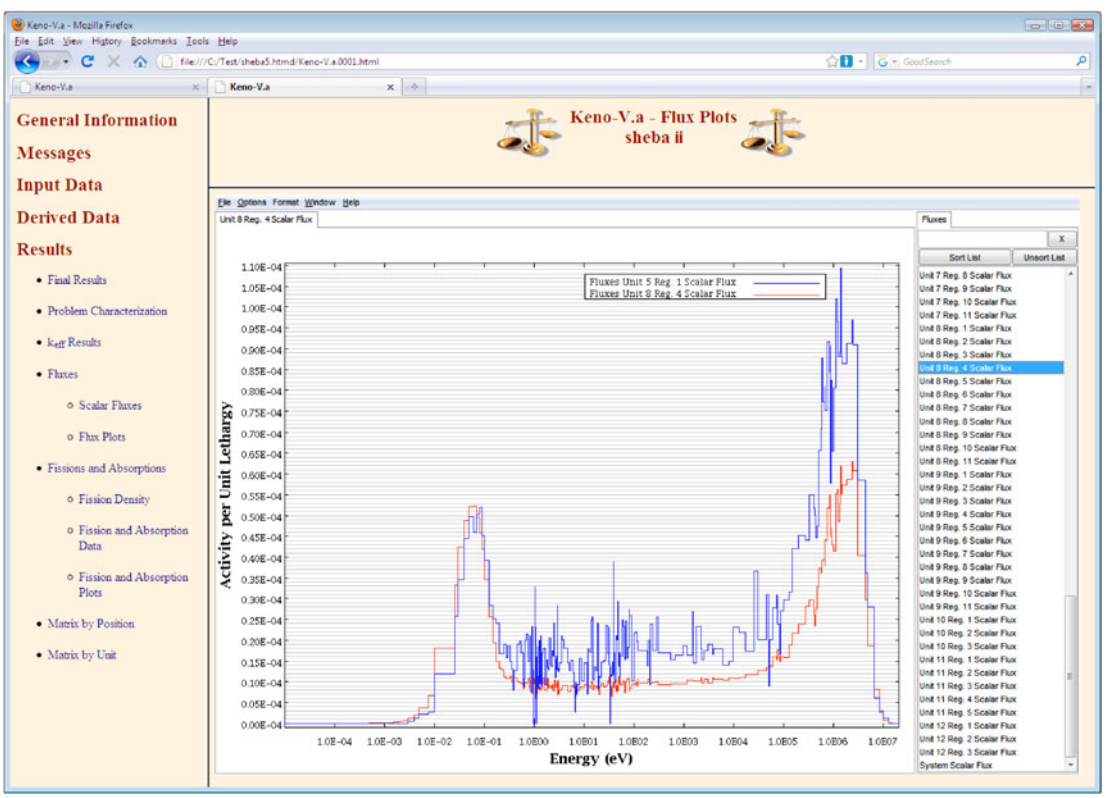

Fig. 6. KENO V.a HTML output showing plot of flux spectra per unit lethargy by region.

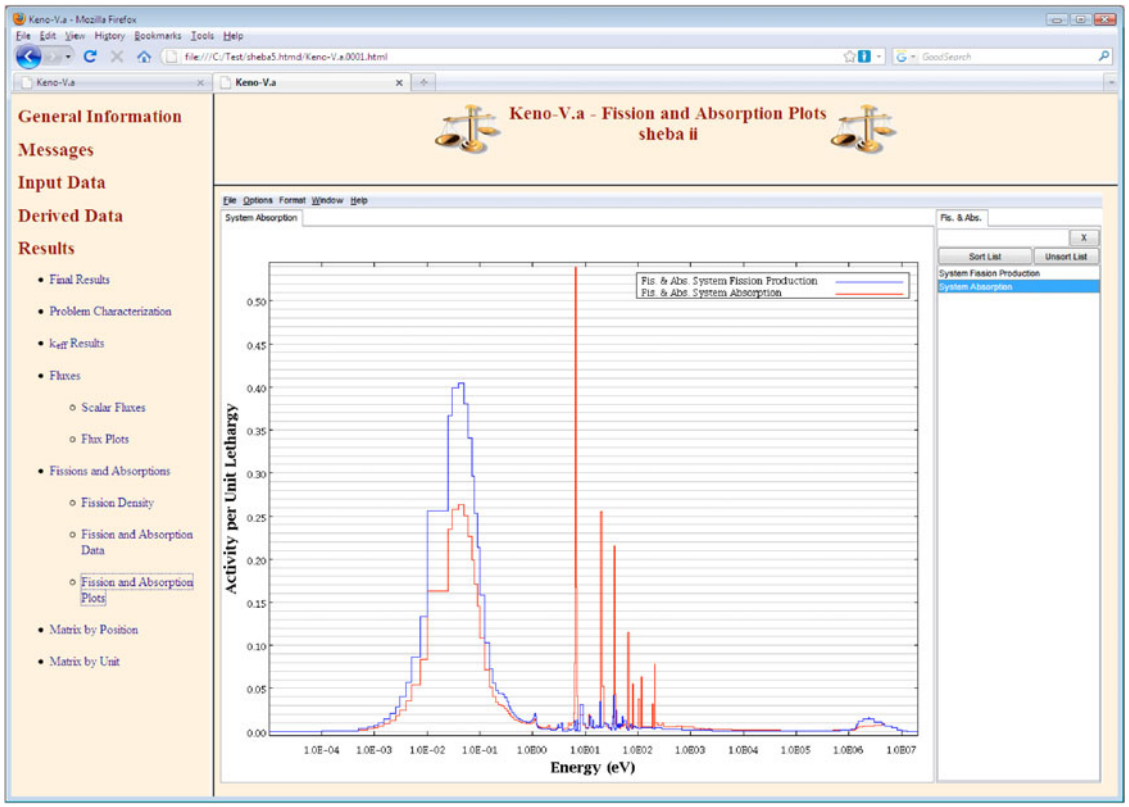

Fig. 7. KENO V.a HTML output showing plot of fission and absorption rates per unit lethargy by region.

set of modules using the AMPX cross-section data processing codes[9] to produce the required continuous-energy cross-section libraries. The essential components of a continuous-energy KENO cross-section library include the following:

1. average number of neutrons (delayed and prompt) produced by fission, $\nu(E)$

2. 1-D continuous-energy cross sections as a function of temperature, $\sigma(E,T)$

3. 2-D pointwise joint probability distributions that describe the energy and angle of particles emerging from a collision, $f(E \rightarrow E', \mu)$

4. probability tables for sampling the cross sections in the unresolved resonance region.

Some continuous-energy radiation transport codes have the ENDF laws and procedures programmed in them. As changes are made to the ENDF formats, the radiation transport code and associated cross-section processing code system must be updated to process the new ENDF laws and procedures. Because AMPX processes the raw ENDF/B data into a continuous-energy library, the burden of treating the ENDF formats lies solely on the AMPX cross-section generation codes, not on the transport code.

The data in the continuous-energy library are stored as discrete points, typically with a tolerance of 0.1%, with the exception of the unresolved resonance data. Because of the statistical nature of the parameters used to describe the unresolved resonance region, probability tables are used to provide cross-section probability distribution functions for energy ranges at specific temperatures within the unresolved region.[10]

VIII. TSUNAMI: SENSITIVITY AND UNCERTAINTY ANALYSES

SCALE contains advanced sensitivity and uncertainty (S/U) analysis capabilities for criticality safety and reactor physics. Both 1-D and 3-D sequences, plus several auxiliary codes, have been developed into a new suite of S/U analysis codes named Tools for Sensitivity and Uncertainty Analysis Methodology Implementation[11–13] (TSUNAMI).

TSUNAMI contains a number of codes that were developed primarily to assess the area of applicability of benchmark experiments for use in criticality code validations. However, the S/U data produced by these codes can be used in a wide range of studies such as assessment of critical experiment applicability for

validation, design of critical experiments, estimation of code bias, and prioritization of needed improvements in nuclear data. Sensitivity coefficients produced by the TSUNAMI sensitivity analysis sequences predict the relative changes in a system's calculated k_{eff} value due to changes in the neutron cross-section data. They use first-order eigenvalue perturbation theory to predict the response of a system k_{eff} value to changes in each constituent groupwise cross-section data value. TSUNAMI produces sensitivity data on a groupwise basis for each region defined in the system model. The TSUNAMI-1D control module uses the 1-D X-Section Dynamics for Reactor Nucleonics (XSDRN) module to generate sensitivity coefficients, while the TSUNAMI-3D control module uses KENO V.a or KENO-VI.

The sensitivity coefficients can be coupled with energy-dependent cross-section covariance data to give an uncertainty in the computed k_{eff}. Both TSUNAMI-1D and TSUNAMI-3D fold the sensitivity data with cross-section covariance data to calculate the uncertainty in the calculated k_{eff} value due to tabulated uncertainties in the cross-section data. A 44-group cross-section covariance data library with data for most ENDF nuclides and reactions is included in SCALE 6 (Ref. 14). This comprehensive covariance library includes data for more than 300 materials. Because covariance data are available in ENDF for a very limited set of nuclides, the covariance data were generated using several computational methods by collaboration of ORNL with Los Alamos National Laboratory and Brookhaven National Laboratory.

The applicability of benchmark experiments to the criticality code validation of a given application can be assessed using S/U-based integral parameters.[11,15] The TSUNAMI-IP (Integral Parameters) utility module combines sensitivity data and cross-section covariance data to produce a number of relational integral parameters that can be used to assess system similarity, including integral indices that quantify the amount of shared sensitivity or uncertainty in the k_{eff} values of an application and a benchmark due to particular nuclide cross sections. An index value of 1.0 indicates that the sensitivities or uncertainties for the application and the benchmark are all generated from the same nuclides and reactions at the same energies, whereas an index value of 0.0 means that the sensitivities or uncertainties of the two systems are completely unrelated. The TSUNAMI methodology has been applied successfully to a wide variety of applications.[16–19]

A premise of the TSUNAMI validation concept is that most computational biases originate with the cross-section data. This assumption is based on extensive data testing of critical benchmark experiments using continuous Monte Carlo codes such as KENO and MCNP, which have small biases due to modeling approximations.[20,21] Multigroup computations with KENO Monte Carlo have found similar agreement.[22] Hence, if the cross-section uncertainties are correctly tabulated, then computational biases should be bounded by nuclear data uncertainties and experimental uncertainties. The Tool for Sensitivity and Uncertainty Analysis of Response Functionals using Experimental Results (TSURFER) is a generalized linear least squares adjustment bias prediction tool that consolidates information from many types of experiments to compute changes in cross-section data and experimental parameters that minimize chi-squared for the set of benchmark experiments. The statistical parameter chi-squared is a measure of the overall discrepancy between the computed and measured results for the selected set of experiments, taking into account the uncertainties in nuclear data as well as the measurements. The bias in an application system is then predicted as the change in the computed result due to the cross-section adjustments that minimize chi-squared.

The Tool for Sensitivity Analysis of Reactivities[13] (TSAR) computes nuclear data sensitivity coefficients for eigenvalue-difference responses such as reactivity and worth coefficients. TSAR reads previously computed sensitivity coefficients for the calculated k_{eff} values at two states of a system (or for two different systems) and then combines them to obtain sensitivity coefficients for the difference. The reactivity sensitivity coefficients are combined with nuclear data covariance information to determine the uncertainty in the reactivity response.

IX. ORIGEN-ARP: SPENT FUEL CHARACTERIZATION, DECAY HEAT, AND RADIATION SOURCE TERMS

The preeminent computer code used internationally to predict spent fuel isotopic evolution and associated radiation sources is ORIGEN, which is one of the key functional modules in SCALE.

The ORIGEN nuclear data libraries distributed in SCALE 6 track 1119 individual fission products generated in the fuel during irradiation, 129 actinides, and 698 light element isotopes associated with structural and/or activation components. The nuclear data (decay data, cross sections, and fission product yields) are based primarily on ENDF/B-VI evaluated nuclear data. Data not available from ENDF/B-VI were obtained from the Evaluated Nuclear Structure Data File[23] (ENSDF), the Fusion Evaluated Nuclear Data Library[24] (FENDL), and the European Activation File[25] (EAF). Explicit fission yields are available for 30 fissile and fissionable actinides. With the release of SCALE 6.1 in 2011, the ORIGEN libraries will be expanded to include 1149 fission products, 174 actinides, and 904 activation products; and nuclear data decay will be upgraded to ENDF/B-VII (Ref. 20). The base ORIGEN cross sections in SCALE 6.1 are developed from a multigroup representation of the JEFF-3.0/A activation files,[26] containing evaluations for 774 target nuclei and 28 different reaction types.

ORIGEN has the ability to accurately predict the neutron and gamma-ray emissions from spent fuel. The

gamma-ray source is generated using a database containing discrete energy photon data for 1132 nuclides. This feature allows the user to generate gamma spectra in any energy-group structure of arbitrary energy resolution. The photon calculation has been validated against experimental data for times <1 s after fission.[27] The neutron source calculation[28] is based on methods from the SOURCES code,[29] using spontaneous fission Watt spectral parameters for 41 actinides and a matrix-dependent (α, n) source method using (α, n) cross sections and yields for 19 target nuclides: ^{7}Li, ^{9}Be, ^{10}B, ^{11}B, ^{13}C, ^{14}N, ^{17}O, ^{18}O, ^{19}F, ^{21}Ne, ^{22}Ne, ^{23}Na, ^{25}Mg, ^{26}Mg, ^{27}Al, ^{29}Si, ^{30}Si, ^{31}P, and ^{37}Cl.

ORIGEN has been extensively validated against destructive radiochemical measurements for more than 100 spent fuel samples from domestic and international programs involving older and modern high-burnup mixed oxide (MOX) and low-enriched uranium (LEU) fuels,[30,31] decay heat measurements for more than 120 assemblies spanning cooling times of up to 30 years,[32,33] and neutron and gamma radiation measurements. The extensive validation of ORIGEN is a critical element in establishing the reliability of the code to support licensing evaluations.

For accurate ORIGEN calculations, the one-group cross sections that are used need to vary as a function of burnup, enrichment, reactor type and operating conditions [e.g., water voiding in boiling water reactors (BWRs)], and fuel assembly design (fuel type and physical configuration). It is crucial to accurately characterize the cross sections for the specific fuel type being analyzed. SCALE contains the Automated Rapid Processing (ARP) module to interpolate pregenerated cross-section libraries distributed with SCALE that cover a wide range of potential fuel types and irradiation conditions and generate problem-dependent ORIGEN cross sections "on the fly." The ORIGEN-ARP sequence couples ARP and ORIGEN to perform rapid and accurate fuel depletion analyses that calculate spent fuel isotopic properties in a few seconds. Because of the pregenerated ORIGEN-ARP cross-section libraries, the accuracy of these calculations is equivalent to that of detailed reactor physics calculations but with the full set of fuel isotopics necessary to accurately calculate radiation sources or spent fuel inventories.

To support spent fuel analyses, SCALE includes ORIGEN-ARP libraries for many commercial light water reactor (LWR) fuel designs used worldwide as well as for European MOX, Canada deuterium uranium (CANDU), advanced gas-cooled reactor (AGR), VVER, RBMK, and Magnox alloy fuel types. Most of these ORIGEN-ARP libraries have been generated using the 2-D neutron transport and depletion capabilities available in the TRITON/NEWT depletion sequence, which can generate fuel rod or assembly-average cross sections that can be used directly by ORIGEN. The spatial and material characteristics are reflected in the spectral effects in the ORIGEN-ARP cross-section libraries developed for the different fuel types. The libraries available in SCALE 6.1 are listed in Table III. Actual geometry models for a selected sample of fuel assembly designs are shown in Fig. 8.

ORIGEN-ARP also has a fast and easy-to-use Windows graphical interface that assists users in performing fuel irradiation and decay calculations, including interactive plotting of results such as calculated neutron and gamma-ray source spectra and nuclide concentration ratios for comparison with measurement results. Virtually any LWR or MOX fuel analysis scoping calculation can

TABLE III

ORIGEN Reactor Libraries Available in SCALE 6.1

Reactor Type	Assembly Design Description
PWR LEU[a] 1.5 to 6.0 wt% < 72 GWd/tonne	Westinghouse CE 14 × 14 Westinghouse CE 16 × 16 Westinghouse 14 × 14 Siemens 14 × 14 Westinghouse 15 × 15 Westinghouse 17 × 17 Westinghouse 17 × 17 OFA
BWR LEU[a] 1.5 to 6.0 wt% < 72 GWd/tonne	GE 7 × 7 GE 8 × 8 ABB 8 × 8 GE 9 × 9 GE 10 × 10 ATRIUM-9 9 × 9 ATRIUM-10 10 × 10 SVEA-64 8 × 8 SVEA-100 10 × 10
VVER LEU[a]	VVER-440 1.6%, 2.4%, 3.6% VVER-440 3.82% VVER-440 4.25% VVER-440 4.38% VVER-1000
RBMK[a] 1.8 to 2.2 wt%	3 rings of pins with 1 (central), 6 (middle), and 12 (outer) in each ring
CANDU	CANDU 37-element natural uranium CANDU 28-element natural uranium
MAGNOX[a]	Natural uranium fuel rod
AGR[a] 1.5 to 4.5 wt%	3 rings of pins with 6 (inner), 12 (middle), and 18 (outer) in each ring
PWR MOX	14 × 14 15 × 15 16 × 16 17 × 17 18 × 18
BWR MOX	8 × 8-2 9 × 9-1 9 × 9 ATRIUM-9 10 × 10 ATRIUM-10

[a]Developed using new 2-D methods.

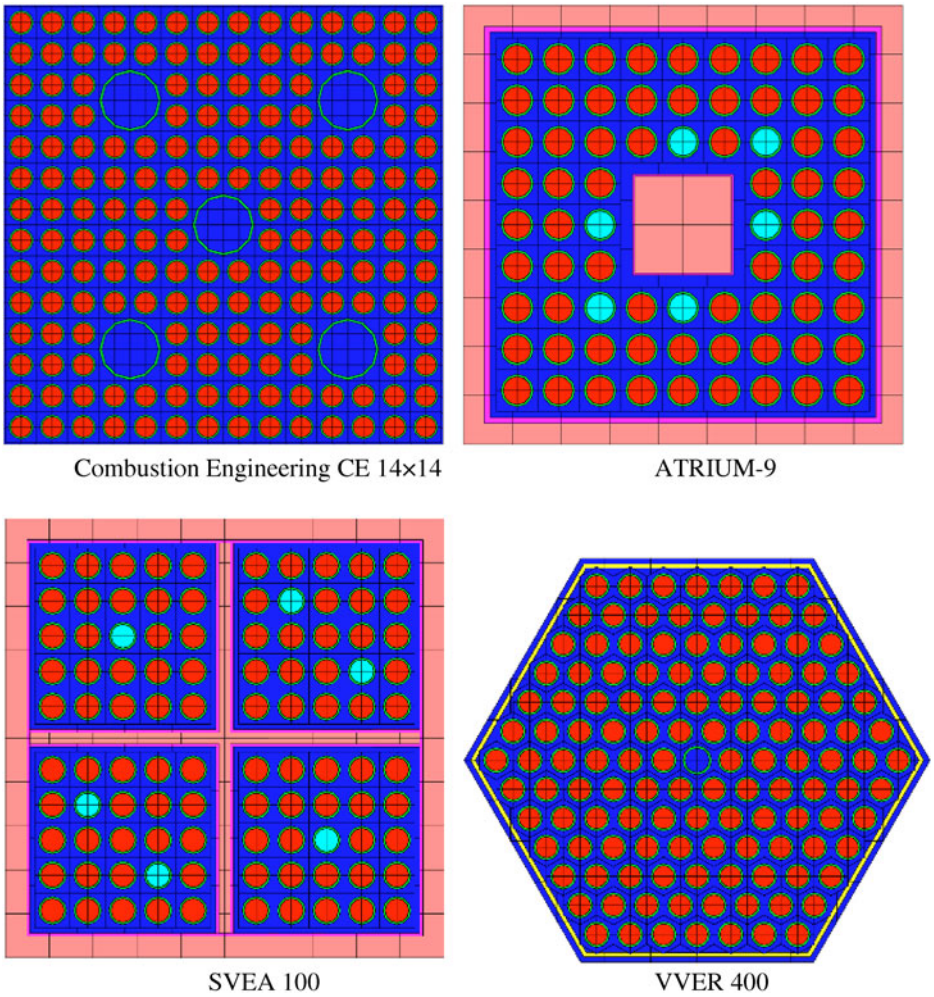

Fig. 8. TRITON fuel assembly models for ORIGEN-ARP libraries.

be set up and executed in <1 min using the Express input screen (Fig. 9).

X. STARBUCS: BURNUP CREDIT ANALYSIS SEQUENCE

The Standardized Analysis of Reactivity for Burnup Credit using SCALE (Refs. 34 and 35) (STARBUCS) is a control module to perform criticality calculations for spent fuel systems employing burnup credit. STARBUCS automates the criticality safety analysis of spent fuel configurations by coupling the depletion and criticality aspects of the analysis, thereby eliminating the need to manually process the spent fuel nuclide compositions into a format compatible with criticality safety codes. STARBUCS automatically prepares the input for all codes in the analysis sequence, executes the codes through the SCALE driver, and performs all module interface and data management functions for the user.

STARBUCS performs a depletion analysis calculation for each spatially varying burnup region (if an axial or horizontal burnup profile is specified) of a spent fuel assembly using the ORIGEN-ARP methodology of SCALE. If a multigroup calculation is to be performed in KENO, the spent fuel compositions are then used to generate resonance self-shielded cross sections for each burnup-dependent fuel region. Finally, a KENO criticality calculation is performed to determine the neutron multiplication factor for the system.

The STARBUCS input format has been designed around the existing depletion analysis and criticality safety sequences of SCALE. Only a minimal amount of input beyond that typically required for a fresh fuel calculation is needed to perform a burnup credit calculation.

STARBUCS was developed to facilitate studies of major burnup credit phenomena, such as those identified in the U.S. Nuclear Regulatory Commission "Interim Staff Guidance 8" (Ref. 36). Specifically, STARBUCS provides the following features and capabilities:

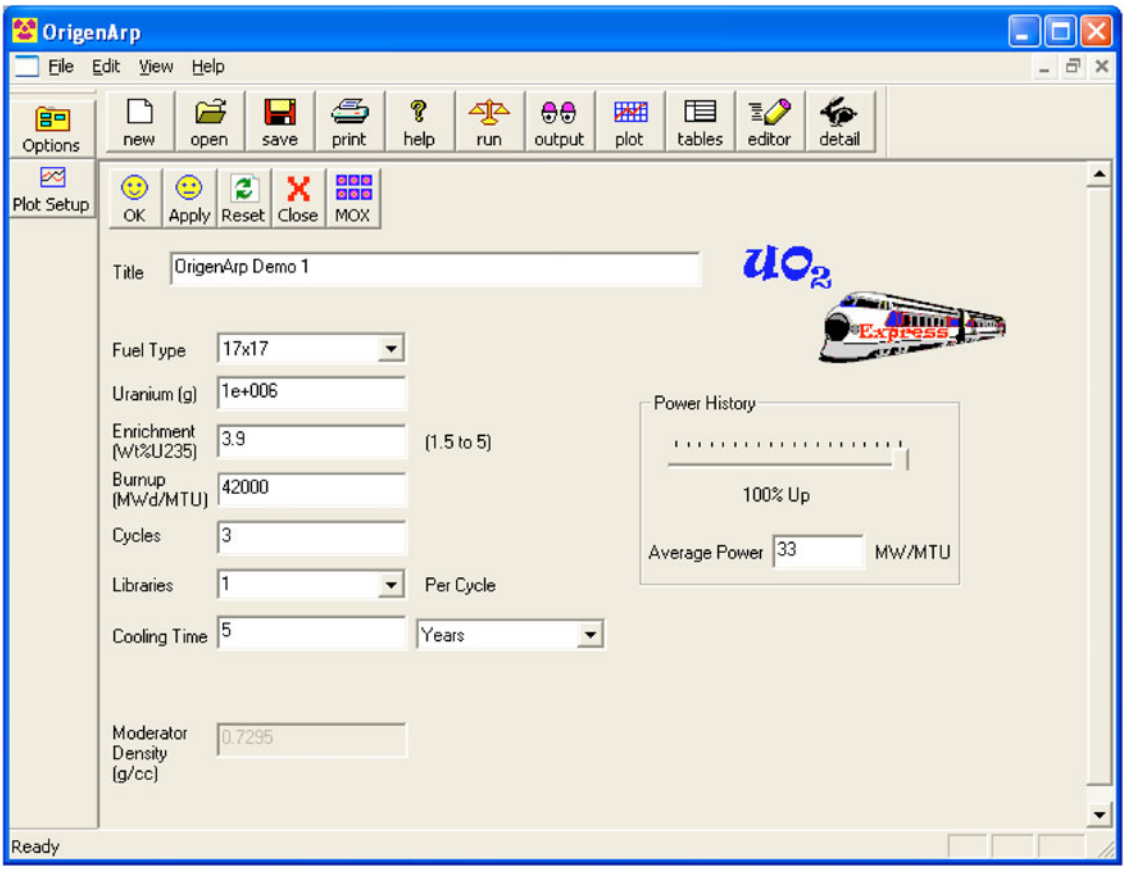

Fig. 9. ORIGEN-ARP Express form.

1. An arbitrary axial and/or horizontal assembly burnup gradient can be modeled.

2. Any or all of the spent fuel actinide or fission product isotopes may be included in the criticality calculation.

3. The burnup calculations can specify any desired operating history.

4. Isotopic correction factors may be input to adjust the calculated isotopic inventories to account for known bias and/or uncertainties associated with the depletion calculations.

5. Virtually any arrangement of spent fuel may be simulated.

For burnup loading curve iterative calculations, STARBUCS employs the search algorithm from CSAS5 to determine initial fuel enrichments that satisfy a convergence criterion for the calculated k_{eff} value of the spent fuel configuration. Two example burnup loading curves are shown in Fig. 10. Any burnup/enrichment points to the left and above the upper curve labeled "Major Actinides" are acceptable for loading in a spent fuel container, based on taking burnup credit for the major actinides. If credit is also taken for 16 primary fission products, the lower curve labeled "Actinides & 16 FPs" would be used instead. If convergence is not achieved in a search pass, the initial fuel enrichment is automatically adjusted. This sequence repeats either until k_{eff} converges to an upper subcritical limit (USL) or until the algorithm determines that a solution is not possible. The procedure is repeated for each requested burnup value. The maximum allowable iterations, USL, tolerance for convergence, and a range of initial fuel enrichments can be set by the user. The lower and upper enrichment bounds as well as the set of requested burnup values must be contained within the range of enrichments and burnups used to generate the ORIGEN-ARP library used by STARBUCS. The control module prepares a STARBUCS input file for each search pass requesting a single criticality calculation using the calculated spent fuel compositions. In the input file, the burnup history data block and/or the fuel mixture compositions are updated based on the outcome of the search sequence.

Additional STARBUCS features available in SCALE 6 include the ability to use either multigroup or continuous-energy criticality calculations with KENO, fewer iterations

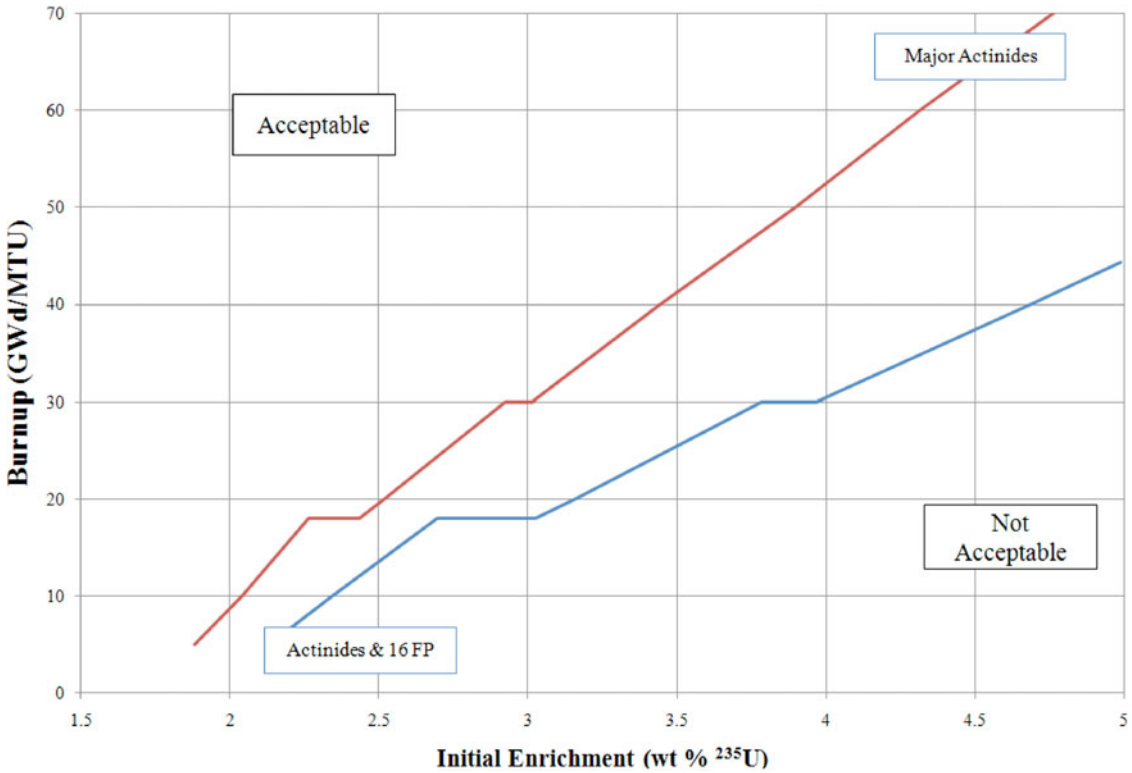

Fig. 10. Example burnup credit loading curves.

to achieve eigenvalue convergence, reduced output, and the capacity to save the input files created by the criticality calculations for use in subsequent calculations, such as sensitivity and uncertainty calculations with the TSUNAMI tools.

XI. NEWT: FLEXIBLE MESH 2-D DISCRETE ORDINATES

SCALE includes 2-D lattice physics analytical capability via the NEWT flexible mesh discrete ordinates code. NEWT is based on the extended step characteristic (ESC) approach[37] for spatial discretization on an arbitrary mesh structure. This discretization scheme makes NEWT an extremely powerful and versatile tool for deterministic calculations in real-world nonorthogonal problem domains. Unlike traditional S_n codes, NEWT is not limited to Cartesian or cylindrical coordinate systems. NEWT's arbitrary geometry, also known as flexible mesh, allows users to combine orthogonal, radial, and other more unusual geometry shapes in the same model.

The input format has been adapted from the SGGP combinatorial input format employed by KENO-VI. The use of a common input format reduces the learning curve in model development for SCALE users and allows easy conversion of most models between the two codes. Although it is limited to two dimensions, use of the SGGP input format provides virtually all the geometric flexibility of Monte Carlo for a deterministic solution. It also provides a means for direct comparisons between Monte Carlo and deterministic methods. If the same cross-section data and virtually identical geometric configurations are used, differences in results can be attributed to differences in the transport techniques.

Deterministic solutions to the transport equation are generally calculated in terms of the particle flux; the flux is the product of particle density and speed and is a useful quantity in the determination of reaction rates that characterize nuclear systems. With the ESC approach, a more flexible and completely arbitrary problem grid may be defined in terms of convex polygons; no limit is placed on the number of sides in a given polygon. Side-averaged fluxes for each polygon in the problem domain are computed and are used to calculate a cell-averaged flux. The process is repeated for each cell in the problem domain, and as with the traditional approach, iteration is performed for convergence.

Lower-order deterministic methods typically applied in lattice analyses (e.g., integral transport and collision probability methods) do not provide the angular resolution necessary to treat strongly anisotropic fluxes, such as those in the vicinity of strong absorbers or in high-leakage cores. This limitation may be exacerbated in MOX fuels as a result of the increased sensitivity of

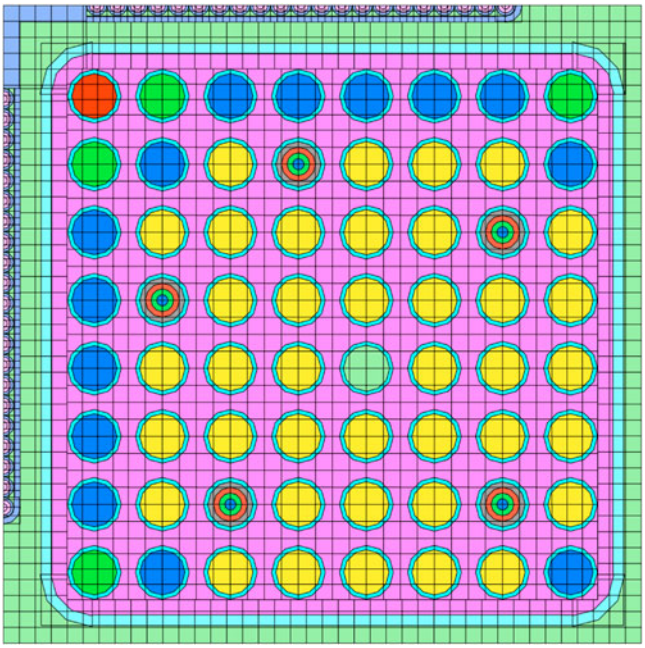

Fig. 11. NEWT grid for BWR fuel assembly.

such fuels to the thermal spectrum. NEWT has been used to demonstrate the effect of minor assumptions on the thermal spectra of MOX fuels.[38]

NEWT's automated grid generation scheme, based on the placement of simple bodies within a problem domain, allows rapid development of a model without the need to manually input a complex and irregular grid structure. Figure 11 shows the computational grid and materials generated by NEWT for a BWR fuel assembly with gadolinium poison rods. The model contains no curved surfaces but instead consists of arbitrary polygons computed by NEWT in which volumes are conserved.

XII. TRITON: 2-D AND 3-D FUEL DEPLETION

The TRITON control module[3,39] automates 2-D and 3-D lattice physics depletion calculations. TRITON provides an automated and simplified approach for setting up and performing complex sets of depletion calculations. TRITON provides multiple sequence options, depending on the nature of the problem to be analyzed, including a single NEWT transport calculation (with problem-specific multigroup cross-section generation), a 2-D depletion calculation that combines multigroup cross-section processing using BONAMI/CENTRM/PMC and NEWT transport calculations with ORIGEN depletion calculations, and a 3-D depletion sequence that uses KENO instead of NEWT.

The rigor of the NEWT solution in estimating angular flux distributions, combined with the world-recognized accuracy of ORIGEN depletion, gives TRITON the capability to perform rigorous 2-D burnup-dependent physics calculations with few implicit approximations. As an illustration of the modeling capability, the thermal flux profile for a MOX assembly surrounded by neighboring LEU assemblies (typical of a MOX core) is shown in Fig. 12. The figure shows the large spatial and spectral changes in the flux between the MOX and LEU assemblies, particularly near the periphery of the assembly where boundary effects become important.

TRITON is also able to perform 3-D Monte Carlo depletion calculations using the KENO V.a or KENO-VI Monte Carlo transport codes. TRITON couples these neutron transport codes with ORIGEN in a method similar to that used in 2-D depletion calculations with NEWT. Because of the general nature of these codes, it is possible for a user to model a lattice of virtually any size and type, such as fuel rods, assemblies, or reactor cores. This capability allows the user to perform detailed calculations, such as tracking the isotopic depletion by individual fuel rods, by axial portions of a fuel rod (in 3-D), or by concentric rings in a rod loaded with burnable poison. Such rigor may be necessary to capture the unique attributes of the advanced, highly heterogeneous fuel assembly designs being developed for current and next-generation reactors. The TRITON 2-D and 3-D depletion sequences have been validated for LWR and MOX applications.[3]

XIII. SAS1: 1-D SHIELDING

Shielding Analysis Sequence No. 1 (SAS1) is a SCALE control module developed for problem-dependent

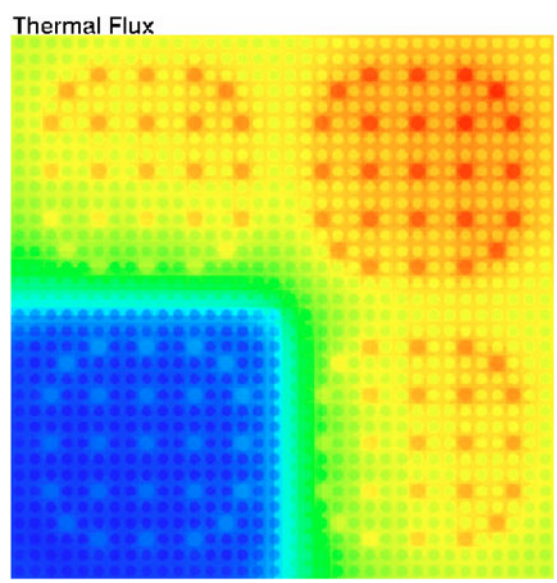

Fig. 12. TRITON/NEWT thermal flux plot for MOX assembly (lower left) surrounded by LEU assemblies.

cross-section preparation and subsequent 1-D shielding calculations. The control module has two analytic sequences—SAS1 and SAS1X. Input for the module is designed to be simple and direct.

The SAS1 calculational sequence module includes execution of a 1-D radiation transport analysis in spherical, cylindrical, or slab geometry and the subsequent calculation of dose rates outside the shield. The radiation transport analysis is performed by the XSDRN module. This module performs the 1-D fixed-source calculation that provides the neutron and/or gamma fluxes used to determine the dose rates. It also calculates the dose rates inside the system. The last step of the SAS1 sequence is a call to the XSDOSE module, which uses XSDRN fluxes and standard flux-to-dose conversion factors available in SCALE to calculate the dose rates for selected points on or outside the system boundary.

The SAS1X sequence follows the steps of the SAS1 sequence except that an additional call is made to XSDRN (prior to the XSDRN shielding calculation) to perform a simple 1-D criticality safety analysis to obtain a boundary source for the subsequent XSDRN shielding analysis. The boundary source option provides an easy means to evaluate the dose from a postulated criticality accident as a function of shield design or detector location.

XIV. MONACO: 3-D MONTE CARLO SHIELDING MODULE

Monaco is a new 3-D Monte Carlo code developed within SCALE for shielding calculations. It is a fixed-source, 3-D generalized geometry, multigroup Monte Carlo radiation transport code based on the Multigroup Oak Ridge Stochastic Experiment (MORSE) Monte Carlo code in earlier versions of SCALE. Monaco uses the same AMPX multigroup cross-section library format and SGGP as KENO-VI.

Users can construct a source by specifying separate spatial, energy, and directional distributions. Available tallies in Monaco include point detectors, region-based flux tallies, and mesh tallies (a set of region tallies defined on a mesh that overlies the physical geometry). Any Monaco tally can be convolved with a response function, either user defined or from a standard list available with each SCALE cross-section library. Mesh tally values and uncertainties can be viewed with the Mesh-View Java plotting software, as shown in Fig. 13.

XV. MAVRIC: MONTE CARLO SHIELDING WITH AUTOMATED 3-D VARIANCE REDUCTION

The new shielding analysis tools in SCALE 6 have been designed using advanced variance reduction methods that are automated for the user. The Monaco with Automated Variance Reduction using Importance Calculations (MAVRIC) sequence performs radiation transport on problems that are too challenging for standard, unbiased Monte Carlo methods. MAVRIC is based on the Consistent Adjoint Driven Importance Sampling (CADIS) methodology,[40,41] which uses an importance map and biased source that are derived to work together. MAVRIC

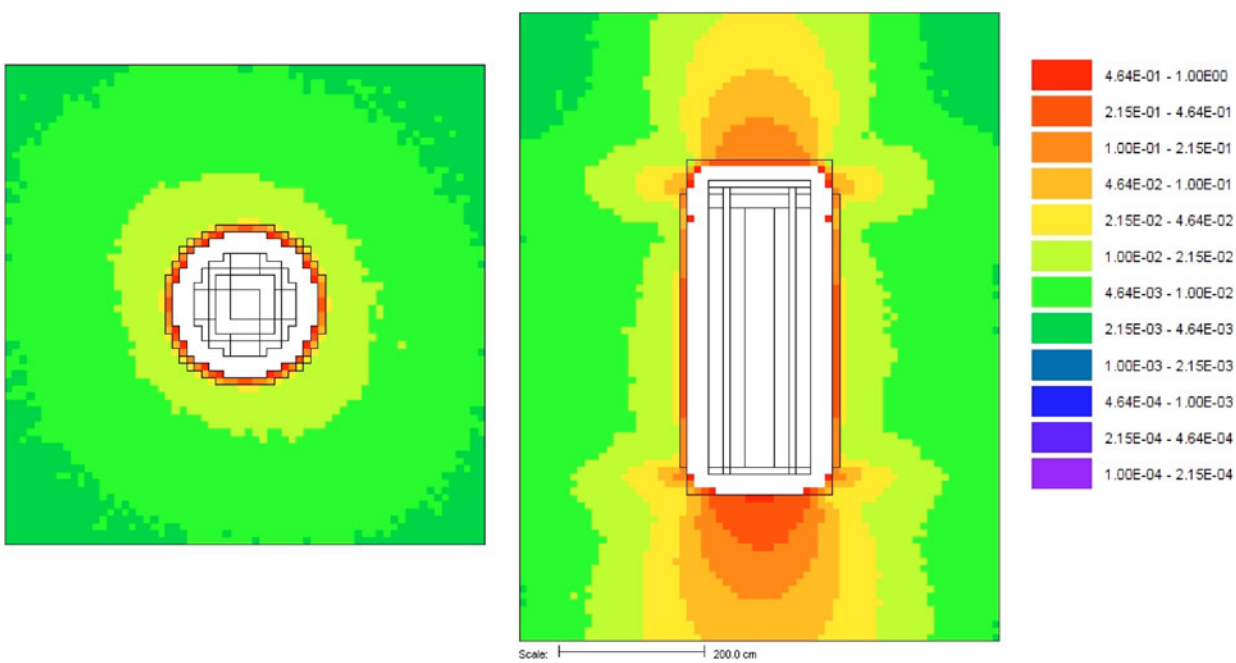

Fig. 13. Monaco mesh tally showing total dose rate (rem/h) outside a spent fuel transport cask from seven sources.

automatically performs a coarse-mesh, 3-D, discrete ordinates calculation using the new Denovo[42] S_N code to determine the adjoint flux as a function of position and energy. This adjoint flux information is then used by MAVRIC to construct a space- and energy-dependent importance map (i.e., weight windows) to be used for biasing during particle transport and a mesh-based biased source distribution. MAVRIC then passes the importance map and biased source distribution to the Monte Carlo transport code Monaco. MAVRIC is completely automated—from a single user input file, it creates the cross sections (forward and adjoint), computes the adjoint fluxes, creates the importance map and biased source, and executes Monaco.

Users can start and stop the calculation at various points so that progress can be monitored and importance maps can be reused for similar problems. The discrete ordinates calculation is based on the Monte Carlo input of sources and responses—so the only additional input required by the user is the listing of mesh planes that will be used to create a mesh geometry model. This same mesh is used for the importance map and the biased source. Results for some simple shielding problems show speedup factors of 50. For dose rate calculations from spent fuel casks, speedup factors of several hundred have been achieved using MAVRIC compared with analog Monaco. Figure 14 shows a comparison of results between analog Monaco and MAVRIC for a three-legged duct.

With advances in computational resources, Monte Carlo methods using mesh tallies are being used to compute fluxes or doses over large areas. For problems that demand that the uncertainty in each mesh cell be less than a specified maximum, computation time is controlled by the cell with the largest uncertainty. This issue becomes quite troublesome in deep-penetration problems, and advanced variance reduction techniques are required to obtain reasonable uncertainties over large areas. To optimize several tallies at once (i.e., calculate the tallies with similar relative uncertainties) or to optimize

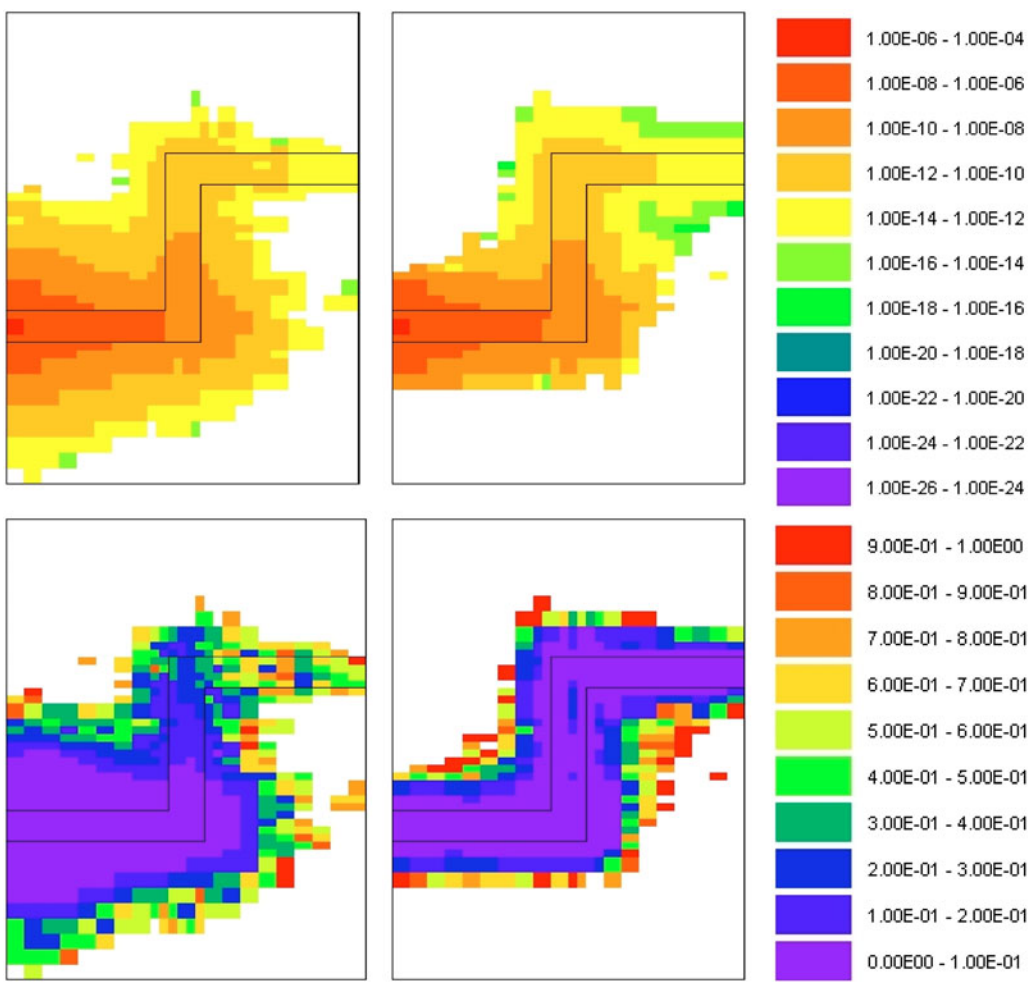

Fig. 14. Comparison of dose rate (rem/h) per source particle (top row) for analog Monaco (left) and MAVRIC using the CADIS methodology (right) for a three-legged duct problem, and the relative uncertainties (bottom row).

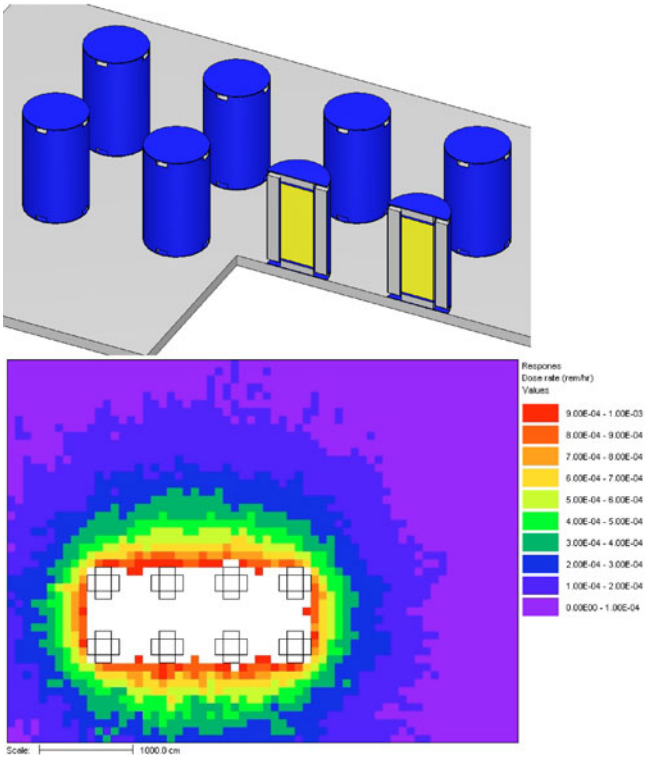

Fig. 15. Dose rates from spent fuel cask array using FW-CADIS.

the calculation of a mesh tally, an extension of the CADIS method has been implemented into the MAVRIC sequence. First, a forward discrete ordinates calculation over a coarse geometry mesh is performed to estimate the tally responses. Then the adjoint problem is created with an adjoint source for each tally to be optimized, weighted inversely by its expected result. As in standard CADIS, the result of the adjoint calculation is used to create a set of target weight windows and a biased source distribution that are then used by Monaco. This forward-weighted CADIS (FW-CADIS) approach[43] is quite useful in many problems, such as the dry storage spent fuel cask array modeled in Fig. 15. The MAVRIC methodology has been verified and validated by comparisons with both measured data and other shielding codes.[44]

XVI. CAAS SAFETY ANALYSES WITH KENO AND MAVRIC

Also included in SCALE 6 is a new capability to perform criticality accident alarm systems (CAAS) safety analyses.[45] CAAS modeling presents challenges because the analysis consists of both a criticality problem and a deep-penetration shielding problem. Modern codes are typically optimized to handle one of these types of problems but not both. The two problems also differ in size—the criticality problem depends on materials relatively close to the fissionable materials, whereas the shielding problem can cover a much larger range. SCALE 6 includes 3-D tools that can be coupled to perform both parts of a CAAS analysis.

The CAAS analysis can be performed using the KENO-VI criticality module and the MAVRIC shielding sequence. First, the fission distribution (in space and energy) is determined via KENO-VI. Along with calculating the system k_{eff}, KENO-VI accumulates the fission distribution over all saved generations. This information is collected on a 3-D Cartesian mesh that overlies the physical geometry model and is saved as a Monaco mesh source file. The mesh source is then used as the source term in MAVRIC. The absolute source strength is set by the user to the total number of fissions (based on the total power released) during the criticality excursion. Further neutron multiplication is prevented in the MAVRIC transport calculation. The user can also request that MAVRIC add fission photons to the mesh source, specifying which isotope to use for the multiplicity (photons per fission) and fission photon energy distribution. To correctly account for the number of source photons released per source neutron, the system average neutrons per fission calculated by KENO-VI is used. Adding fission photons to the neutron source is optional; for example, in modeling neutron-only detectors, adding and following the fission photons in the transport calculation is unnecessary and would slow the calculation. MAVRIC can be optimized to calculate a specific detector response at one location using the CADIS methodology or to calculate multiple responses/locations with roughly the same relative uncertainty using FW-CADIS.

With this two-step approach, users have a great deal of flexibility in modeling CAAS problems. The KENO-VI step and the MAVRIC step could both use the same geometry and materials definitions or could have different levels of detail included in each. For best results, a possible scheme would be to model the critical system geometry with only the closest surrounding materials in fine detail. The radiation transport geometry used by MAVRIC could omit small details that are unimportant to its analysis, while including large building-level components that are important. The fission source distribution from one KENO-VI criticality calculation could be used in a number of different MAVRIC building/detector models, with each MAVRIC calculation optimized for a given type of detector.

XVII. GEEWIZ: WINDOWS USER INTERFACE FOR SCALE

As part of development efforts to improve SCALE's ease of use, a Windows user interface for SCALE has been created. The SCALE Graphically Enhanced Editing Wizard (GeeWiz) serves as a user control center for

execution of many automated SCALE sequences. GeeWiz provides input menus and context-sensitive help to guide users through the setup of their input. It includes a direct link to the KENO3D 3-D visualization tool to allow users to view the components of their geometry model as it is constructed. Once the input is complete, the user can click a button to run SCALE and another button to view the output. GeeWiz is compatible with the primary SCALE sequences: CSAS5, CSAS6, MAVRIC, TSUNAMI-1D, TSUNAMI-3D, STARBUCS, and TRITON.

GeeWiz provides a simple user interface with toolbar buttons to access the primary functions of the program. The main toolbar has buttons that invoke a variety of commands and options, including

1. create a new problem
2. open an input file
3. save an input file
4. execute SCALE
5. view output (in text or HTML format)
6. view 2-D color geometry model plots (if plot data are entered)
7. access online help
8. view the model in KENO3D
9. plot results in Java Plots Especially Nice Output (Javapeño).

Examples of the GeeWiz user interface are displayed in Figs. 16 and 17. The Geometry form (Fig. 16) allows the user to easily navigate through the units that define the geometry model. This form includes all options for specifying KENO geometry models. The Array form (Fig. 17) provides an intuitive point-and-click interface for creating and modifying arrays to be used in the KENO geometry. The GeeWiz integrated user interface enables new users to quickly learn how to perform analyses with SCALE and use many of its visualization tools.

XVIII. KENO3D: INTERACTIVE 3-D VISUALIZATION

Criticality safety analyses often require detailed modeling of complex geometries. Developing and checking the accuracy of these models can be enhanced by effective

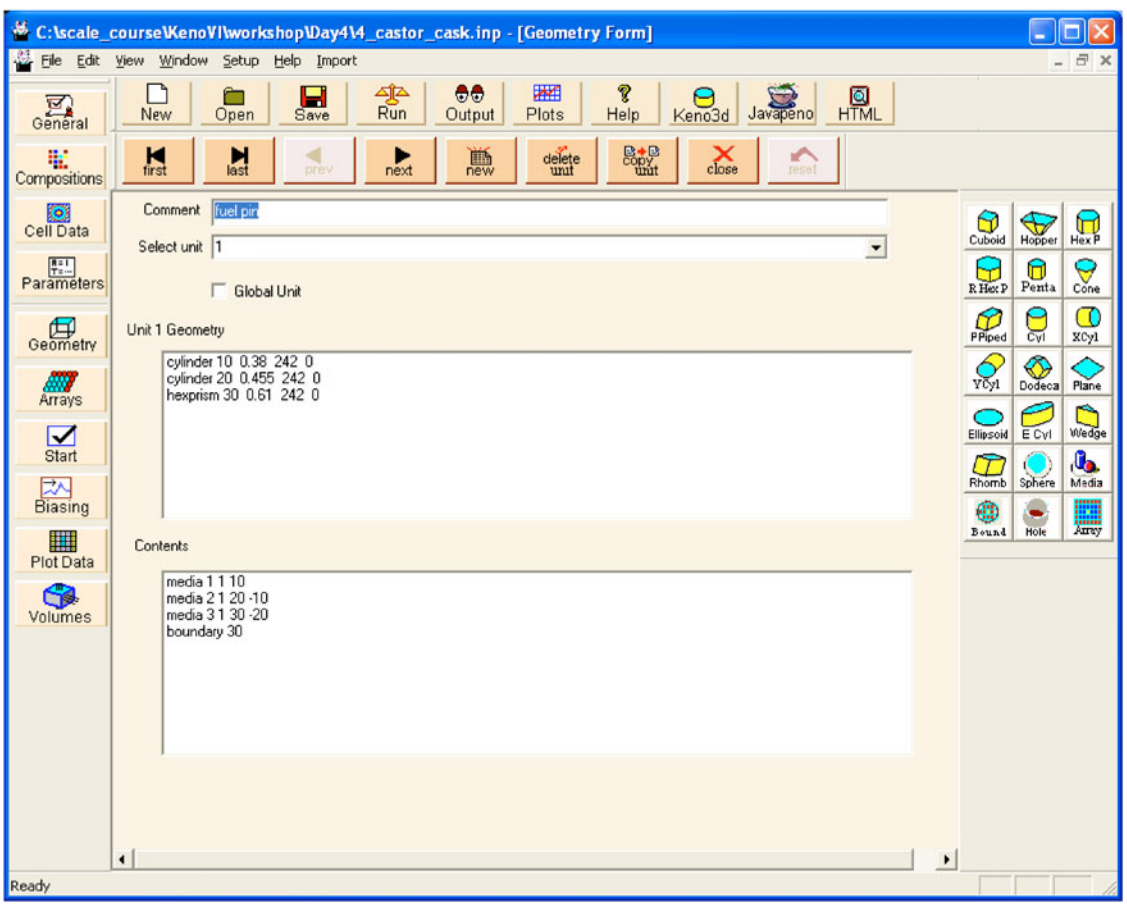

Fig. 16. Geometry form in GeeWiz.

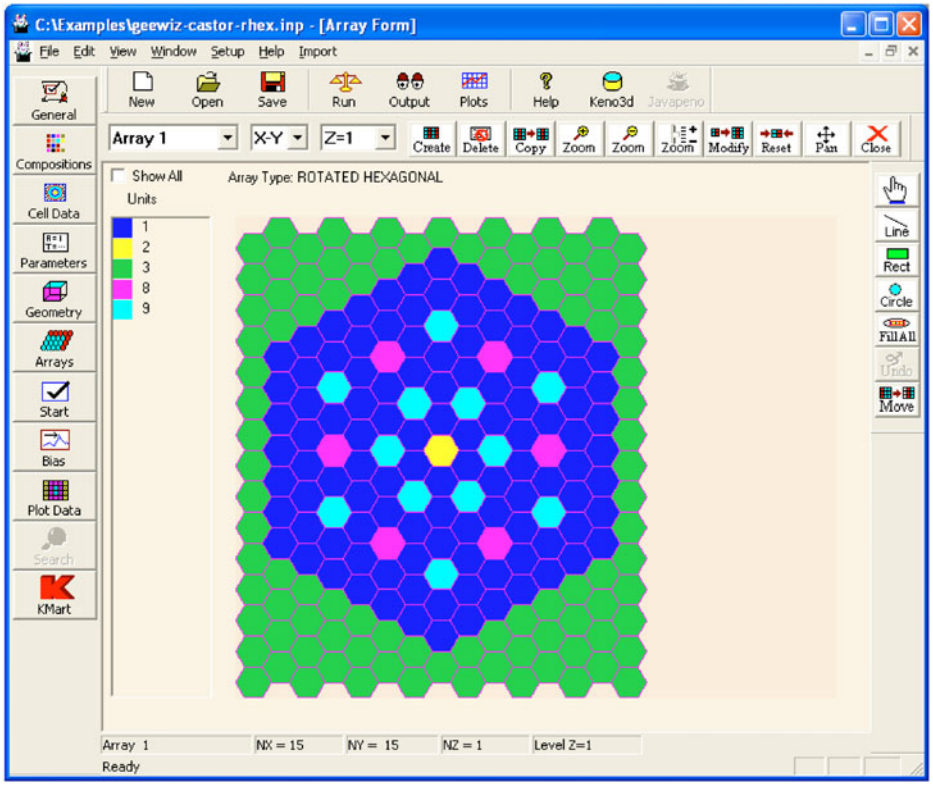

Fig. 17. GeeWiz array form for rotated hexagonal array in KENO-VI.

visualization tools. To address this need, SCALE includes a powerful state-of-the-art visualization tool called "KENO3D." KENO3D enables KENO V.a and KENO-VI users to interactively display their 3-D geometry models. The interactive options include

1. shaded or wireframe images
2. standard views, such as top view, side view, front view, and isometric (3-D) view
3. rotating the model
4. zooming in on selected locations
5. selecting parts of the model to display
6. editing colors and displaying legends
7. displaying properties of any unit in the model
8. creating cutaway views
9. removing units from the model
10. copying image to the clipboard to paste in other applications.

KENO3D reads existing KENO models from SCALE input files and attempts to verify that the KENO geometry input conforms to the code input guidelines. KENO3D prints a warning message for illegal geometry input, and if possible, displays the illegal KENO V.a geometry to facilitate debugging of the input. A display of a sample LWR fuel assembly burnup credit cask model is shown in Fig. 18.

KENO3D has a fully integrated help system to aid users. It has several unique options that provide users with increased flexibility in visualizing portions of a model in greater detail or in visualizing parts of larger models that may be too large to provide a useful image when viewed in their entirety. KENO3D has the capability to overlay results produced by KENO on the 3-D geometry model. As an example, a KENO model of the Solution High Energy Burst Assembly (SHEBA) solution reactor (uranyl nitrate in an annular steel tank) with the fission rate overlaid on the geometry is shown in Fig. 19.

XIX. JAVAPEÑO: INTERACTIVE PLOTTING OF CALCULATED RESULTS

Javapeño is a powerful interactive 2-D and 3-D plotting program. Although originally designed to plot TSUNAMI sensitivity data, it has been enhanced to work with data files generated by several SCALE modules and other data sources, including SCALE cross-section or covariance data. Javapeño is written entirely in Java and can be executed on several platforms, including Windows, Linux, Macintosh, and UNIX. Javapeño plots

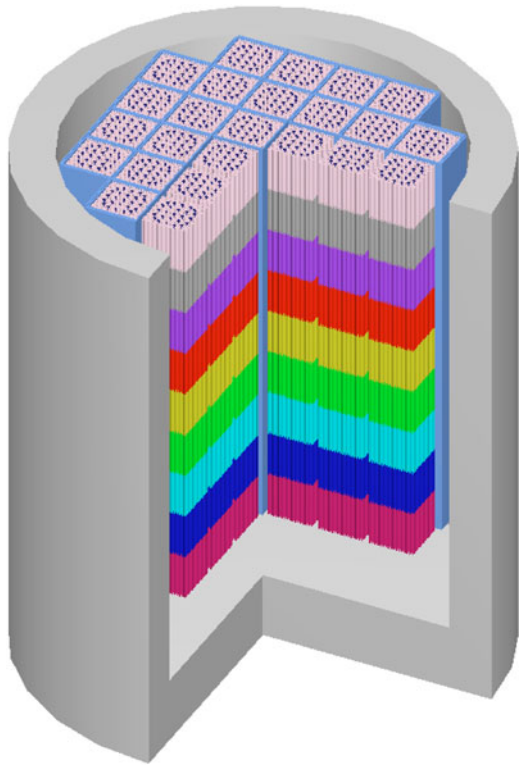

Fig. 18. KENO3D cutaway view of LWR burnup credit cask model.

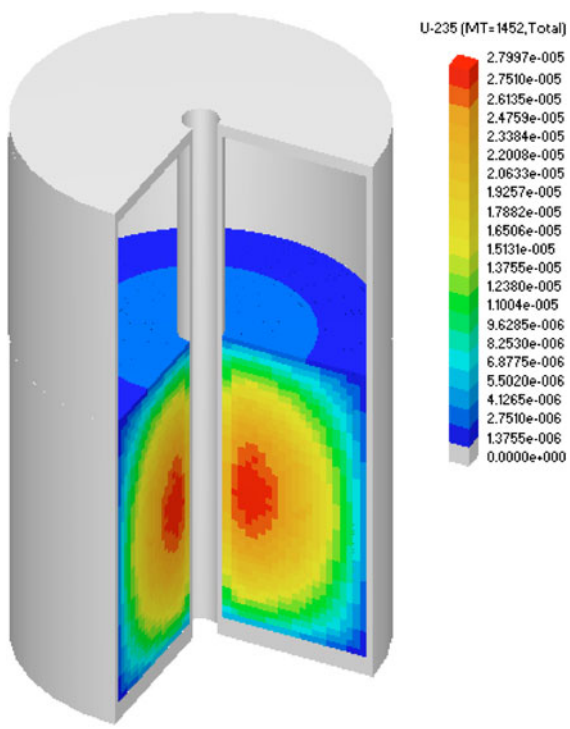

Fig. 19. SHEBA-2 fission density profile (per fission neutron) in KENO3D.

can be printed directly from the software package or can be exported to a variety of graphics formats to use in reports or presentations.

Javapeño plots sensitivity, reaction rate, or flux data as a function of energy group normalized by the unit lethargy for each group, thus eliminating the relative group width from the analysis. Figure 20 contains a Javapeño plot of the ^{239}Pu fission k_{eff} (or eigenvalue) sensitivity profiles for two MOX polystyrene compact critical experiments.[46] The dashed red curve (nse55t4-01) is the first experiment in Table IV of Ref. 46; the solid blue curve (nse55t5-01) is the first experiment in Table V of Ref. 46 (color online). The characteristics of these experiments are given in Table IV of this paper. The plot shows that the first experiment is much more sensitive to the ^{239}Pu fission cross section in the thermal range. The second experiment is much more sensitive in the resonance and fast ranges.

XX. TRAINING, USER SUPPORT, AND VALIDATION

ORNL offers several hands-on onsite training courses each year. In addition, courses are frequently conducted at user facilities or international locations such as the Organisation for Economic Co-operation and Development (OECD) Nuclear Energy Agency (NEA) Data Bank in Paris, France. Approximately 1000 users have participated in SCALE training courses since they were first offered in 1993; roughly one-third of those were foreign nationals.

Technical support is also provided to users via e-mail and the SCALE Web site.[47] The Web site contains useful information such as user notebooks, software updates, validation reports, and other publications. Newsletters have been published semiannually for 20 years to inform users of updates and important technical issues and are posted on the Web site as well.

Extensive validation of SCALE modules and data libraries has been performed over the past three decades. Numerous criticality safety validation reports for KENO (Refs. 21 and 48 through 52) and TRITON/ORIGEN validations versus measured spent fuel assay data[30,31,53–55] and decay heat[32,33] have been published. The new MAVRIC shielding capability has also been recently validated.[44]

XXI. SUMMARY

SCALE 6 can be used to perform nuclear safety analyses using state-of-the-art computational capabilities for

1. problem-dependent multigroup cross-section processing
2. criticality safety (continuous energy Monte Carlo)

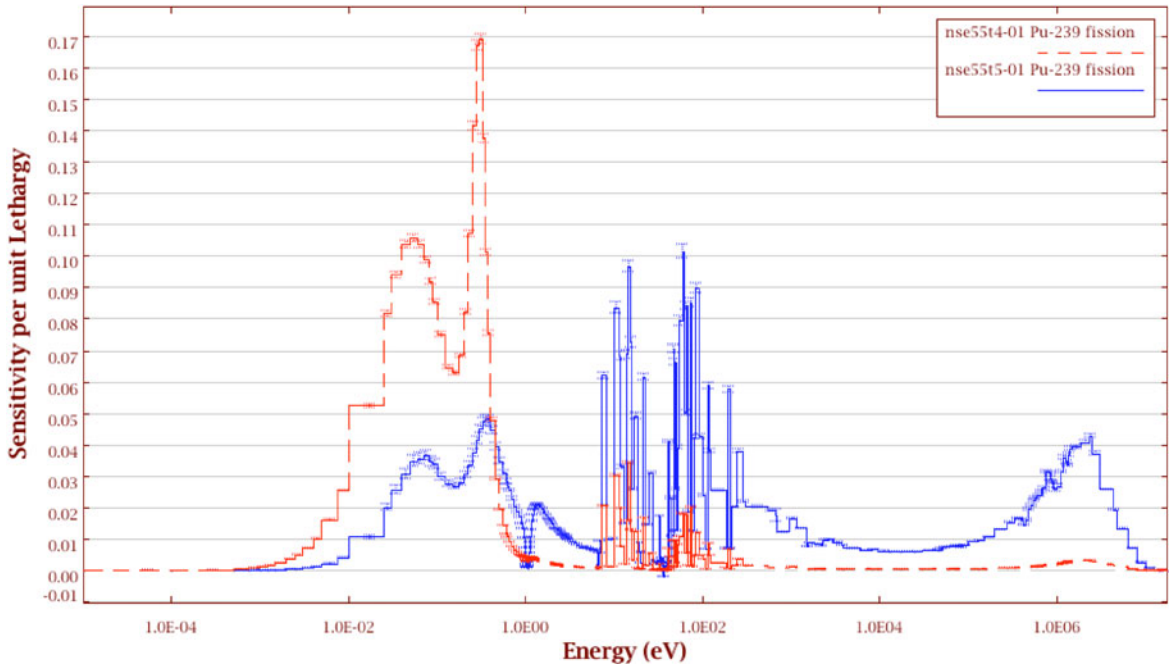

Fig. 20. Javapeño plot of ^{239}Pu fission k_{eff} sensitivity profiles from MOX polystyrene compact critical experiments.

TABLE IV

MOX Polystyrene Compact Critical Experiments

Experiment	nse55t4-01 (Ref. 46)	nse55t5-01 (Ref. 46)
H/(U + Pu)	30.6	2.8
Pu/(U + Pu)	0.146	0.303
^{240}Pu (wt%)	7.97	11.5
EALF[a]	0.143	39.7

[a]Energy of average lethargy-causing fission.

3. radiation shielding (Monte Carlo with automated 3-D variance reduction)
4. lattice physics and depletion (2-D discrete ordinates and 3-D Monte Carlo)
5. spent fuel characterization, including source terms and decay heat
6. sensitivity/uncertainty (1-D discrete ordinates and 3-D Monte Carlo)
7. burnup credit (3-D Monte Carlo).

SCALE 6 includes ENDF/B-VI and ENDF/B-VII multigroup and continuous-energy cross-section data and a comprehensive covariance data library for more than 300 nuclides. The package contains 3-D visualization, 2-D and 3-D plotting, and user interfaces to facilitate problem setup, execution, and review. It is distributed by the Radiation Safety Information Computational Center[56] and the OECD/NEA Data Bank and is used in approximately 40 nations worldwide.

A comprehensive plan has been created for future SCALE methods development activities in all applications areas. The list of tasks is continuously revised and expanded as current development activities are completed and new priorities are identified. Planned methods development activities after the release of SCALE 6.1 currently include a redesign of the basic SCALE computational architecture to provide coarse-level parallelization, internal multithreading, generalized coupling between different computation methods, and more efficient exchange of data between computational modules.

REFERENCES

1. "SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation," ORNL/TM-2005/39, Version 6, Vols. I–III; see also CCC-750, Radiation Safety Information Computational Center, Oak Ridge National Laboratory (Jan. 2009).

2. M. L. WILLIAMS and M. ASGARI, "Computation of Continuous-Energy Neutron Spectra with Discrete Ordinates Transport Theory," *Nucl. Sci. Eng.*, **121**, 173 (1995).

3. M. D. DeHART and S. M. BOWMAN, "Reactor Physics Methods and Analysis Capabilities in SCALE," *Nucl. Technol.*, **174**, 196 (2011).

4. I. C. GAULD, G. RADULESCU, G. ILAS, B. D. MURPHY, M. L. WILLIAMS, and D. WIARDA, "Isotopic Depletion and Decay Methods and Analysis Capabilities in SCALE," *Nucl. Technol.*, **174**, 169 (2011).

5. M. L. WILLIAMS, "Resonance Self-Shielding Methodologies in SCALE," *Nucl. Technol.*, **174**, 149 (2011).

6. S. GOLUOGLU and M. L. WILLIAMS, "Modeling Doubly Heterogeneous Systems in SCALE," *Trans. Am. Nucl. Soc.*, **93**, 963 (2005).

7. S. GOLUOGLU, "Analysis of a Computational Benchmark for a High-Temperature Reactor Using SCALE," *Proc. Int. Topl. Mtg. Reactor Physics (PHYSOR '06)*, Vancouver, British Columbia, Canada, September 10–14, 2006, American Nuclear Society (2006).

8. S. GOLUOGLU, L. M. PETRIE, Jr., M. E. DUNN, D. F. HOLLENBACH, and B. T. REARDEN, "Monte Carlo Criticality Methods and Analysis Capabilities in SCALE," *Nucl. Technol.*, **174**, 214 (2011).

9. M. E. DUNN and N. M. GREENE, "AMPX-2000: A Cross-Section Processing System for Generating Nuclear Data for Criticality Safety Applications," *Trans. Am. Nucl. Soc.*, **86**, 118 (2002).

10. M. E. DUNN and L. C. LEAL, "Calculating Probability Tables for the Unresolved-Resonance Region Using Monte Carlo Methods," *Proc. Int. Conf. New Frontiers of Nuclear Technology: Reactor Physics, Safety and High-Performance Computing (PHYSOR 2002)*, Seoul, Korea, October 7–10, 2002, paper 11C.03, American Nuclear Society (2002).

11. B. T. REARDEN, "Perturbation Theory Eigenvalue Sensitivity Analysis with Monte Carlo Techniques," *Nucl. Sci. Eng.*, **146**, 367 (2004).

12. B. L. BROADHEAD, B. T. REARDEN, C. M. HOPPER, J. J. WAGSCHAL, and C. V. PARKS, "Sensitivity- and Uncertainty-Based Criticality Safety Validation Techniques," *Nucl. Sci. Eng.*, **146**, 340 (2004).

13. B. T. REARDEN, M. L. WILLIAMS, M. A. JESSEE, D. E. MUELLER, and D. A. WIARDA, "Sensitivity and Uncertainty Analysis Capabilities and Data in SCALE," *Nucl. Technol.*, **174**, 236 (2011).

14. M. L. WILLIAMS and B. T. REARDEN, "Sensitivity/Uncertainty Analysis Capabilities and New Covariance Data Libraries in SCALE," *Nucl. Data Sheets*, **109**, 2796 (Dec. 2008).

15. S. GOLUOGLU, C. M. HOPPER, and B. T. REARDEN, "Extended Interpretation of Sensitivity Data for Benchmark Areas of Applicability," *Trans. Am. Nucl. Soc.*, **88**, 77 (2003).

16. D. E. MUELLER, B. T. REARDEN, and D. A. REED, "Evaluation of Fission Product Critical Experiments and Associated Biases for Burnup Credit Validation," *Proc. IAEA/CSN Int. Workshop Advances in Applications of Burnup Credit for Spent Fuel Storage, Transport, Reprocessing, and Disposition*, Cordoba, Spain, October 27–30, 2009 (2010).

17. D. E. MUELLER, B. T. REARDEN, and D. F. HOLLENBACH, "Application of the SCALE TSUNAMI Tools for the Validation of Criticality Safety Calculations Involving ^{233}U," ORNL/TM-2008/196, Oak Ridge National Laboratory (Jan. 2009).

18. G. RADULESCU, D. E. MUELLER, and J. C. WAGNER, "Sensitivity and Uncertainty Analysis of Commercial Reactor Criticals for Burnup Credit," NUREG/CR-6951 (ORNL/TM-2006/87), Oak Ridge National Laboratory (Dec. 2007).

19. B. T. REARDEN, W. J. ANDERSON, and G. A. HARMS, "Use of Sensitivity and Uncertainty Analysis in the Design of Reactor Physics and Criticality Benchmark Experiments for Advanced Nuclear Fuel," *Nucl. Technol.*, **151**, 133 (2005).

20. M. B. CHADWICK et al., "ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology," *Nucl. Data Sheets*, **107**, 2931 (2006).

21. S. GOLUOGLU, M. E. DUNN, L. M. PETRIE, and T. S. SUMNER, "Development and Validation of the New Continuous Energy Capability in the Criticality Safety Code KENO," *Proc. Int. Conf. Physics of Reactors (PHYSOR '08)*, Interlaken, Switzerland, September 14–19, 2008.

22. M. L. WILLIAMS and G. ILAS, "ENDF/B-VII Nuclear Data Libraries for SCALE-6," *Proc. Topl. Mtg. Advances in Nuclear Fuel Management (ANFM IV)*, Hilton Head Island, South Carolina, April 12–15, 2009, American Nuclear Society (2009).

23. "Evaluated Nuclear Structure Data File—A Computer File of Evaluated Experimental Nuclear Structure Data Maintained by the National Nuclear Data Center," ENSDF decay file as of April 2003, Brookhaven National Laboratory.

24. A. B. PASHCHENKO, H. WIENKE, J. KOPECKY, J.-Ch. SUBLET, and R. A. FORREST, "Neutron Activation Cross-Section Data Library for Fusion Applications," IAEA-NDS-173, Rev. 1, International Atomic Energy Agency (October 1998).

25. R. A. FORREST, J. KOPECKY, and J.-Ch. SUBLET, "The European Activation File: EAF-2003 Cross Section Library," UKAEA FUS-486, UKAEA/EURATOM Fusion Association (Dec. 2002).

26. J.-Ch. SUBLET, A. J. KONING, R. A. FORREST, and J. KOPECKY, "The JEFF-3.0/A Neutron Activation File—EAF-2003 into ENDF-6 Format," JEFDOC-982, Commissariat à l'Energie Atomique (Nov. 2003); http://www.nea.fr/html/dbdata/JEFF/ (current as of August 3, 2010).

27. I. GAULD, "Validation of ORIGEN-S Decay Heat Predictions for LOCA Analysis," *Proc. Int. Topl. Mtg. Reactor Physics (PHYSOR'06)*, Vancouver, British Columbia, Canada, September 10–14, 2006, American Nuclear Society (2006).

28. I. C. GAULD, E. F. SHORES, and R. T. PERRY, "New Neutron Source Algorithms in the ORIGEN-S Code," *Proc. Topl. Mtg. Radiation Protection and Shielding Division*, Santa Fe, New Mexico, April 14–17, 2002, American Nuclear Society (2002).

29. E. F. SHORES, "SOURCES 4C: A Code for Calculating (α, n), Spontaneous Fission, and Delayed Neutron Sources and Spectra," LA-UR-02-1839, Los Alamos National Laboratory (Apr. 2002).

30. G. ILAS, I. C. GAULD, F. C. DIFILIPPO, and M. B. EMMETT, "Analysis of Experimental Data for High Burnup PWR Spent Fuel Isotopic Validation—Calvert Cliffs, Takahama, and Three Mile Island Reactors," NUREG/CR-6968 (ORNL/TM-2008/071), Oak Ridge National Laboratory (Feb. 2010).

31. G. ILAS, I. C. GAULD, and B. D. MURPHY, "Analysis of Experimental Data for High Burnup PWR Spent Fuel Isotopic Validation—ARIANE and REBUS Programs (UO_2 Fuel)," NUREG/CR-6969 (ORNL/TM-2008/072), Oak Ridge National Laboratory (Feb. 2010).

32. B. D. MURPHY and I. C. GAULD, "Spent Fuel Decay Heat Measurements Performed at the Swedish Central Interim Storage Facility," NUREG/CR-6971 (ORNL/TM-2008/016), Oak Ridge National Laboratory (Feb. 2010).

33. I. C. GAULD, G. ILAS, B. D. MURPHY, and C. F. WEBER, "Validation of SCALE 5 Decay Heat Predictions for LWR Spent Nuclear Fuel," NUREG/CR-6972 (ORNL/TM-2008/015), Oak Ridge National Laboratory (Feb. 2010).

34. I. C. GAULD and S. M. BOWMAN, "STARBUCS: A Prototypic SCALE Control Module for Automated Criticality Safety Analyses Using Burnup Credit," NUREG/CR-6748 (ORNL/TM-2001/33), Oak Ridge National Laboratory (Oct. 2001).

35. G. RADULESCU and I. C. GAULD, "Enhancements to the Burnup Credit Criticality Safety Analysis Sequence in SCALE," *Proc. Topl. Mtg. Nuclear Criticality Safety Division: Realism, Robustness and the Nuclear Renaissance (NCSD 2009)*, Richland, Washington, September 13–17, 2009, American Nuclear Society (2009).

36. "Issue: Burnup Credit in the Criticality Safety Analyses of PWR Spent Fuel in Transport and Storage Casks," Spent Fuel Project Office Interim Staff Guidance—8, Rev. 2, U.S. Nuclear Regulatory Commission (Sep. 27, 2002).

37. M. D. DeHART, "An Advanced Deterministic Method for Spent-Fuel Criticality Safety Analysis," *Trans. Am. Nucl. Soc.*, **78**, 170 (1998).

38. M. D. DeHART, "A Deterministic Study of the Deficiency of the Wigner-Seitz Approximation for Pu/MOX Fuel Pins," *Proc. Int. Conf. M&C'99—Madrid, Mathematics and Computations Meeting*, Madrid, Spain, September 27–30, 1999, p. 689 (1999).

39. M. D. DeHART, "High-Fidelity Depletion Capabilities of the SCALE Code System Using TRITON," *Trans. Am. Nucl. Soc.*, **97**, 598 (2007).

40. J. C. WAGNER and A. HAGHIGHAT, "Automated Variance Reduction of Monte Carlo Shielding Calculations Using the Discrete Ordinates Adjoint Function," *Nucl. Sci. Eng.*, **128**, 186 (1998).

41. J. C. WAGNER, E. D. BLAKEMAN, and D. E. PEPLOW, "Forward-Weighted CADIS Method for Variance Reduction of Monte Carlo Calculations of Distributions and Multiple Localized Quantities," *Proc. Int. Conf. Mathematics, Computational Methods & Reactor Physics (M&C 2009)*, Saratoga Springs, New York, May 3–7, 2009, American Nuclear Society (2009).

42. T. M. EVANS, A. S. STAFFORD, R. N. SLAYBAUGH, and K. T. CLARNO, "Denovo: A New Three-Dimensional Parallel Discrete Ordinates Code in SCALE," *Nucl. Technol.*, **171**, 171 (2010).

43. D. E. PEPLOW, T. M. EVANS and J. C. WAGNER, "Simultaneous Optimization of Tallies in Difficult Shielding Problems," *Nucl. Technol.*, **168**, 785 (2009).

44. D. WIARDA, M. E. DUNN, D. E. PEPLOW, T. M. MILLER, and H. AKKURT, "Development and Testing of ENDF/B-VI.8 and ENDF/B-VII.0 Coupled Neutron-Gamma Libraries for SCALE 6," NUREG/CR-6990 (ORNL/TM-2008/047), Oak Ridge National Laboratory (Feb. 2009).

45. D. E. PEPLOW and L. M. PETRIE, Jr., "Criticality Accident Alarm System Modeling with SCALE," *Proc. 2009 Int. Conf. Advances in Mathematics, Computational Methods, and Reactor Physics (M&C 2009)*, Saratoga Springs, New York, May 3–7, 2009, American Nuclear Society (2009).

46. S. R. BIERMAN and E. D. CLAYTON, "Critical Experiments to Measure the Neutron Poisoning Effects of Copper and Copper-Cadmium Plates," *Nucl. Sci. Eng.*, **55**, 58 (1974).

47. SCALE Web site: http://www.ornl.gov/sci/scale (current as of August 3, 2010).

48. P. B. FOX and D. F. HOLLENBACH, "KENO-VI Validation," ORNL/TM-2004/60, Oak Ridge National Laboratory (May 2005).

49. P. B. FOX and L. M. PETRIE, "Validation and Comparison of KENO V.a and KENO-VI," ORNL/TM-2001/110, Oak Ridge National Laboratory (May 2002).

50. S. M. BOWMAN, W. C. JORDAN, J. F. MINCEY, C. V. PARKS, and L. M. PETRIE, JR., "Experience with the SCALE Criticality Safety Cross-Section Libraries," NUREG/CR-6685 (ORNL/TM-1999/322), Oak Ridge National Laboratory (Oct. 2000).

51. J. J. LICHTENWALTER, S. M. BOWMAN, M. D. DeHART, and C. M. HOPPER, "Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages," NUREG/CR-6361 (ORNL/TM-13211), Oak Ridge National Laboratory (Mar. 1997).

52. M. B. EMMETT and W. C. JORDAN, "Guide to Verification and Validation of the SCALE-4 Criticality Safety Software," NUREG/CR-6483, ORNL/TM-12834, Oak Ridge National Laboratory (Nov. 1996).

53. G. RADULESCU, I. C. GAULD, and G. ILAS, "SCALE 5.1 Predictions of PWR Spent Nuclear Fuel Isotopic Compositions," ORNL/TM-2010/44, Oak Ridge National Laboratory (Mar. 2010).

54. M. D. DeHART and S. M. BOWMAN, "Improved Radiochemical Assay Analyses Using TRITON Depletion Sequences in SCALE," *Proc. Int. Conf. Advances in Applications of Burnup Credit to Enhance Spent Fuel Transportation, Storage, Reprocessing and Disposition*, London, United Kingdom, August 29–September 2, 2005, IAEA-TECDOC-CD-1547, Session 2, p. 99, International Atomic Energy Agency (May 2007).

55. I. C. GAULD, "Strategies for Application of Isotopic Uncertainties in Burnup Credit," NUREG/CR-6811 (ORNL/TM-2001/257), Oak Ridge National Laboratory (June 2003).

56. SCALE 6 package, Radiation Safety Information Computational Center, http://www-rsicc.ornl.gov (current as of August 3, 2010); see also Nuclear Energy Agency, http://www.nea.fr (current as of August 3, 2010).