



# SCALE Newsletter

Number 39

January 2009

## Special Points of Interest:

SCALE workshops in March 2009 at ORNL, \$300 discount until February 9, 2009

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## New Capabilities in SCALE 6

SCALE 6 will be available from the Radiation Safety Information Computational Center (RSICC) beginning the first week of February. You can go to <http://rsicc.ornl.gov/rsiccnew/order.htm> to order it. It should be available from the OECD/NEA Data Bank in late February.

The following items highlight new capabilities that are included in SCALE 6.

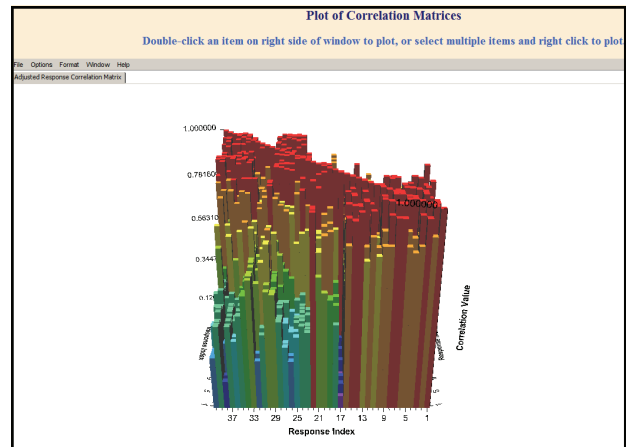
- Continuous energy (CE) capability in KENO V.a and KENO-VI (see [July 2008 issue](#) for details)
- CE and 238-group ENDF/B-VI.8 and ENDF/B-VII.0 (latest ENDF release) cross-section libraries with full-range Bondarenko factors in multigroup libraries
- MAVRIC/Monaco 3-D Monte Carlo shielding modules with automated variance reduction (see [January 2008 issue](#) for details)
  - \* Uses SCALE Generalized Geometry Package (same as KENO-VI)
  - \* Flexible source description: separable spatial, energy, and directional distributions
  - \* Tally options: region tally, point detectors, mesh tally
  - \* Uses CADIS methodology to perform automated 3-D variance reduction
  - \* Creates a biased source distribution and weight windows in space and energy
  - \* Uses FW-CADIS (Forward Weighted CADIS) to optimize multiple tallies simultaneously or produce mesh tallies with more uniform relative uncertainties
  - \* Graphical displays of mesh tallies, weight windows, source distributions, intermediate flux files, and tally convergence with Java viewer ([page 4](#))
- ENDF/B-VII coupled neutron/gamma shielding cross-section libraries for use with MAVRIC/Monaco (200 neutron/47 gamma groups and 27 neutron/19 gamma groups)
- Criticality accident alarm system (CAAS) analysis using CSAS6/KENO-VI criticality sequence and MAVRIC/Monaco shielding sequence ([page 3](#))
- TRITON/NEWT enhancements ([page 5](#))
  - \* Depletion with doubly heterogeneous unit cells (e.g., pebble bed or prismatic fuel)
  - \* Automatic group collapse for depletion calculations
  - \* Extended limits for number of depletion materials and depletion steps
  - \* Improved treatment of depletion by flux vs depletion by power for nonpower rods
  - \* Full support for fixed source calculations
  - \* Improved treatment for sigma-transport calculations (current weighted)
  - \* Improved accuracy in calculations where critical buckling is supplied
  - \* Addition of arbitrarily high-order product quadrature set
  - \* New fast reactor ORIGEN-S library for fast reactor analysis with TRITON
  - \* Tracking of trace element nuclides in TRITON depletion calculations
  - \* Full support for all OPUS capabilities including stacked OPUS specifications within a single TRITON calculation
- TSUNAMI-3D with KENO-VI (SCALE 5.1 used only KENO V.a with TSUNAMI)

(Continued on page 2)

## New Capabilities in SCALE 6

(Continued from page 1)

- Flexible mesh grids in KENO V.a and KENO-VI for TSUNAMI or criticality accident alarm system (CAAS) analyses
- HTML output for KENO-VI (SCALE 5.1 included HTML output for KENO V.a)
- Covariance library with data for more than 300 materials based on
  - \* LANL covariance data for light nuclei up to and including F-19
  - \* "Integral method" in thermal and resonance range for other nuclides (ORNL)
  - \* Nuclear model techniques in fast range for other nuclides (BNL, LANL)
- TSURFER S/U data adjustment tool to examine measured and calculated data and adjust integral experiment values within uncertainties to produce consistency between measured and calculated results ([page 7](#))
- Reactivity sensitivity analysis tool TSAR ([page 7](#))
- New USLSTATS (**U**pper **S**ubcritical **L**imits **STAT**istic**S**) entirely rewritten in Java with integrated user interface for input, output, and plotting ([page 4](#))
- VIBE (Validation, Interpretation, and Bias Estimation) Java user interface to filter TSUNAMI files and sort/filter sensitivity data ([page 4](#))
- ExSITE (**Ex**ensible **SCALE** **I**ntelligent **T**ext **E**ditor) Java user interface for TSUNAMI-IP, TSURFER, and TSAR ([page 4](#))
- STARBUCS burnup credit cask loading curve search
- MCDancoff (Monte Carlo Dancoff) control module to calculate Dancoff factors in complicated 3-D geometries using Monte Carlo integrations in a modified version of KENO-VI called KENO\_Dancoff



TSURFER Correlation matrices

## TSUNAMI-3D Enhancements with KENO V.a and KENO-VI

The TSUNAMI-3D sensitivity/uncertainty (S/U) sequence was enhanced to include the generalized geometry capabilities of KENO-VI. A new flexible mesh capability was added to KENO-VI to accumulate the angular moments of the forward and adjoint multigroup flux solutions. The same flexible mesh was added to KENO V.a to reduce resource requirements for TSUNAMI-3D calculations with KENO V.a. The order of flux moment expansions has been increased to calculate moments through any order requested by the user. Previously, moments could be computed only through third order. The implicit sensitivities previously

computed with the resource-intensive CENTRMST code are now computed using BONAMIST and the new full-range Bondarenko factors in the SCALE 6 ENDF/B-VI and ENDF/B-VII multigroup cross-section libraries, significantly decreasing the CPU time and memory requirements for most models. CENTRMST will not be included in SCALE 6. Additionally, the calculation of the fission spectrum and chi sensitivities was modified to produce constrained sensitivities that maintain the requirement that the integral of chi always be maintained as 1.0.

## CAAS Analysis Using CSAS6/KENO-VI and MAVRIC/Monaco

Modeling criticality accident alarm systems presents challenges since the analysis consists of both a criticality problem as well 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 now contains fully 3-D tools to perform both parts of a CAAS analysis.

CAAS analysis can be performed with SCALE 6 using the KENO-VI criticality code and the new MAVRIC shielding sequence. First, the fission distribution (in space and energy) is determined via KENO-VI. This distribution is saved to a file using a user-specified 3-D mesh grid and an energy structure from the cross-section library. MAVRIC (Monaco with Automated Variance Reduction using Importance Calculations) then uses the fission distribution as the source for a shielding calculation. MAVRIC is designed to implement advanced variance reduction methods to calculate dose rates or detector responses for difficult shielding problems.

The CAAS capability in SCALE 6 is a two-step approach using KENO-VI and MAVRIC. The first step is the determination of the source distribution, done with the CSAS6 (Criticality Safety Analysis Sequence 6) control sequence, which uses the KENO-VI functional module. Along with calculating the system  $k_{eff}$ , KENO-VI has been modified to accumulate the fission distribution over all saved generations. This information is collected on a 3-D Cartesian mesh that overlays the physical geometry model and is saved as a Monaco mesh source file.

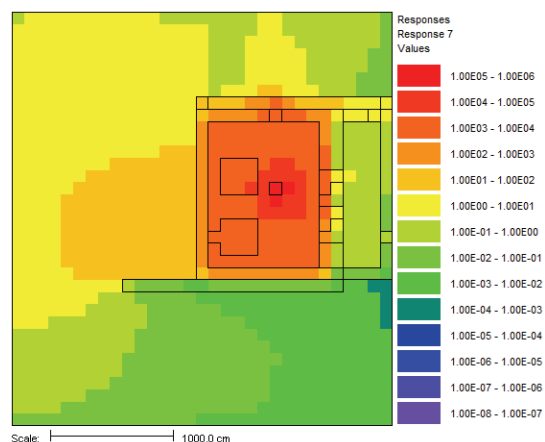
The mesh source is then used in the second step as the source term in MAVRIC. The absolute source strength is set by the user based on the total number of fissions (based on the total power released) during the criticality excursion. Further neutron multiplication is prevented in the MAVRIC transport calculation. If further fissions were allowed, Monaco would add neutrons to its particle bank faster than they could be removed (since the system is at or above critical) and would never finish.

The user can also tell MAVRIC to 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  $\nu$ -bar (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 would only slow down the calculation.

For the transport part, MAVRIC can be optimized to calculate one specific detector response at one location using the Consistent Adjoint Driven Importance Sampling (CADIS) methodology<sup>1</sup> or to calculate multiple responses/locations with roughly the same relative uncertainty using forward weighted CADIS (FW-CADIS). For calculating mesh tallies of fluxes or dose rates, MAVRIC also uses FW-CADIS to help balance the Monaco Monte Carlo calculation such that low-flux voxels are computed with approximately the same relative uncertainty as high-flux voxels.

With this two-step approach, users have a great deal of flexibility in modeling CAAS problems. The CSAS6/KENO-VI step and the MAVRIC/Monaco 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 could omit small details but would include large building-level components. The fission source distribution from one KENO-VI calculation could be used in a number of different MAVRIC building/detector models, with each MAVRIC calculation optimized for a given type of detector.



Calculated doses for hypothetical criticality accident in the Oak Ridge Critical Experiments Facility

<sup>1</sup>J. C. Wagner and A. Haghghat, "Automated Variance Reduction of Monte Carlo Shielding Calculations Using the Discrete Ordinates Adjoint Function," *Nucl. Sci. Eng.*, **128**, 186–208 (1998).

## New Java User Interfaces in SCALE 6

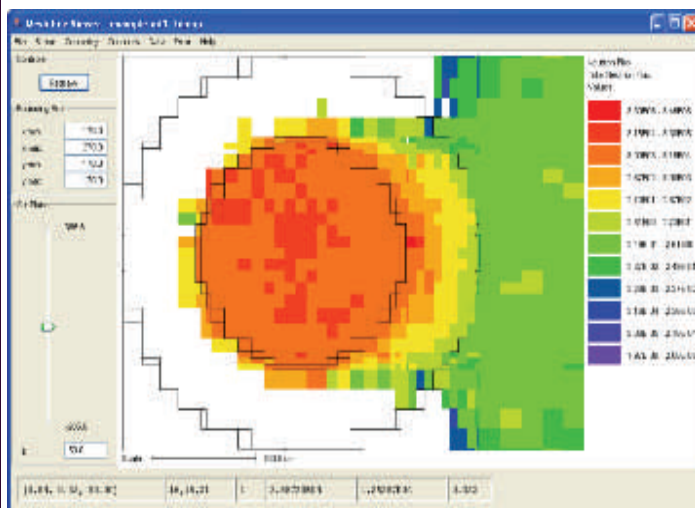
**MeshView** allows the user to display 3-D data using contour slices. Slices can be made through any of the three dimensions. Data can be shown using linear or logarithmic contours. Various geometry data can be shown as edges with the data or as solid color regions without the data. For data sets with uncertainties, the uncertainties can also be shown using contour slices. As the mouse is moved around the image, a status bar below the image lists the location, cell indices, geometry index, data value, data uncertainty and the relative uncertainty for each cell. MeshView can be used to show scalar fluxes from Denovo discrete ordinates calculations in MAVRIC and mesh tallies, mesh importance maps, and mesh-based sources from Monaco, as well as other 3-D mesh-based data files.

The **ChartPlot** interactive 2-D plotter allows the user to display data in a variety of ways in order to more fully investigate the data. Data can be shown on linear or logarithmic axes, with or without axis titles, a chart title, or a legend. Each series of data in the chart can be shown as points with different markers, as lines of variable width, as both markers and lines, with or without error bars in either dimension, and in different colors. Linear least-squares fits can be made to subsets of series data. ChartPlot is used to display Monaco tally convergence data as well as lines of data through 3-D mesh-based data files using MeshView.

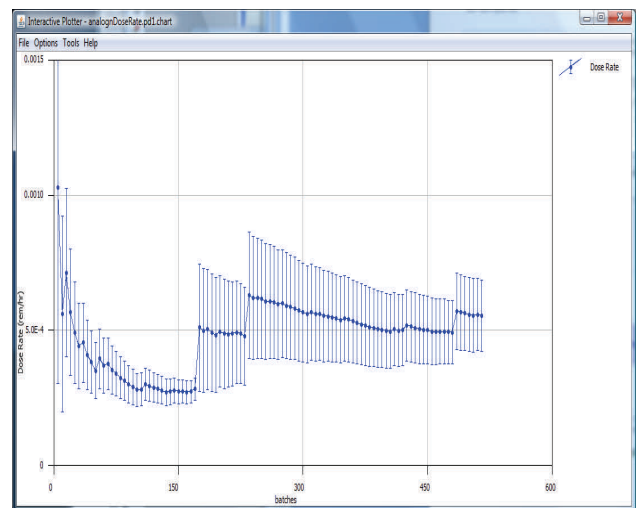
**VIBE** (Validation, Interpretation and Bias Estimation) is a new interactive Java code developed for SCALE 6. VIBE will scan a file system and locate all available TSUNAMI

sensitivity data files, which can include sensitivity data for the user's application as well as files from the ICSBEP Handbook. Because a sensitivity data file can contain millions of data points, VIBE will help the user consolidate these data by collapsing the data along one dimension (energy) and then allowing the user to sort and filter the data along other dimensions (nuclide, reaction, sensitivity values, etc.). Once the data are parsed with VIBE, the user can select the benchmark most similar to the application, based on sensitivity criteria. Lists of matching files can be stored in groups and passed to the SCALE 6 ExSITE input generator where further options for TSUNAMI-IP and TSURFER are set and the TSUNAMI-IP and TSURFER analysis is conducted. VIBE is also capable of querying the DICE database distributed with the ICSBEP Handbook to display the characteristic parameters of each benchmark (enrichment, EALF, H/X, etc.), along with the experimental and computed  $k_{eff}$  values and uncertainties in a tabular format. These data can be exported for further analysis, such as traditional trending analysis with USLSTATS for comparison with the TSUNAMI results.

**USLSTATS** (Upper Subcritical Limit STATisticS) is a new interactive Java version of the criticality safety validation tool for bias, bias uncertainty, and upper subcritical limit trending analysis that was formerly written in Fortran. The SCALE 6 version of USLSTATS provides improved results over previous Fortran versions and provides a convenient interactive interface for input preparation, analysis, and visualization of results.



Contour plot of neutron flux from MeshView



Convergence plot for the neutron dose rate from ChartPlot

## TRITON Enhancements in SCALE 6

### *Automated Library Generation to Support Non-LWR Systems*

The 44-group ENDF/B-V library in SCALE was collapsed from the 238-group ENDF/B-V library based on a typical LWR spectrum. Neither the 238-group ENDF/B-VI library nor the ENDF/B-VII library has been collapsed to a broad-group format, because of concern over the possible misuse of such libraries for non-LWR applications. An automated library generation capability has been added to TRITON to simplify the process of creating a reactor-specific broad group library.

An algorithm was developed and implemented that allows TRITON calculations to automatically collapse a 238-group library to 49 energy groups for depletion calculations, using the spectrum of the system being depleted. A single fine-group calculation is performed; the fluxes from this calculation are then used to collapse the initial 238-group master library to 49 energy groups. The depletion calculation is then performed using the newly created 49-group master library. This allows the user to perform depletion calculations in 49 groups using ENDF/B-VI and ENDF/B-VII data, for which no general broad-group library is available, without having to manually create the library. Other group structures and applicability of the current group structure to non-LWR reactor concepts remain to be evaluated.

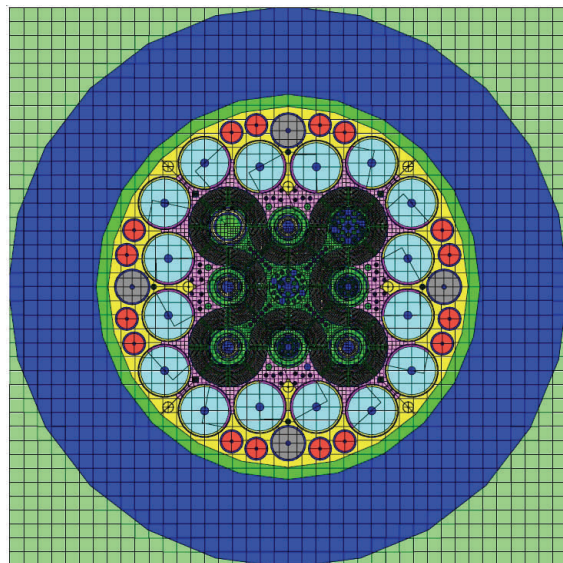
### *Fixed Source Calculations in NEWT*

The original release of NEWT provided the capability to support fixed source calculations, but only with a very primitive source specification option. This fixed source input option was removed in SCALE 5.1, primarily because of a lack of testing as other parts of the code were changed. The coding has been tested and revised as necessary in SCALE 6, and a more robust input structure has been developed for specification of fixed sources. This has required the introduction of a new *MATERIALS* block structure, although the old structure will remain in place for the foreseeable future to allow for backwards compatibility. Both input methods are

described in the updated manual. This implementation has been tested by first running an eigenvalue calculation, and then taking the fission neutron distribution from that calculation to use as a source in an identical fixed source calculation, which reproduced the results of the first calculation.

### *Tracking of Trace Element Nuclides in Depletion Calculations*

The ability to input trace elements into TRITON has been developed. Although ORIGEN-S is able to track approximately 1500 nuclides in depletion calculations, the current format of TRITON input allows specification of initial quantities for only the approximately 300 nuclides available on SCALE's multigroup ENDF cross-section libraries. It is occasionally desirable to track inventories of trace elements (e.g., impurities or nuclides present in preburned or recycled fuel) that are not available in an ENDF cross-section library. Trace element input allows isotopic masses to be input and passed directly to ORIGEN-S for tracking. Although the transport calculation does not include cross sections for these nuclides, the trace quantities and typically small cross sections make such nuclides unimportant in the transport solution.



TRITON/NEWT model of Advanced Test Reactor (ATR)

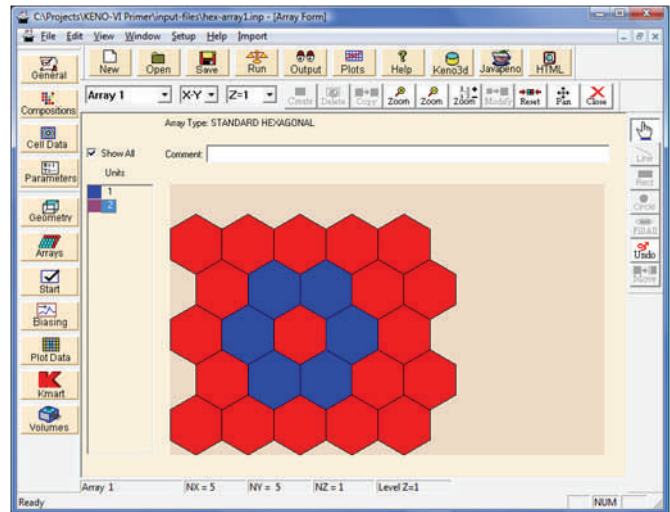


## Primers for KENO V.a, KENO-VI, and TSUNAMI in SCALE 6

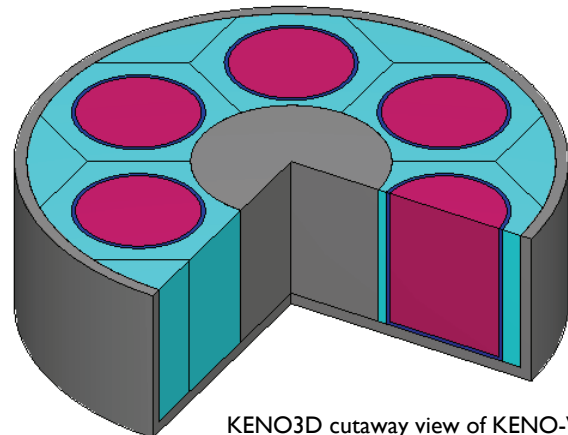
New primers for KENO-VI and TSUNAMI are included in the SCALE 6 package. The KENO V.a Primer that was released with SCALE 5.1 ([January 2006 issue](#)) is also included. The primers are designed to teach new users how to use these SCALE modules for criticality safety and sensitivity/uncertainty analyses. The primers provide step-by-step examples with many color figures illustrating the use of the interactive user interface tools in SCALE, such as GeeWiz, KENO3D, Javapeño, ExSITE, and USLSTATS.

The primers present an overview of the basic requirements for input and allow the user to quickly run a simple problem with each module. Each subsequent section provides a list of basic objectives that identifies the goal of the section and the individual software features that are covered in detail in the sample problems in that section. Each document contains over 100 color figures illustrating the GeeWiz input screens and the sample geometry models. The primer is written as a “getting started” manual for new users and complements the training provided in the SCALE workshops at Oak Ridge National Laboratory (ORNL).

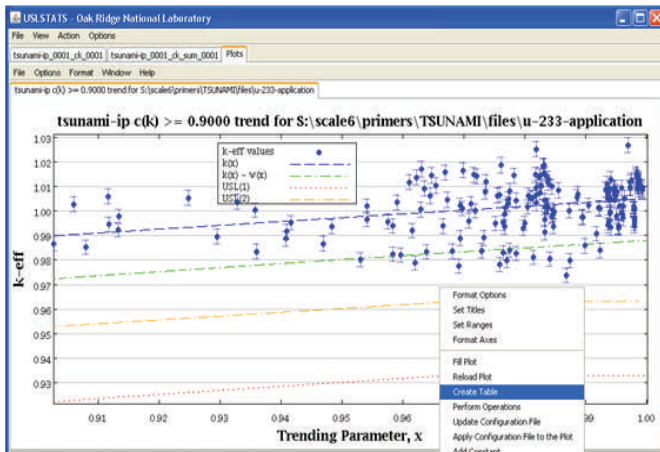
Although the primers are self-contained, they are intended as companion volumes to the SCALE manual. While the primers provide specific examples, the SCALE manual provides complete information on the use of each module.



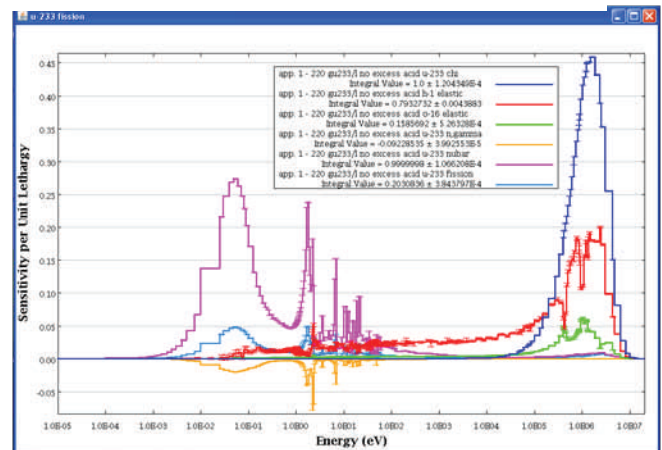
KENO-VI array input in GeeWiz



KENO3D cutaway view of KENO-VI array



USLSTATS plot (TSUNAMI Primer)



Javapeño sensitivity plot (TSUNAMI Primer)

## New TSURFER and TSAR Sensitivity/Uncertainty Tools

TSURFER (Tool for Sensitivity and Uncertainty analysis of Response Functionals using Experimental Results) is a bias prediction tool that consolidates information from many types of experiments to compute changes in cross-section data and experimental parameters, within their uncertainties, that would minimize computational biases. The bias in an application system is then predicted from the cross-section adjustments that would minimize bias.

TSAR (Tool for Sensitivity Analysis of Reactivities) is a tool that 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. TSAR can play a key role in emphasizing data gained from replacement-type criticality experiments and projecting biases in specific cross-section data to an application bias using TSURFER.

## STARBUCS Burnup Credit Cask Loading Curve Search

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. If convergence is not achieved in a search pass, the initial fuel enrichment is automatically adjusted. This sequence repeats until either  $k_{eff}$  converges to an upper subcritical limit or until the algorithm determines that a solution is not possible. The procedure is repeated for each requested burnup value. The maximum allowable iterations, upper subcritical limit, 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 applicable ORIGEN-ARP library. The control module prepares a STARBUCS input file for each search pass

requesting a single criticality calculation using the calculated spent fuel compositions. In this 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 V.a or KENO-VI, reduced number of iterations required to achieve eigenvalue convergence, reduced printed 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 in SCALE.

## Updates and Corrections to SCALE 6

Click [here](#) to see a summary of code and data modifications that have been made to the configuration-controlled version of SCALE at ORNL since the previous issue of the *SCALE Newsletter*.

*Words to the Wise . . .***KENO3D Errors for Dodecahedral Arrays**

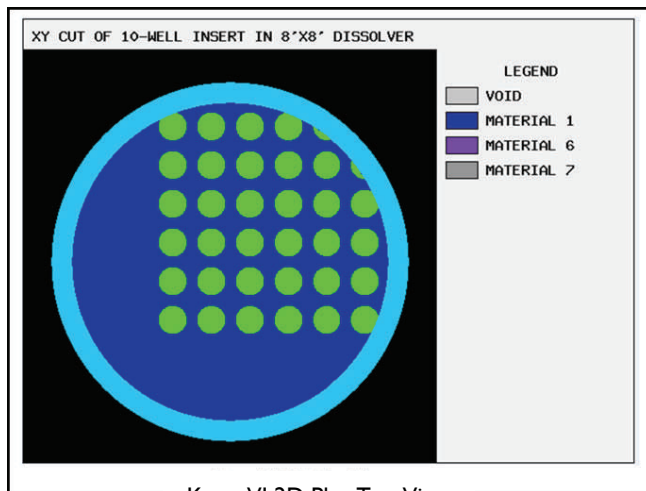
As noted on page 222 of the SCALE 5 Notebook, an error has been identified in KENO3D. This error occurs for KENO-VI models with dodecahedral arrays. As shown in the figures below, the error is the incorrect placement of the array in the surrounding geometry region. The first plot shows the actual placement of the array in KENO-VI obtained from a 2-D plot by KENO-VI, while the second plot shows the incorrect placement depicted by KENO3D. Note that the difference in the number of spheres between the two plots occurs because the plot by KENO-VI shows a 2-D slice through a specific axial location, while the KENO3D plot shows all spheres that can be seen from a top view, regardless of their axial location.

This error would impact only those users who used KENO3D as their only method to check geometry

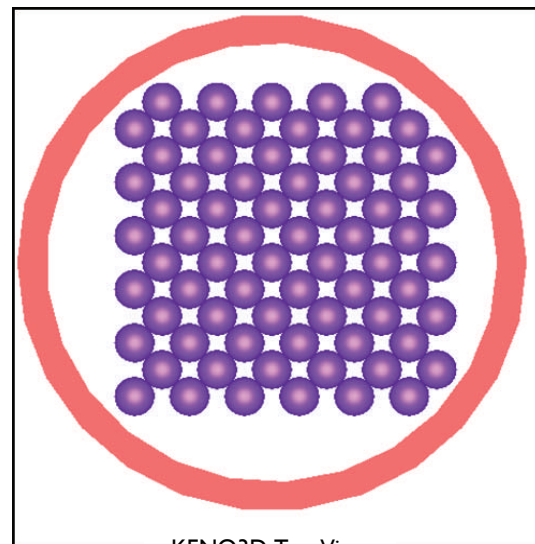
models. Note that if other checks are applied by the user (e.g., 2-D plots from KENO-VI or checks on mass balance), the error should be readily detected. Also note that the erroneous geometry would have to be a legal KENO-VI geometry for the case to run. (This reduces the likelihood of this error going undetected.)

An update to KENO3D that disables viewing dodecahedral arrays will be issued shortly after the release of SCALE 6. All users should use the 2-D plot option in KENO-VI to check geometry models with dodecahedral arrays.

ORNL is developing a new 3-D Java viewer for KENO that uses the KENO Fortran source code to perform ray tracing so that the user sees exactly what is modeled in KENO. The release date for this new tool is anticipated in late 2009.



Keno-VI 2D Plot Top View



KENO3D Top View

## SCALE 6 Lattice Physics and Depletion Course (TRITON/ORIGEN-ARP) at OECD/NEA Data Bank

The OECD/NEA Data Bank will host a training course on TRITON and ORIGEN-ARP, March 2–6, 2009. This hands-on training course will demonstrate and teach the use of advanced lattice physics and depletion tools

available in SCALE 6. For more information please refer to the [announcement](#) and [registration form](#) in the current Data Bank newsletter.



## Spring 2009 SCALE Training Courses at ORNL

Date	Title	Registration Fee*
March 9–13, 2009	SCALE Sensitivity/Uncertainty Course (TSUNAMI) (Experienced KENO users only)	\$1800
March 23–27, 2009	SCALE Lattice Physics and Depletion Course (ORIGEN-ARP/TRITON)	\$1800
March 30–April 3, 2009	SCALE Criticality Safety and Radiation Shielding Course (KENO-VI/MAVRIC)	\$1800

After February 9, 2009, the registration fee will increase to \$2100. A discount of \$300 for each additional week of training will be applied for registration in multiple courses.

Please note: Foreign nationals **must** register **at least 40 days** in advance to obtain security clearance.

For more information and online registration, please visit <http://www.ornl.gov/sci/scale/training.htm>.



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