Oak Ridge National Laboratory

SCALE Newsletter

Number 28 July 2003

Special points of interest:

- SCALE 5 release set for December 2003
- SCALE ORNL workshops in November 2003

Inside this Issue:

SCALE 5: POWERFUL NEW NUCLEAR SAFETY ANALYSIS TOOLS

Version 5 of the SCALE computer software system developed at Oak Ridge National Laboratory (ORNL), is scheduled for release in December 2003. SCALE 5 has bee rewritten in Fortran 90 and contains several significant new modules and sequences for nuclear safety analyses and marks the most important update to SCALE in more than a decade. This issue highlights the capabilities of these new modules and sequences, including: continuous energy flux spectra for processing multigroup problem-dependent cross sections; one-dimensional (1-D) and three-dimensional (3-D) sensitivity and uncertainty analyses for criticality safety evaluations; two-dimensional (2-D) flexible mesh discrete ordinates code; automated burnup-credit analysis sequence; and 1-D material distribution optimization for criticality safety.

Cross-Section Processing Enhancements

The cross-section processing capabilities in SCALE 5 have been expanded over the capabilities in SCALE 4.4a. Currently in version 4.4a, only one unit cell can be specified, and all other materials are treated as infinite homogeneous medium. Resonance data must be manually added to the MORE DATA block to account for the geometry and lattice effects of materials not specified in the unit cell. In SCALE 5, the user may specify multiple unit cells. Each unit-cell specification contains the cell type (infinite homogeneous medium, multi-region, or lattice cell), cell geometry type, and appropriate material and geometry data. Any number of unit cells may be specified, but each material may appear in only one unit cell. All materials not specified in a unit cell are processed as infinite homogeneous media.

NITAWL-III is an upgrade of NITAWL-II and has the capability to process multipole data, thus enabling it to process an ENDF/B-VI cross-section library with the Reich-Moore resonance parameters converted to multipole parameters. NITAWL uses the Nordheim Integral Treatment to process cross-section data in the resolved resonance range. As in the previous version, each resonance is processed individually, not accounting for the change in the background cross section due to other overlapping resonances.

The most significant enhancement to SCALE's cross-section processing capabilities is the new CENTRM continuous energy module. For complete information, see the CENTRM article on the next page.

KENO V.a / KENO-VI Improvements

The KENO V.a and KENO-VI Monte Carlo criticality safety codes have been extensively modified for SCALE 5. Most of these modifications are transparent to the user. Like all the modules in SCALE 5, the codes have been completely rewritten in Fortran 90. The large array that previously contained the cross-section and geometry data has been eliminated. In SCALE 5 the memory needed to store data in arrays are allocated dynamically as needed and deallocated when no longer needed. This greatly simplifies the overall program logic and removes the need for supergrouping. As a result, the supergrouping option has been eliminated.

A new algorithm is used to determine the standard deviation associated with the system k_{eff}. This algorithm accounts for the serial correlation between successive generations, thus producing a more realistic standard deviation.

The codes calculate a system mean-free path by first calculating a mean-free path for each generation. An average mean free path over all generations and its standard deviation are then calculated. Region mean-free paths can also be calculated using the region macroscopic total cross section and the region fluxes.

The criticality search capabilities in SCALE 5 have been expanded to allow each unit cell to be explicitly identified with either a unit or a material that is being modified in KENO V.a. A search case may alter the material densities, the pitch of cells in a lattice, or simple geometry boundaries. Since multiple unit cells are now allowed, a critical search may now be performed on lattices containing more than one fuel pin type. As the geometry or

(See KENO V.a /KENO-VI page 2)

KENO V.a / KENO-VI

Continued from page 1

KENO uses a new algorithm that accounts for serial correlation between successive generations to calculate the standard deviation of k_{eff}.

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.

Several new geometry and array types have been added to KENO-VI. New geometry types include: X-cylinder, Y-cylinder, Z-cylinder, rotated hexprism, pentagon, X-plane, Y-plane, and Z-plane. Three additional array types are available: dodecahedral, which is a 3-D stack of dodecahedrons; standard hexagonal, which differs from the existing hexagonal array type as shown in Figures 1 and 2; and rotated hexagonal, which is a standard hexagonal array rotated 90 degrees (Figure 3).

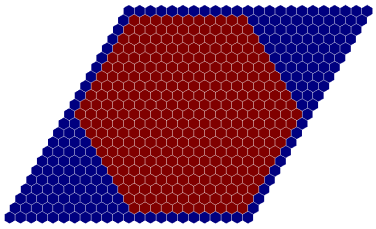


Fig. 1 Hexagonal array.

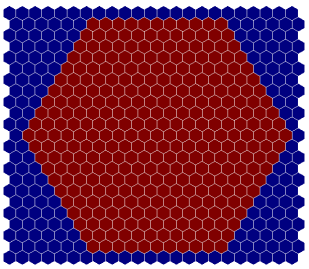


Fig. 2 New Standard hexagonal array.

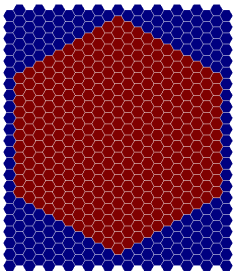


Fig. 3 New Rotated hexagonal array.

CENTRM: Continuous Energy Flux Spectra for Multigroup Cross Sections

CENTRM/PMC provide multigroup cross sections with the accuracy of continuous energy data.

The resolved resonance processor modules CENTRM (**C**ontinuous **En**ergy **Tr**ansport **M**odule) and PMC (**P**ointwise **M**ultigroup **C**onverter) provide significant new capabilities in SCALE 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, PMC collapses the pointwise continuous energy cross sections into multigroup cross sections for each nuclide in each material in the unit cell. Other modules in SCALE 5, such as KENO, can then use these multigroup cross sections.

Discrete-level inelastic cross-section data can also be processed by CENTRM/PMC. Thermal upscattering is optionally available. CENTRM/PMC avoids many of the inherent assumptions in NITAWL by calculating a problem-dependent flux profile, thus making it a far more rigorous cross-section treatment. Effects from overlapping resonances, fissile material in the fuel and surrounding moderator, and inelastic level scattering are explicitly handled in CENTRM/PMC.

A separate set of CENTRM and PMC input files are required for each unit cell. For a SCALE sequence utilizing CENTRM/PMC, the control module produces the input files for CENTRM and PMC based on the unit-cell data specified in the problem. If a lattice unit cell is specified, the code converts the cell description to an equivalent Wigner-Seitz cell for processing. When the CENTRM/PMC option is specified, the WORKER utility module is initially run to produce a working format cross-section library. Then CENTRM and PMC are executed for each unit cell specified plus an additional time to process all the nuclides contained in materials not specified in a unit cell.

CENTRM/PMC provide multigroup cross sections with the accuracy of continuous energy data.

TSUNAMI: Sensitivity and Uncertainty for Criticality Safety Analysis

ORNL has invested a significant effort in the development of sensitivity and uncertainty (S/U) analysis capabilities for criticality safety. Both 1-D and 3-D sequences plus several auxiliary codes have been developed into a new suite of sensitivity and uncertainty analysis codes called TSUNAMI (**T**ools for **S**ensitivity and **UN**certainty **A**nalysis **M**ethodology **I**mplementation).

TSUNAMI contains a number of codes that were developed primarily to assess the degree of applicability of benchmark experiments for use in criticality code validations. However, the sensitivity and uncertainty data produced by these codes can be used in a wide range of studies. 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. TSUNAMI produces sensitivity data on a groupwise basis for each region defined in the system model. The TSUNAMI-1D control module uses XSDRNPM, while TSUNAMI-3D control module uses KENO V.a to generate forward and adjoint neutron flux moments and calculate k_{eff}. First–order perturbation theory is used to compute sensitivity coefficients from both cross-section and flux data.

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. Multigroup cross-section covariance data libraries for available ENDF/B-V nuclides and reactions are included in SCALE 5.

The applicability of benchmark experiments to the criticality code validation of a given application can be assessed using S/U-based integral indices. The TSUNAMI-IP (Indices and Parameters) code utilizes sensitivity data and cross-section covariance data to produce a number of relational integral indices that can be used to assess system similarity.

SMORES: Material Optimization for Criticality Safety Analysis

A new SCALE control module named SMORES (**S**CALE **M**aterial **O**ptimization and **RE**placement **S**equence) has been developed as part of the Applicable Ranges of Bounding Curves and Data (AROBCAD) Task undertaken by the DOE Nuclear Criticality Safety Program. The purpose of SMORES is to perform automated 1-D optimization for criticality safety analysis.

The SMORES sequence consists of three major steps that are repeated as needed:

- preparation of the cross sections and mixing table used for the transport and optimization calculations,
- 1-D neutron transport calculation of the angular forward and adjoint fluxes, and
- calculation of effectiveness functions and optimization of the system with respect to a parameter, either (1) the calculated k_{eff} value of a system or (2) the minimum amount of fissile material in a system that will yield a desired k_{eff} value.

The cross-section processing is performed using either BONAMI/NITAWL-III or BONAMI/CENTRM/PMC. The processed cross sections are then used to create a problem-dependent self-shielded macroscopic cross-section library that corresponds to the most recent configuration in the optimization process.

The forward and adjoint neutron transport calculations of the system are performed using the XSDRNPM module. This module performs the 1-D criticality calculation that provides the neutron fluxes that are used to determine the effectiveness functions, as well as the k_{eff} of the current system.

Finally, SMORES calls the SWIF functional module, which has been developed at the University of California, Berkley. SWIF optimizes a specified parameter (k_{eff} or minimum fissile mass) by calculating the effectiveness functions (equal volume replacement reactive worth) using the forward and adjoint fluxes calculated by XSDRNPM and problem-dependent cross sections. Since the optimization process is iterative, the above steps are repeated until convergence is achieved or the maximum number of iterations is reached. If the maximum number of iterations is reached before convergence, a restart option can be used to change the

(See SMORES page 4)

SMORES

Continued from page 3

convergence criteria for continued optimization with a new maximum number of iterations. Along with a standard output file, several plot-oriented output files are created to allow rapid processing for visualization using Javapeno (included with SCALE) or other standard plotting packages. Hence, the system k_{eff}, material concentrations, and fissile mass as a function of iteration number can easily be plotted. Figure 4 shows a plot of fissile mass vs iteration for a minimum critical mass search.

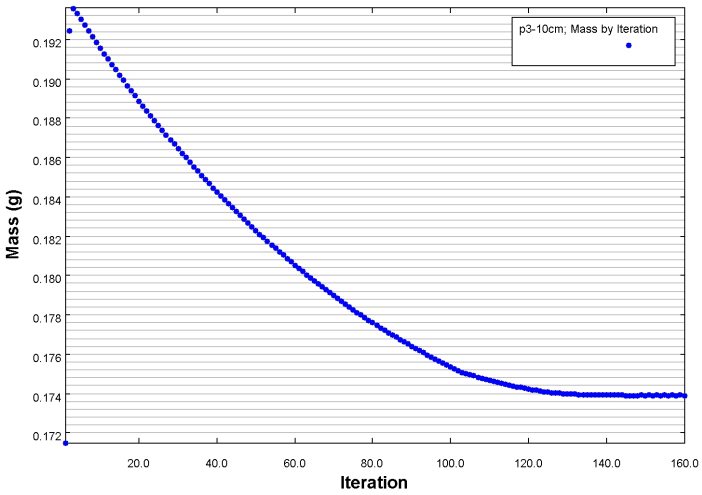


Fig. 4 SMORES minimum critical mass.

Javapeno: Interactive Plotting of Calculated Results

Javapeno (**Java** **P**lots **E**specially **N**ice **O**utput) is a Java program originally designed to plot data from the TSUNAMI sensitivity sequences. It has been expanded to plot the SMORES material optimization sequence results and the groupwise reaction-rate and flux data calculated by KENO V.a/KMART and KENO-VI/KMART6.

Javapeno 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 5 contains a Javapeno plot of the Pu-239 fission sensitivity profiles for two mixed oxide (MOX) polystyrene compact critical experiments. The plot shows that the first experiment (red line) is much more sensitive to the Pu-239 fission cross section in the thermal range, while the second experiment (blue line) is much more sensitive in the resonance and fast ranges.

Javapeno plots can be printed directly from the software package, or can be exported to a variety of graphics formats to use in reports or presentations. Because of the cross-platform capabilities of Java, Javapeno can execute on any computer for which the Java Runtime Environment is available.

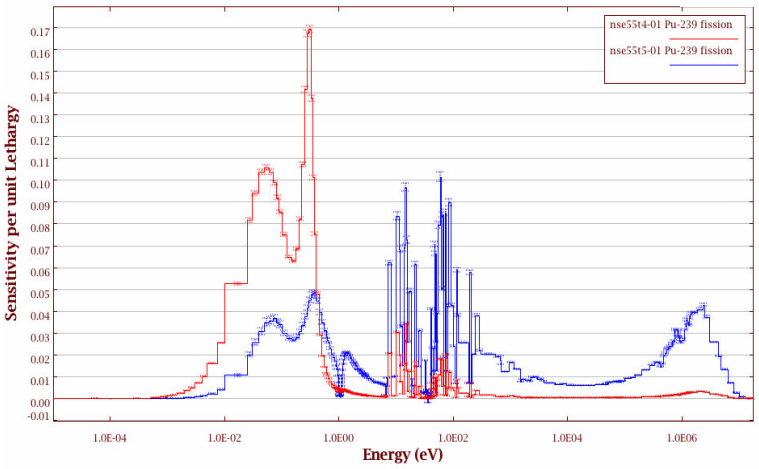


Fig. 5 Javapeno plot of Pu-239 fission sensitivity profiles from two MOX critical experiments.

STARBUCS: Burn-up Credit Analysis Sequence

STARBUCS (**St**andardized **A**nalysis of **R**eactivity for **Bu**rnup **C**redit using SCALE) is a new sequence to perform criticality calculations for spent fuel systems employing burnup credit. STARBUCS automates the criticality 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 of a spent fuel assembly using the ORIGEN-ARP methodology of SCALE. The ORIGEN-ARP methodology serves as a faster alternative to the SAS2H depletion analysis sequence in SCALE, while maintaining calculational accuracy. The spent fuel compositions are then used to generate resonance self-shielded cross sections for each burnup-dependent fuel region using the SCALE CSAS control module. Finally, a KENO V.a or KENO-VI criticality calculation is performed using the spatially-varying cross sections to determine the neutron multiplication factor for the system.

The STARBUCS control module is designed to facilitate burnup credit criticality analysis by automating and linking the depletion analysis and criticality calculations. The input format has been designed around the existing depletion and criticality safety analysis sequences of SCALE. Only a minimal amount of input beyond that typically required for a fresh-fuel criticality safety calculation is needed to perform a burnup-credit calculation. STARBUCS has been designed specifically to allow analysts and reviewers to assess the major burnup credit phenomena identified in the NRC Interim Staff Guidance 8 (ISG-8). Specifically, STARBUCS allows the user to:

- Input an arbitrary axial and/or horizontal assembly burnup gradient. The spatial burnup distribution may be controlled entirely by the user. Optionally, built-in "bounding" axial profiles may be selected by the user. A maximum of 100 axial and 10 horizontal zones may be defined.
- Any or all of the spent fuel actinide or fission product isotopes may be included in the criticality calculation. The user may select from any of the more than 1000 nuclides in the ORIGEN-S libraries, provided cross sections are available for the KENO calculation (more than 300 nuclides are available in the SCALE ENDF/B-V libraries). This allows the fission product margin to be readily evaluated. Optionally, the user may request all nuclides to be included to obtain "best-estimate" results.
- The burnup calculations can specify any desired operating history. The user may specify the assembly-average specific fission power, cycle lengths, cycle down time, and post irradiation cooling time. This allows the user to readily evaluate power history and cooling time effects.
- Isotopic correction factors may be input to adjust the calculated isotopic inventories to account for known biases and/or uncertainties associated with the depletion calculations.
- Virtually any arrangement of spent fuel may be simulated. STARBUCS is not restricted to spent fuel transport and storage cask analysis. Any KENO geometry model is permissible. For example, spent fuel arrays in a storage pool could be easily simulated.

NEWT: Flexible Mesh 2-D Discrete Ordinates Code

SCALE 5 introduces 2-D analytical capability via the NEWT (**NEW** **T**ransport algorithm) flexible mesh discrete ordinates code. Unlike traditional S_n codes, NEWT is not limited to Cartesian or cylindrical coordinate systems. NEWT's arbitrary geometry, or flexible mesh, allows users to combine orthogonal, radial, and other more unusual geometry shapes in the same model.

NEWT is unique in the domain of discrete ordinates methods because it is based on a nonorthogonal, flexible mesh scheme that allows accurate representation of complex geometric configurations that are normally impossible to model with discrete ordinates methods without significant approximations. Using a discrete ordinates approximation to the transport equation on an arbitrary grid, NEWT provides a robust and rigorous determi-

(See NEWT page 6)

NEWT

Continued from page 5

nistic solution for nonorthogonal configurations. 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 mixed oxide fuels due to the increased sensitivity of such fuels to the thermal spectrum. NEWT has already been used to demonstrate the effect of minor assumptions on the thermal spectra of MOX fuels.

NEWT offers several calculational options. It may be used to calculate the eigenvalue of a system, to perform a fixed source calculation, or to calculate the critical (X-Y) buckling of a lattice. It allows the specification of axial buckling or calculates axial buckling based on a specified height, to account for axial leakage effects. NEWT can collapse cross sections to an appropriately weighted group structure subset, in the form of an AMPX working-format library.

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. Figures 6 and 7 show two computational grids generated by NEWT for a hypothetical fuel assembly. The geometry input specifications are identical, but a more refined grid is specified for the second model. Note that these models contain no curved surfaces, but instead consist of arbitrary polygons computed by NEWT in which volumes are conserved.

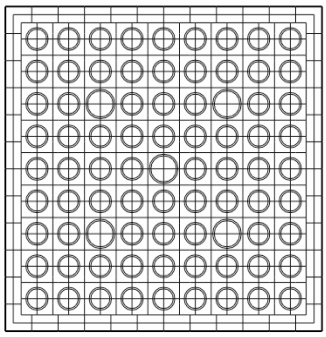


Fig. 6 NEWT coarse grid for fuel assembly.

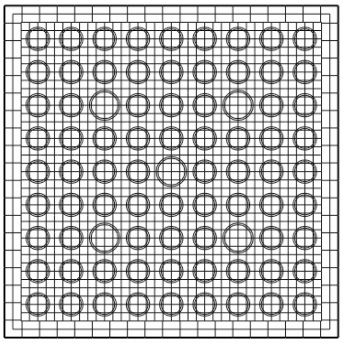


Fig. 7 NEWT refined grid for fuel assembly.

TRITON: 2-D Lattice Depletion and More

The TRITON control module (originally developed as a prototype named SAS2D) brings to NEWT the automated and simplified approach for setting up and performing complex sets of calculations, a hallmark of the SCALE system.

TRITON provides multiple sequence options, depending on the nature of the problem to be analyzed, e.g., a single NEWT transport calculation (with problem-specific multigroup cross-section generation) or ORIGEN-S depletion calculations that iterate between NEWT-based transport calculations. However, in a departure from the traditional province of SCALE applications, TRITON will provide the capability to generate few-group cross-section data for use in subsequent nodal diffusion calculations. TRITON supports branch calculations that allow calculation of cross sections and their first derivatives with respect to fuel and moderator temperature, moderator density, soluble boron concentration, and control rod insertion, as a function of burnup. These cross sections are stored in a database format that can be retrieved and processed as appropriate for use by core analysis codes.

The rigor of the NEWT solution in estimating angular flux distributions combined with the world-recognized accuracy of ORIGEN-S depletion gives TRITON the capability to perform rigorous burnup-dependent physics calculations with few implicit approximations. Such rigor may be necessary to capture the unique attributes of MOX fuel behavior as well as that of advanced, highly heterogeneous LWR fuel assembly designs being deployed in current-generation reactors.

SCALE KENO V.a Criticality Safety Course Agenda (November 3-7, 2003) ORNL

Monday
Overview of SCALE System
Introduction to CSAS
Standard Composition Library
Material Information Processor
Resonance Self-Shielding
Unit Cell Geometry - Lattice Cell/Multiregion
Gee Wiz Demo
Problem Session 1

Tuesday
KENO V.a Parameters
KENO V.a Geometry
KENO V.a Plot Data
Problem Session 2

Wednesday
Introduction to KENO V.a Output
KENO3D Tutorial
Holes
Arrays
Problem Session 3

Thursday
KENO V.a Output - How to Read It
Start Data
Bias Data
Boundary Data
Mixing Table Data
Search Data
Problem Session 4

Friday
Monte Carlo Uncertainties
Introduction to TSUNAMI-3D
Code and Data Validation Issues
Conclusion / Questions and Answers

The course will conclude with lunch on Friday.

SCALE Source Terms & Shielding Course Agenda (November 10-14, 2003) ORNL

Monday
Overview of SCALE System
Introduction to SCALE Shielding Sequences
ORIGEN-ARP
Plotting ORIGEN Results with OPUS/PlotOPUS
OrigenArp / PlotOPUS Demonstration
ORIGEN-ARP Problem Definitions
ORIGEN-ARP Problem Session
How to Create ORIGEN-ARP Libraries

Tuesday
Material Information Processor
SAS2 Depletion/Decay/Source Terms Analysis Sequence
SAS2 Problem Definitions
SAS2 Problem Session

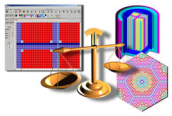
Wednesday
Introduction to NEWT/TRITON
SAS1 1-D Shielding Sequence
SAS1X 1-D Combined Criticality/Shielding Sequence
SAS1 Problem Session

Thursday
SAS4 3-D Monte Carlo Shielding Analysis Sequence
SAS4 Variance Reduction Techniques
SAS4 MARS Geometry Option
SAS4 Validation/Limitations
ESPN Demo
SAS4 Problem Definitions
SAS4 Problem Session

Friday
QADS 3-D Point Kernel Shielding Analysis Sequence
QADS Problem Definitions
QADS Problem Session
Shielding Course Wrap-up

The course will conclude with lunch on Friday.

For more information and online registration, please visit www.ornl.gov/scale/trcourse.html



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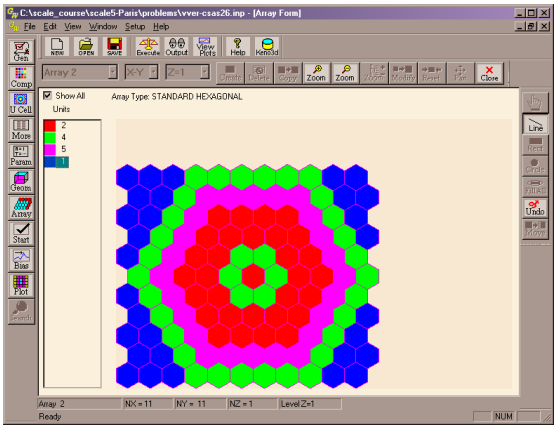
We've moved!
Note our new address above.

GeeWiz: A Complete Graphical User Interface for KENO V.a and KENO-VI

One of the latest SCALE development efforts is the SCALE Graphically Enhanced Editing Wizard (GeeWiz). The GeeWiz Graphical User Interface (GUI) is compatible with KENO V.a and KENO-VI in SCALE 4.4a or 5 and runs on Windows personal computers (PCs). It replaces the CSPAN and CSPAN-VI Windows GUIs for KENO V.a and KENO-VI, respectively. GeeWiz provides input menus and context-sensitive help to guide users through the setup of their input. It includes a direct link to KENO3D to allow the user 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 several important new SCALE 5 features:

- multiple unit cells for cross-section processing,
- new criticality sequences using the CENTRM continuous-energy module, and
- new geometry and array options in KENO-VI.



Example of the versatile array input form in GeeWiz.

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