Oak Ridge National Laboratory

SCALE Newsletter

Number 33 January 2006

Special points of interest:

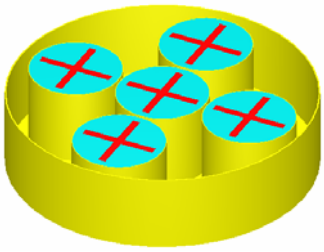
- SCALE 5.1 scheduled for summer 2006
- SCALE workshops in March/April at ORNL

Inside this issue:

New KENO V.a Primer Using GeeWiz and KENO3D

A new version of the KENO V.a Primer has been published on CD-ROM and distributed to all registered SCALE 5 users by the Radiation Shielding Information Computational Center (RSICC). The primer is designed to teach new users how to use KENO V.a with the GeeWiz user interface in SCALE 5. It also includes a section on the use of the KENO3D visualization tool to plot models and overlay them with calculated results.

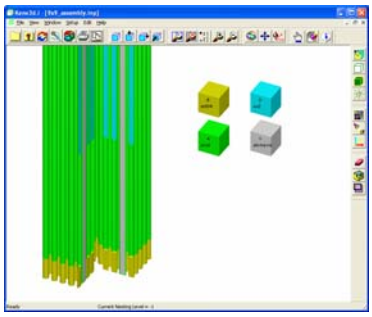
The primer gives an overview of the basic requirements for KENO V.a input and allows the user to quickly run a simple criticality problem with KENO V.a. Each subsequent section provides a list of basic objectives that identifies the goal of the section and the individual



SCALE/KENO V.a features that are covered in detail in the sample problems in that section. The document contains over 100 color figures illustrating the GeeWiz input screens, the KENO V.a geometry, and the sample KENO V.a models. The primer is written as a "getting started" manual for new KENO V.a users and complements the training provided in the SCALE workshops at Oak Ridge National Laboratory (ORNL).

Although the primer is self-contained, it is intended as a companion volume to the KENO V.a documentation in the SCALE manual. The primer provides specific examples using SCALE/KENO V.a for criticality safety analyses, while the SCALE manual provides complete information on the use of SCALE/KENO V.a and all its modules.

A primer for KENO-VI is planned for publication in 2007.



SCALE 5.1 Release Scheduled for Summer

The release of SCALE 5.1 has been moved to this summer due to a number of unexpected issues. Once these are resolved, the package will be ready for testing and packaging by RSICC.

Some of the significant new features in SCALE 5.1 include

- Improved 2-D geometry in TRITON/NEWT based on KENO-VI SCALE Generalized Geometry Package (SGGP)
- ENDF/B-VI cross-section libraries (both multigroup and continuous energy)
- Problem-specific broad-group cross-section library collapse in TRITON
- 3-D Monte Carlo–based depletion with KENO V.a or KENO-VI coupled to ORIGEN-S in TRITON
- Doubly heterogeneous unit cell capability for resonance treatment
- Improved resonance and thermal treatments in CENTRM
- New ORIGEN-ARP libraries generated with 2-D TRITON/NEWT models
- HTML output in KENO V.a
- Enhanced sensitivity/uncertainty tools in TSUNAMI

For more-detailed information on these topics, refer to the January 2005 issue.

Speed Improvements to SAMS for Large Problems

For problems with a very large number of nuclides, SAMS runs about 100 times faster.

An updated version of the SAMS sensitivity module (to be released in SCALE 5.1), which is used by the TSUNAMI sequences in SCALE, provides substantially improved performance for problems with many nuclides. The results of the calculations are identical in the previous and new versions. The table below shows a few examples of runtime improvements in SAMS. This same level of speedup will not be seen on problems with only a few nuclides. Those problems typically ran in a few seconds in SCALE 5.

This new version will provide additional screen messages regarding the progression of the calculation of the implicit sensitivities. The user will have the option to turn off these messages. If multiple executions of TSUNAMI-1D and/or TSUNAMI-3D are requested from the same input file, the second and subsequent .sdf files will have sequential numbers appended to their file names (e.g., testcase.0002.sdf). Previously, requesting more than one execution from the same input file would result in all .sdf files being overwritten by the last case in the file.

Number of Nuclides	SAMS runtime (SCALE 5)	SAMS runtime (SCALE 5.1)
288	160 minutes	1.33 minutes
21,968	>9 days	119 minutes
47,269	>21 days	<12 hours

Words to the Wise . . .
Error in Dancoff Factor for SCALE 5 Slab Cell Cases

Users were notified of this error by email on October 13, 2005.

An error has been identified in SCALE 5 for input files that use the ASYMSLABCELL or SYMMSLABCELL option and the new SCALE 5 input format (keywords "READ COMP"). If SCALE 5 is executed using input files developed with the SCALE 4 format, the input file will not properly convert to a SCALE 5 input format and a fatal error will result before any calculations are performed.

The impact of the erroneous Dancoff factor calculation on the system k_{eff} value is problem dependent. Analyses performed at ORNL indicate that the error in k_{eff} can be potentially significant if the ASYMSLABCELL option is used. The impact of the error on k_{eff} is relatively minor for cases where the SYMMSLABCELL option is used. The error in the calculated k_{eff} value depends upon the slab thicknesses and the fuel enrichment. If a user's application applies the ASYMSLABCELL option and sufficient critical benchmarks with the ASYMSLABCELL are included in the SCALE 5 validation set, then the impact of the error may already be accounted for in the bias and uncertainty applied in the safety case.

The ASYMSLABCELL option is seldom used. To determine whether they have been impacted by this error, users should check for input files that use the keywords ASYMSLABCELL or SYMMSLABCELL and use the SCALE 5 input format (search for the keywords "READ COMP"). If such cases are found, replace the ASYMSLABCELL or SYMMSLABCELL input with an equivalent MULTIREGION geometry specification and use SLAB geometry. Tests at ORNL have confirmed that the MULTIREGION specification with the SLAB option will produce the correct prediction of k_{eff} .

More Words to the Wise …
Potential Problem with CENTRM Cases

The PMC discrepancy may result in non-conservative calculated k_{eff} values for cases where well-moderated fuel is surrounded by a material with high iron, cadmium, hafnium, or nickel content that is inside a strong thermal absorber such as boron or gadolinium.

ORNL has identified a potential problem for a limited class of criticality safety cases when the CENTRM/PMC codes are used to perform resonance self-shielding of the cross sections. Note that the CSAS sequences use NITAWL by default. This problem is related only to the optional use of CENTRM/PMC. The problem is caused by PMC normalizing the 2-D thermal scattering matrix data to 1-D thermal scattering data that do not correspond to the 2-D data. The normalization process has been modified to correct the problem. It is recommended that all SCALE 5 users download the updated version of PMC from the SCALE website.

A discrepancy was identified for a model of an infinite array of LWR fuel assemblies in a poisoned storage geometry. Each assembly was located in a water-flooded square steel basket structure with a wall thickness of 0.75 cm. A half-thickness Boral plate was placed on the outside of the basket such that the Boral plate between each assembly had an areal loading of 0.0225 g ^{10}B / cm^2. This model generated a calculated k_{eff} value of 1.019 +/- 0.0004 using CENTRM and 1.034 +/- 0.0004 using NITAWL. In this particular case, the problem occurred where thermal neutrons traveled through iron (Fe) to be absorbed by ^{10}B. A spike occurred in the calculated flux at approximately 3 eV due to the error in the normalized Fe scattering data. This flux spike resulted in excessive neutron absorption by the ^{10}B and an under predicted k_{eff} value. The normalization error in PMC became significant because the mixture with erroneous thermal scattering data lay between the thermalized neutron source (i.e., water-moderated fuel) and a strong thermal absorber – in this case ^{10}B. When ^{10}B was removed, the problem disappeared.

The occurrence of this discrepancy depended on the geometry configuration and the materials involved. More than 200 critical experiment benchmark models with similar geometry and/or materials were checked, but none of them showed a discrepancy. Next a large series of calculations were performed with a simplified version of the original geometry to determine what other nuclides could cause a similar behavior. The Fe was replaced by each available nuclide in the SCALE ENDF/B-V cross-section libraries. Although about 50 nuclides exceeded a cutoff value of greater than 1% error in the calculated k_{eff} value, most resulted in conservative values such that the erroneous k_{eff} values were higher than the correct values. Those nuclides that resulted in nonconservative values were Fe, ^{106}Cd, ^{180}Hf, ^{139}La, Ni, ^{102}Pd, ^{96}Ru, ^{98}Ru, ^{144}Sm, ^{120}Te, and ^{135}Xe. Iron is the only nuclide that is considered likely to be used between the moderator and absorber materials. Other less likely nuclides are nickel, hafnium, and cadmium. Additional analysis indicates that replacing the boron in the outermost region with another strong thermal absorber such as gadolinium has similar effects.

The PMC discrepancy may result in nonconservative calculated k_{eff} values for cases where well-moderated fuel is surrounded by a material with high iron, cadmium, hafnium, or nickel content that is inside a strong thermal absorber such as boron or gadolinium. Users who have performed criticality safety analyses using CENTRM/PMC (i.e., "PARM=CENTRM" in the input file) to perform the cross-section resonance self-shielding should examine their models for cases that meet these criteria. Previous calculated results should be compared with results from cases using NITAWL or the updated version of PMC with CENTRM. We do not expect that this discrepancy will seriously impact our users due to the restricted conditions in which it might occur.

Using SCALE 4 Input Files with Dancoff Factors in CENTRM Calculations

CENTRM cases must use multiple unit cells rather than Dancoff factors input in MORE DATA.

Recently our staff was rerunning SCALE 4 LWR criticality safety benchmark files with SCALE 5 and CENTRM. Several cases showed significant differences in the calculated k_{eff} values. These cases all have multiple unit cells. The inputs were prepared in the 1990s with SCALE 4, so Dancoff factors had to be input using MORE DATA for multiple cells. (The ability to explicitly calculate Dancoff factors for multiple cells was introduced in SCALE 5.) NITAWL is able to use the MORE DATA specifications, but CENTRM is not. Beginning with SCALE 5.1, CENTRM will become the default resolved-resonance processor in SCALE, although NITAWL remains available as an option. SCALE 4 format input files must be modified to use multiple unit cells rather than MORE DATA, so that CENTRM can properly calculate all lattice effects.

More Words to the Wise ...
Violation of KENO-VI Geometry Restrictions Can Produce Incorrect Results

Holes and arrays allow very complex problems to be constructed without having to explicitly specify every region in every location. A unit may be specified once and then used in multiple locations by placing that unit in holes and arrays. These holes and arrays may then be placed within other holes and arrays, a process referred to as "nesting." There are certain restrictions that must be observed when using holes and arrays.

1. Holes may share surfaces with but must not intersect other holes or the boundary of the unit that contains the hole.
2. A hole in a unit contained in an array must not intersect the array boundary.
3. A higher-level array boundary must not cross a nested array boundary.

Examples of the violations of these restrictions are shown in Figures 1-3, respectively. Note that each of these examples could be modeled in KENO-VI with alternative methods that do not violate the restrictions.

These restrictions stem from the algorithm used to perform the particle tracking through the geometry. The particle is tracked only to the level of the unit and array (if applicable) in which it is currently contained. If the particle is in a unit that contains a hole, it will continue its motion in the unit until it is either absorbed or crosses out of the unit. If the unit in the hole intersects the boundary of the unit that contains the hole, it is possible for the particle to leave the hole and not be in the unit that contains the hole, thus causing the particle to terminate (i.e., be lost from the problem). Similarly, a particle in a nested array that intersects the boundary of the array in which it is nested may leave the nested array and not be in the higher-level array, thus causing the particle to terminate. In both situations it is possible to calculate results that are nonconservative. The magnitude of the error in k_{eff} in such a case is dependent upon the problem geometry, materials, and model setup.

KENO-VI users need to be aware of restrictions in the use of holes and arrays in the SCALE Generalized Geometry Package (SGGP) in KENO-VI. In some very limited cases, KENO-VI may not be able to detect violations of these restrictions in a geometry model. It is possible to create a problem with holes and/or nested arrays that will run to completion with no error messages but produce incorrect results. In addition, it is likely that the 2-D plots generated by KENO-VI or the 3-D images from KENO3D may not show any problem with the geometry setup even though the restrictions have been violated.

Section F17.4.4, Page F17.4.40, of the SCALE 5 manual, under the subheading "HOLE," includes a brief incomplete summary of these geometry restrictions. These restrictions will be documented completely in the SCALE 5.1 manual. Plans are being developed to add the capability to KENO-VI in SCALE 5.1 to either remove or identify the violation of these restrictions in geometry models and terminate execution. Until such capability is implemented, users must take care to ensure that the KENO-VI geometry restrictions are not violated when using holes and nested array.

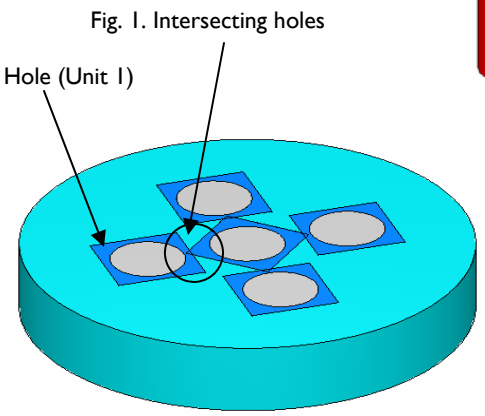


Fig. 1. Intersecting holes

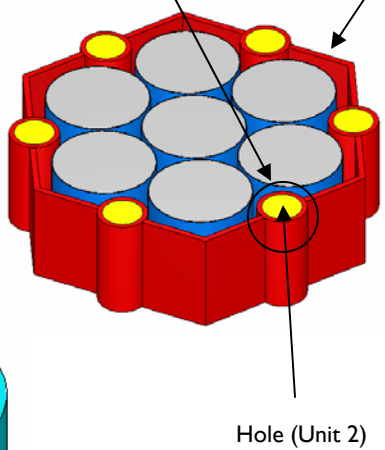


Fig. 2. Holes intersecting array boundary

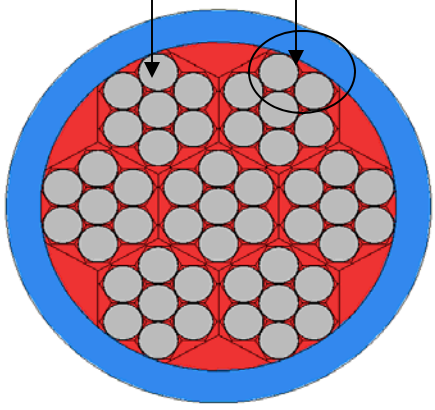


Fig. 3. Large array boundary intersecting nested arrays

Minor Corrections and Updates to SCALE 5

The following list provides an abbreviated summary of code and data modifications that have been made to the configuration-controlled version of SCALE at ORNL since the release of SCALE 5. These modifications will be available later this year in the SCALE 5.1 release.

AIM: An error that prevented successful conversion of an ASCII library to binary was corrected. The Sigma-p value was not being transferred to the binary library. (MRR 05-009)

ALPO: The transport correction of the transfer array was corrected. (MRR 05-053)

ARP: Flux activation option (cross-section interpolation on fluence) was added to allow activation calculations in ORIGEN-ARP. The interpolation method for all cases was upgraded to use the Lagrange method and apply Lagrange interpolation to all parameters. Previously a power coefficient fit was used for interpolation of burnup, and linear interpolation was used for other parameters. (MRR 05-017)

AWL: The conversion of the temperature of the 2-D thermal transfer array was corrected. (MRR 05-054)

HEAT TRANSFER MODULES: All heat transfer modules have been removed from SCALE. (MRR 05-008)

ICE: The upscatter cross section was added to the group-independent library. (MRR 05-061)

KENO V.a: KENO V.a has been updated to add HTML-formatted output. (MRR 05-075)

KENO VI: Changes were made to correct a problem with arrays containing hexprisms and rotated hexprisms that could enter an infinite loop if a particle crosses from one array position to another at an X-Y corner in a hexprism. (MRR 05-095)

MALOCS: The collapsing of chi (χ) matrices from flux weighting to $\nu\Sigma_f$* flux weighting was corrected. (MRR 05-001)

MORSE/MARSLIB: The code was updated to correct a fatal error that occurred while tracking a source particle in an array. (MRR 05-048)

MORSE: Several minor corrections were made. (1) SAS4 axial problems where INTZR >50 now run correctly. (2) Problems with fissions allowed now store input data correctly. Previously, if the number of regions exceeded the number of media, an array dimension was exceeded. (3) Some problems were previously normalized with an incorrect weight. (This was machine dependent.) (MRR 05-041)

NITAWL: Corrections were made to infinite dilution and sensitivity library calculations. (MRR 05-067)

OPUS: Minor updates were made for compatibility with SCALE 5.1. An error was corrected in the element ranking that occurred when more than approximately 30 elements were requested. Modifications were also made to correct an error in the plot axis labels when case comparisons were performed for spectral plots. (MRR 05-050)

ORIGEN-S: A correction was made to the neutron balance and multiplication tables printed by ORIGEN-S. The neutron absorption was previously calculated incorrectly, causing the neutron multiplication factor to be incorrect. This error was isolated to the neutron balance printout. (MRR 05-030)

ORIGEN-S: (1) The Taylor series expansion method of estimating step flux was replaced with explicit matrix calculation for improved accuracy and stability. The number of Taylor expansion terms was found to be insufficient for problems involving low flux and very long irradiation time, and the previous method used only the actinide compositions to estimate change in flux over the irradiation interval. The method was modified to perform an explicit ORIGEN matrix exponential simulation to estimate interval midpoint compositions and flux. (2) The power-to-flux calculation was modified to operate with or without fissionable material for activation problems; changes also allow irradiation calculations to use multiple zero power steps. (3) An array deallocation bug in the neutron source routine for problems that have no neutron-emitting nuclides was fixed. (4) An option was added to print fission rates and relative fission rates to provide output required for the American Nuclear Society (ANS) decay heat standard. (5) Other miscellaneous print and format fixes were implemented. (MRR 05-020)

(Continued on page 6)

Minor Corrections and Updates to SCALE 5

(Continued from page 5)

PICTURE: Minor modifications were made to make it compatible with current version of SCALELIB and to fix a problem with colors that occurred on AIX systems. (MRR 05-044)

PMC: An improved calculation for the elastic removal/within-group cross-section values has been implemented. Minor errors were corrected. (MRR 05-033)

SAMS: The code has been updated to reduce the memory requirements when running TSUNAMI-3D problems. Screen data output has also been added to update the user as the calculation progresses. (MRR 05-004)

SAS4: A potential round-off error was corrected that might have selected an index outside a Fortran array. (MRR 05-042)

TRITON: (1) The capability was added to perform a broad-group collapse of the AMPX master-format cross-section library at the end of a t-newt calculation using the problem-specific flux spectrum. (2) The capability was added to perform both a forward and adjoint case in a single t-newt calculation. (MRR 06-001)

WORKER: An error was corrected because the code did not interpolate on temperature when producing a master library for PMC. This discrepancy can result in CENTRM/PMC generating incorrect cross sections for cases with temperatures higher than room temperature. The impact of this discrepancy apparently is minimal. While conceptually it is better to interpolate first, and then apply the resonance correction to the interpolated matrix, applying the same correction to all matrices and then interpolating gives nearly the same resulting k_{eff}. (MRR 05-103)

MPDKXGAM: The Master Photon data library, MPDKXGAM, containing discrete and continuous-energy gamma lines and intensity data, was revised to correct double accounting of some photons associated with decay transitions to or from a metastable nuclide. The problem occurred because some nuclear data evaluations included the gamma emission data with the parent nuclide of the transition, while other evaluations included the data with the metastable daughter product. The library was regenerated, ensuring that the sources of the evaluation for both parent and daughter nuclides were consistent. The updated library now yields photon release energies (MeV/s) calculated from the gamma spectra that agree with the decay gamma heating values (based on Q values) to well under 1%. The changes have no impact on previous calculations at most practical decay times of interest (days to years). For very short decay times (less than 1 day), the correction is on the order of 1%. For decay times less than 5 minutes, the correction is about 5%, with the original SCALE 5 library giving a slightly larger (more conservative) photon energy yield. In addition, the library size was reduced by removing the photon emission data for nuclides that were not in the ORIGEN-S decay library. This change resulted in a revised library of 1132 nuclides with explicit photon emission data. (DRR 05-001)

STANDARD COMPOSITION LIBRARY: Data for all individual nuclides were changed from atom fractions to weight percents to improve precision. New standard compositions Al_2O_3, GD_2O_3, GRANITE, LIMESTONE, and ThF_4 were added. (DRR 05-003)

Spring 2006 SCALE Training Courses at ORNL

Date	Title	Registration Fee
March 20–24, 2006	**KENO-VI Criticality Safety Course**	$1800
March 27–31, 2006	**ORIGEN-ARP/TRITON Course**	$1800
April 3–6, 2006	**TSUNAMI Sensitivity/Uncertainty Tools (Experienced KENO users only)**	$1800

Early registration deadline is Feb. 27. Fees will increase by $300 after this date.
A discount of $300 per each additional week for registration to multiple courses.
Foreign nationals must register at least 40 days prior to the training course.

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

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