Oak Ridge National Laboratory

SCALE Newsletter

Number 34 July 2006

Special points of interest:

- SCALE 5.1 release scheduled for September 30, 2006
- SCALE workshops in Oct./Nov. at ORNL; $300 discount until September 22

Inside This Issue:

SCALE 5.1 in Final Testing

The SCALE 5.1 package is currently being tested at the Oak Ridge National Laboratory (ORNL) in preparation for its public release. The release is anticipated to occur by September 30. Some of the new capabilities of SCALE 5.1 are highlighted in this newsletter. For more information on improvements to SCALE that will be included in version 5.1, please refer to the January and July 2005 issues.

New ORIGEN-ARP Libraries in SCALE 5.1

The LWR libraries previously released with SCALE 5.0 were created using the 1-D depletion sequence SAS2. New cross-section libraries have been generated with the 2-D TRITON/NEWT depletion sequence for seven PWR, nine BWR, and five VVER assembly configurations, as listed in Table I. The range of the parameters was extended, as compared with the previous release, to include burnups up to 72 GWd/MTU and fuel enrichments up to 6 wt % ^{235}U. Unless otherwise noted in Table I, the new libraries were generated for six fuel enrichment values: 1.5, 2.0, 3.0, 4.0, 5.0, and 6.0 wt % ^{235}U. In the case of the BWR assembly designs, five values of coolant density were considered: 0.1, 0.3, 0.5, 0.7, and 0.9 g/cm^3, whereas for the PWR and VVER a core-average value was used for the moderator density. Three of the four VVER-440 configurations considered are characterized by a radial enrichment profile, and two of these contain burnable absorber rods.

Table I. New LWR libraries for ORIGEN-ARP

Reactor type	Assembly design description
PWR	Westinghouse CE 14 x 14 Westinghouse CE 16 x 16 Westinghouse 14 x 14 Siemens 14 x 14 Westinghouse 15 x 15 Westinghouse 17 x 17 Westinghouse 17 x 17 OFA (Optimized Fuel Assembly).
BWR	GE 7 x 7 GE 8 x 8 ABB 8 x 8 GE 9 x 9 GE 10 x 10 ATRIUM-9 (9 x 9) ATRIUM-10 (10 x 10) SVEA-64 (8 x 8) SVEA-100 (10 x 10)
VVER	VVER-440 flat enrichment 1.6%, 2.4%, 3.6% VVER-440 profiled enrichment, average 3.82% VVER-440 profiled enrichment, average 4.25% VVER-440 profiled enrichment, average 4.38% VVER-1000

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New ORIGEN-ARP Libraries in SCALE 5.1

(continued from page 1)

New ORIGEN-ARP libraries include seven PWR, nine BWR, and five VVER libraries based on 2-D models.

An important aspect of the work was collecting, from various sources, assembly data for each of the designs considered. Because there are small variations in the parameters characterizing the assemblies of a specific design, these gathered data were analyzed in order to build a representative analysis model, typical for a large number of applications involving assemblies of that type. Most of the assembly information was taken from multiple sources, such as the *2004 World Nuclear Industry Handbook* and various technical reports issued by the U.S. Nuclear Regulatory Commission (NRC) or ORNL. Typical values were used if data were not available. All PWR assemblies were modeled with no absorber rods/devices inserted into the guide or instrument tubes. The level of detail in the models is illustrated in Fig. 1 for two assembly designs, BWR (GE-9 x 9-7), left, and VVER (VVER-1000), right.

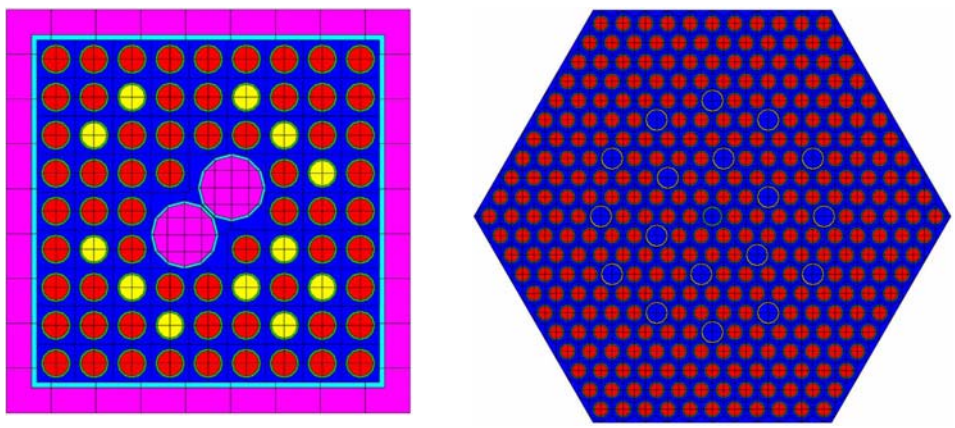

Figure 1

New Covariance Libraries for TSUNAMI in SCALE 5.1

New covariance libraries contain data for nearly all nuclides in ENDF/B-V and –VI.

For SCALE 5.1, a total of four cross-section covariance libraries are being released; 44GROUP-V5COV, 44GROUPV6COV, 44GROUPV5REC, and 44GROUPV6REC. The first two libraries represent a *basic* set with only the covariance data included in the ENDF/B formal release, about 50 nuclides corresponding to ENDF/B-V and ENDF/B-VI, respectively. The last two represent a *recommended* set with covariance information for nearly every nuclide in the cross-section library. The recommended sets contain the ENDF/B-V and ENDF/B-VI data plus a large number of nuclides for which covariance information is included based on integral uncertainty data. Each of these libraries contains cross-section covariance information in the SCALE 44 neutron-energy-group structure. While conceptually it is possible to process the cross-section covariance information into the SCALE 238 group structure, very little additional information would be available. The capability to use a cross-section covariance group structure that is the same as or a subset of the cross-section library group structure was built into the SCALE sensitivity/uncertainty codes so that these covariance libraries could be used with 238-group calculations.

Each of the four covariance libraries described above processed all of the information that was contained in the cross-section uncertainty files. Because many of the specific reactions that contain uncertainty data are not actually used by the TSUNAMI processing codes, the files were thinned to contain only the reactions utilized by TSUNAMI. These reactions include: total, elastic, inelastic, (n,2n), fission, chi, (n,gamma), (n,p), (n,d), (n,t), (n,He-3), (n,alpha), and nu-bar.

KENO-VI Array and Hole Enhancements in SCALE 5.1

Recent enhancements to KENO-VI address limitations discussed in the January 2006 issue of the *SCALE Newsletter*.

As discussed in the January 2006 issue, KENO-VI has certain restrictions that must be observed when using holes and arrays. These restrictions stem from the algorithm used to perform particle tracking through the geometry.

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.

In SCALE 5.1 , KENO-VI has been enhanced to address these limitations. If the first or second restriction is violated, KENO-VI terminates and writes an error message stating why the problem terminated and the unit, location, and direction of the particle crossing the boundary where the intersection occurs. The third restriction has been removed in SCALE 5.1.

The removal of the restriction on nested array boundaries allows the user to set up complex problems much more simply and avoids the possibility of erroneous k_{eff} calculation. For example Figure 2 illustrates where a nested array boundary that overlaps a higher-level array boundary. Because the previous version of the geometry package tracked particles only in the current array level, the particle was required to exit a lower-level array before exiting a higher-level array. In the new version, the particle is tracked in the current array level and all higher-level arrays. This allows the particle to determine the shortest distance to any array crossing and to possibly cross out of multiple arrays simultaneously.

Another example of a problem that can be modeled easily using the new geometry capabilities is a reactor composed of multiple fuel assemblies, each composed of multiple fuel pins, and control blades that move between the assemblies. Each fuel assembly may be set up as an array of fuel pins. The reactor core is then modeled as an array of fuel assemblies with a boundary that consists of the reactor vessel and the control blades. Figure 3 shows an example of this type of configuration. A particle in a fuel assembly crossing into a control blade crosses out of the fuel assembly array and the array of fuel bundles before crossing into a control blade.

These updates highlight our continuing software maintenance efforts to address limitations and potential problems and to make SCALE more accurate and easier to use.

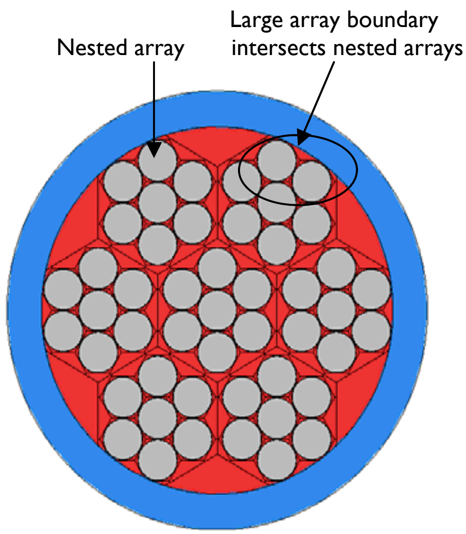

Figure 2

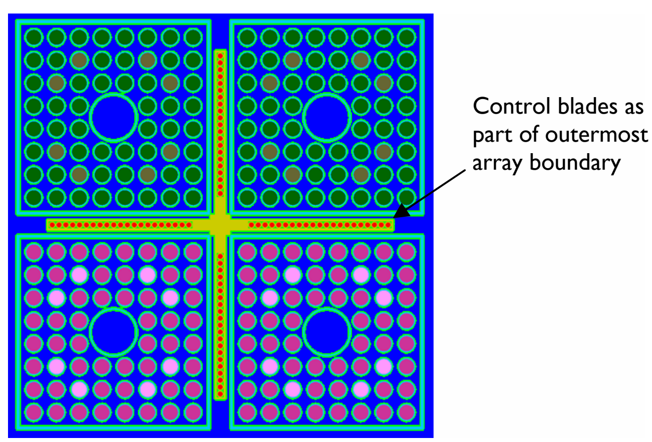

Figure 3

GeeWiz/KENO3D Calculate KENO-VI Volumes

KENO-VI volumes can be calculated quickly and analytically by KENO3D in SCALE 5.1.

The SCALE KENO-VI program does not calculate volumes for model bodies by default. The reason is that the calculation of volumes in KENO-VI is more difficult than in KENO V.a due to the generalized geometry in KENO-VI that allows body intersections. Although volumes are not needed for the calculation of k_{eff}, they are necessary for the calculation of other parameters such as fluxes and fission densities. They are also required for TRITON6/KENO-VI fuel depletion calculations to correctly normalize the power densities.

The GeeWiz user interface and KENO3D visualization tool have been enhanced to calculate KENO-VI volumes analytically and write those volumes directly to a KENO-VI input file. This new feature is a significant capability that will prove useful for applications that use a KENO-VI (i.e., SCALE Generalized Geometry Package) model and require accurate volumes for model bodies.

KENO3D is a visualization tool that allows users to interactively view the components of their geometry model as it is constructed. Internally, KENO3D uses constructive solid geometry to build the faceted or wireframe model bodies for display. KENO3D has the capability to calculate volumes of individual bodies. Previously, the volume calculation was used internally by KENO3D when performing Boolean operations (e.g., subtracting bodies and intersecting bodies). With the need for accurate volume calculations for KENO-VI geometry models, the volume calculation was extended to calculate the volumes for each medium in the model and to write the volumes to a file that is formatted for reading by KENO-VI or GeeWiz.

The calculation of volumes in KENO3D has been optimized for models where all units and arrays are bounded by rectangular solids. If a unit or array is bounded by a rectangular solid, then each body can be tested to see if its bounding box intersects that of the rectangular solid. For rectangular geometries, if the bounding boxes do not intersect, then the model bodies do not intersect. If the model bodies do not intersect, then the volume of each object as constructed in its unit of origin is simply added to the accumulated volume for that medium.

The intersection of boxes is significantly faster than the intersection of bodies. For a shipping cask model containing approximately 200,000 bodies, the execution time required to accurately calculate volumes was reduced from 30 minutes to less than 1 second by using the bounding box optimization. With rectangular geometries, when a unit or array bounding box does intersect an object's bounding box, the more-costly calculation using intersections is required for that object. In most practical applications, only a subset of object boundaries intersects unit or array bounds; therefore, execution time would still be reduced by box optimization.

Volumes can be calculated directly with KENO3D; however, as an aid to GeeWiz users, a volume calculation capability was added to the GeeWiz Volume dialog. If the user selects the "Keno3D Volumes" button, KENO3D is called to calculate volumes and create an ASCII volume file formatted for input into SCALE. Subsequently, if the user selects the "Attach Volumes" button, the volume data will be added directly to the media records in every region in the SCALE input file.

Corrections and Updates to SCALE 5

The attached file provides a summary of code and data modifications that have been made to the configuration-controlled version of SCALE at ORNL since January 2006. These modifications will be available later this year in the SCALE 5.1 release.

Fall 2006 SCALE Training Courses at ORNL

Date	Title	Registration Fee*
October 23–27, 2006	**ORIGEN-ARP/TRITON**	$1800
October 30–November 2, 2006	**TSUNAMI Sensitivity/Uncertainty Tools (Experienced KENO users only)**	$1800
November 6–10, 2006	**KENO V.a**	$1800

*A late fee of $300 will be applied after September 22, 2006.
A discount of $300 for each additional week will be applied for registration in multiple courses.
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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