SCALE Newsletter

Computational Physics and Engineering Division
Nuclear Engineering Applications Section
Oak Ridge National Laboratory
SCALE Web Site: http://www.cad.ornl.gov/scale
SCALE Electronic Notebook: http://www-rsicc.ornl.gov/ENOTE/enotscal.html

Number 20 **July 1999**

KENO V.a Training Course November 1 – 5

The SCALE staff at ORNL will be offering a KENO V.a Criticality Safety Training Course November 1–5, 1999, at Oak Ridge National Laboratory (ORNL). Training will include use of the new CSPAN input graphical user interface (GUI) and the KENO3D geometry visualization program. The course will emphasize hands-on experience solving practical problems on PCs. Workgroups of two persons each will be used. No prior experience in the use of SCALE is required to attend. The registration fee is $1,800 (**$300 discount if you register by October 1**). A copy of the SCALE software and manual on CD may be obtained for an additional fee of $300. Registrations will be accepted on a first-come basis. **Registration forms submitted directly from the Web are preferred (http://www.cad.ornl.gov/cad_nea/text/scale_course_reg.html)**. Registration via FAX or e-mail is also acceptable. The registration fee must be paid by check or travelers checks. We apologize that we are NOT able to accept credit card payments. The course agenda is presented below. A registration form is also included in this issue.

Monday
- Overview of SCALE
- Introduction to CSAS
- Resonance Self-Shielding
- Standard Composition Library
- Material Information Processor Library Input
- Unit Cell Geometry
- Problem Session 1

Tuesday
- Review of Problem Session 1
- KENO V.a Parameters / Geometry
- KENO V.a Plot Data
- CSPAN / KENO3D Demonstration
- Problem Session 2

Wednesday
- Review of Problem Session 2
- KENO V.a Output - How to Read it
- Holes / Arrays
- Problem Session 3

Thursday
- Review of Problem Session 3
- Start Types, Biasing, Boundary Conditions
- Criticality Search Data
- Problem Session 4

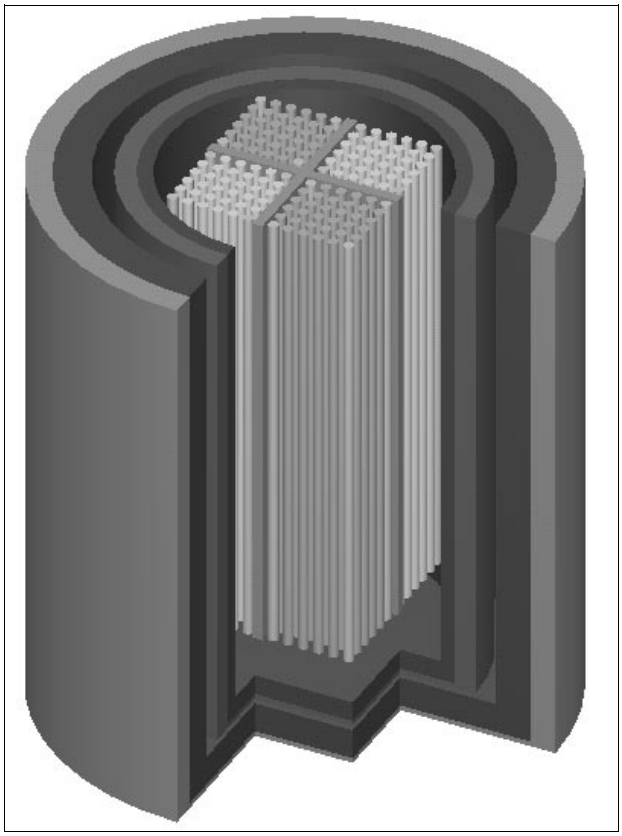
Friday
- Review of Problem Session 4
- Monte Carlo Uncertainties
- Code and Data Validation Issues

Class size is limited, and courses are subject to cancellation if minimum enrollment is not obtained one month prior to the course. Course fees are refundable up to one month before each class. Classes are cosponsored by the Radiation Safety Information Computational Center (RSICC). **Foreign nationals must register by October 1**. For further information, contact Kay Lichtenwalter, x4s@ornl.gov, 423-574-9213.

In This Issue ...

KENO3D Visualization Tool for KENO Geometry Models

Criticality safety analyses often require detailed modeling of complex geometries. Checking the accuracy of these models can be enhanced by effective visualization tools. To address this need, ORNL has recently developed 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



✓Shaded or wireframe images
✓Top, side, front, and isometric (3-D) views
✓Rotate the model
✓Zoom in on selected locations
✓Select parts of the model to display
✓Edit colors and display legends
✓Display properties of any unit in the model
✓Create cutaway views
✓Hide entities in the model
✓Print or save image to common graphics formats

KENO3D reads existing CSAS/KENO V.a or CSAS6/KENO VI input files. It 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, it displays the illegal KENO V.a geometry to facilitate debugging of the input. Problems with more than 200,000 KENO V.a bodies have been successfully tested and displayed. The figure above displays a sample light-water reactor (LWR) fuel assembly shipping container model. KENO3D is written in Visual C++ using ACIS 3-D Toolkit from Spatial Technology.

KENO3D was demonstrated at the American Nuclear Society June meeting in Boston. A production version for KENO V.a geometry models and an alpha test version for KENO VI geometry models is expected to be available from RSICC by the end of 1999 as a separate software package. A notice will be placed on the SCALE Web site.

CSPAN Input GUI to Replace CSASIN

The CSASIN input processor for CSAS/KENO V.a has been a popular tool for new and occasional users for several years. CSASIN is an MS-DOS application that was developed in the early 1990s before the release of Microsoft Windows 3.0. About one year ago we discovered that CSASIN was incompatible with Pentium II class PCs (see *Words to the Wise*). A new graphical user interface (GUI) is being developed as a replacement for CSASIN to assist users in the input setup and execution of any SCALE criticality safety analysis sequence (CSAS). The GUI, known as CSPAN (Criticality Safety Input Processor for Analysis) will run on Windows 95, 98, and NT PCs. The program provides input menus and context-sensitive help to guide the user through input setup. It contains a direct link to KENO3D to allow the user to view the components of their geometry model. Once input is complete, the user can click a button to run the CSAS case. CSPAN will be available on the SCALE Web site in late 1999 or early 2000.

KENO3D and CSPAN to Be Shown at ICNC '99

KENO3D and CSPAN will be demonstrated at the Sixth International Conference on Nuclear Criticality Safety (ICNC '99) meeting in Versailles, France, September 20-24, 1999. At the poster session on Monday evening, September 20, these new programs will be featured in the ORNL presentation: *SCALE Graphical Developments for Improved Criticality Safety Analyses*. If you are attending ICNC '99, please visit our booth.

SCALE Web Updates

Users are encouraged to visit the SCALE Web site (www.cad.ornl.gov/scale) often for current information and updates on SCALE. Listed below are the latest updates.

- The KENO3D Movie, a seven-minute video prepared for the Super Computing 98 conference, introduces our new three-dimensional (3-D) visualization tool for KENO V.a and KENO VI.
- Information and registration for the SCALE KENO V.a Training Course, November 1 – 5.
- Updates to KENO VI and CSAS6 are available on the Download page. These updates include corrections for infinite loop problems reported by users. See "SCALE Minor Modifications" for details.
- The report, *ARP: Automatic Rapid Process for the Generation of Problem-Dependent SAS2H/ORIGEN-S Cross-Section Libraries*, ORNL/TM-13584, is available to download from the Validation page. This report includes a significant number of validation cases using the ORIGEN-ARP methodology.

How to Compare SCALE Sample Problem Output Files

We frequently receive questions from users about how to compare their sample problem results with those distributed with SCALE. The differences for most of the non-Monte Carlo functional module sample problems should be fairly small. The output files for these codes can be compared using the Unix "diff" or the DOS "fc" commands. CPU times printed in XSDRNPM will be different.

For the KENO V.a and VI sample problems, you can extract the lines containing the words "generations skipped" using either the Unix "grep" command or the DOS "find" command. For MORSE, open each output file and search for "uncoll". This will take you to a table of detector responses. Compare this table.

For the control modules, here are some suggested keywords to use for finding the portion of the output you want to compare.
CSAS - same as KENO V.a; also grep or find "search pass"; note that the search cases (CSAS4 or CSAS4X) may have a different number of search passes, meaning more k_{eff} calculations in one of the output files.
CSAS6 - same as KENO VI.
SAS1 - look at the dose results from XSDOSE. To do this, grep or find the phrase "(total"
SAS2 - same as SAS1; grep or find "lambda" to get the XSDRNPM eigenvalues; open file and search for "gamma sources determined". Neutrons source spectra are printed above this line and gamma source spectrum are printed below it.
SAS3 and **SAS4** - same as MORSE.

Fortran 90 Compiler Required for SCALE 4.4 on Unix Workstations

Several users have contacted us with problems they have encountered trying to compile SCALE 4.4 on Unix workstations using a Fortran 77 compiler. The abstract on SCALE from RSICC clearly specifies that a Fortran 90 compiler is required. The SCALE and RSICC staffs are unable to assist users who attempt to install SCALE with a Fortran 77 compiler.

CSASIN Fails on Pentium II and III PCs

As noted in several entries in the SCALE Electronic Notebook, the CSASIN input processor for CSAS/KENO V.a fails to run on Pentium II and III and possibly other new PCs. Our staff is currently developing a new Windows 95/98/NT replacement for CSASIN named CSPAN. CSPAN is scheduled to be available for public release by the end of the year.

SCALE Minor Modifications

The following minor corrections and updates have been made since the release of SCALE 4.4. These modifications will be included in the next public release of SCALE.

MIPLIB: (1) Updates were made to allow number density input for an element that has multiple isotopes. (2) The XSDRNPM mesh generation algorithm was modified to address two problems: (a) insufficient number of mesh intervals for thick reflectors of low-absorbing material and (b) too many mesh intervals for high-absorbing regions. New input options to override the automatic mesh generation were added too. (3) Consistent with MRR 99-011, the default value of PTC was reduced from 10^{-4} to 10^{-5}. Although this enhancement was designed primarily for CSAS1X, it potentially affects all control modules that use XSDRNPM (MRRs 98-064 and 99-015).

XSDRNPM: (1) The Fortran source for XSDRNPM was converted to Fortran 90 free format. (2) The input/output units were all moved to the 0$ array. (3) The energy of the average lethargy causing fission was added to the balance tables. (4) The output files from the balance tables and the activities were modified and converted to ASCII files. (5) A new file was created that contains the input and derived data from a problem. (6) The flux file was changed to double precision. (7) The code was modified *not* to run with fluxes out of core unless explicitly requested in the input. (8) The coarse mesh generation algorithm used in rebalancing the inner iterations was modified to correct a problem that prevented convergence of a very small class of problems. (9) The code was modified to recycle if the final iteration performed after convergence failed the convergence test. For group banding cases, flux convergence is now reset after initial convergence to an order of magnitude less than overall convergence to prevent looping through iterations and never converging. (10) The default value for flux convergence tolerance, PTC, was reduced from 10^{-4} to 10^{-5} . (11) Errors were corrected in the printing of activities by interval when an undocumented option was selected. This previously undocumented option is now documented in the XSDRNPM input description (MRRs 98-065 and 99-011).

SAS2: (1) The code was updated for compatibility with the revisions to XSDRNPM. The routines that wrote the XSDRNPM input files needed to be changed to account for the changes to XSDRNPM input. Subroutine COPYNX had to be changed to add the 0$ array to the XSDRNPM input file, and to move setting the logical unit number of the flux output file from the 2$ array to the 0$ array. (2) Calls to subroutine EPSIG were changed for consistency with MIPLIB modifications in MRR 99-015 (MRRs 99-004 and 99-020).

UNIXLIB: Changes to update XSDRNPM required a double-precision ERF function. This function is part of the Fortran intrinsic library for DEC Alpha's and the IBM RS/6000, but is not part of that library for the HP or the SUN workstations. This modification provided an update for the necessary routines to compute the double-precision ERF when it is not part of the intrinsic library (MRR 99-006).

SAS4: The code was updated to change the convergence criteria because the criteria in XSDRNPM were changed. Also added an input variable NDAB to allow the user to specify the number of direct-access blocks allocated (MRR 99-008).

BONAMI: The code was updated to correct a problem that caused cases to fail when zero number density input is used (MRR 99-007).

ARPLIB: The code was updated to accept either lower- or upper-case input (MRR 99-001).

PRISM: The code was updated to accept either lower- or upper-case input (MRR 99-002).

XSECLIST: The code was updated to accept either lower- or upper-case input (MRR 99-003).

XSDOSE: An option to turn off angular-flux print was added and the default was made to be no angular-flux print (MRR 99-009).

MODIFY: (1) Subroutine LODATA was updated for compatibility with changes to MIPLIB to allow number density input for an element with multiple isotopes. (2) Program MODIFY was changed for consistency with the change in the direct-access file made to MIPLIB in MRR 99-015 (MRRs 99-010 and 99-017).

KENO VI: (1) The code was modified to detect intersecting HOLEs in the global unit. A problem will now terminate if intersecting HOLEs are detected in the global unit. Intersecting HOLEs are illegal in KENO VI geometry but were not detected in the global unit in SCALE 4.4. Intersecting HOLEs in units other than the global unit are detected during tracking of particles through the intersecting regions. (2) The code was corrected to define LCHK as a logical variable in

subroutine POSIT. In addition, an IMPLICIT NONE statement has been added to the beginning of the subroutine. All variables have been explicitly typed as appropriate. (3) The code was updated to fix a roundoff problem that sometimes caused particles to get into an infinite loop when they transferred from one array location to another but in the process missed the unit boundary (MRRs 99-012, 99-016, and 99-022).

CSAS6: The argument list for the call to subroutine PRTPLT was modified for consistency with changes made to KENO VI in MRR 99-012 (MRR 99-019).

ORIGEN-S: A new subroutine was added to provide the user the option of more significant digits in the output tables. Unit 71 was set as the default file number for the binary file containing concentrations and spectral data (MRR 99-014).

KMART: An error that resulted in calculated volumes of zero for hemicylinders and arrays (if an array number was skipped) was corrected (MRR 99-018).

MORSE: The program was updated to correct a problem in determining the day of the week for dates after December 31, 1999 (MRR 99-021).

SUBLIB: Subroutine YREAD turned off the normal invalid character check done by the free-form- reading routines, but does not make any checks of its own for invalid characters. This can lead to erroneous results in some cases where a user mispunches a character when entering the array data to KENO. Checks were added to the array-reading routine to give warning messages if illegal characters are read (MRR 99-023).

SAS4 Sample Problems: SAS4 sample problems 1, 3, and 5 were updated to remove references to variables FR1, FR2, FR3, and FR4, which became obsolete in SCALE 4.4 (DRR 99-001).

XSDOSE Sample Problem: The XSDOSE section of the SCALE Manual documents the output of the sample problem and includes the printing of the fluxes. The input was modified to turn on the new angular flux print option in XSDOSE (see MRR 99-009) (DRR 99-002).

KENO V.a Sample Problems: Input data for sample problems 17 and 18 were changed. The number of neutrons started in sample problem 18 was changed to agree with the number per generation. Problem 17 was changed to specify the NBK parameter because the default was not large enough (DRR 99-003).

238-group and 44-group libraries: Changes were made because problems were discovered with $\bar{\nu}$ for ^{238}Np, ^{250}Cf, ^{253}Cf, ^{249}Bk, ^{242}Am, and ^{233}Pa. The corrections for ^{250}Cf, ^{233}Pa, and ^{249}Bk were very minor and should have no important effects. However, significant errors were identified in $\bar{\nu}$ for ^{238}Np, ^{253}Cf, and ^{242}Am. In addition, these three nuclides do not have fission cross sections specified in the fast region in ENDF/B-V. This omission is obviously wrong, and because it could lead to very non-conservative answers for k_{eff}, these three nuclides were removed from the library (DRRs 99-004 and 99-005).

SCALE KENO V.a Training Course Registration Form

Oak Ridge National Laboratory, Oak Ridge, Tennessee

November 1– 5, 1999

Please use the registration form on the Web if possible

(www.cad.ornl.gov/cad_nea/text/scale_course_reg.html)

I am registering (check one):

☐ **Before October 1** Fee: $1,500

☐ **After October 1** Fee: $1,800

Do you want to receive a copy of SCALE on CD ($300 extra)? ☐ **Yes** ☐ **No** Fee: $ 300

Total Fee $ _____

Name _____

Citizenship _____

Organization _____

Mailing address _____

_____

_____

E-mail: _____

Telephone: _____ **Fax:** _____

Your level of experience (circle one for each):

	Very High	High	Medium	Low	None
Criticality					
CSAS/KENO V.a	4	3	2	1	0
Other_____	4	3	2	1	0

What types of problems/applications do you want to be able to analyze with SCALE after attending the course?

Please mail this form and registration fee payment to:

SCALE Training Course
c/o Kay Lichtenwalter
Oak Ridge National Laboratory
P.O. Box 2008, Bldg. 6011, MS 6370
Oak Ridge, Tennessee 37831-6370
FAX 423-576-3513
E-mail: x4s@ornl.gov

Classes may be canceled if minimum enrollment is not obtained.
Course fees are refundable up to one month before each class.

SCALE Newsletter
Oak Ridge National Laboratory
P.O. Box 2008 MS-6370
Oak Ridge, TN 37831-6370

FAX: (423) 576-3513
E-mail: scalehelp@ornl.gov
Internet: www.cad.ornl.gov/scale

SCALE Newsletter is published twice a year by Oak Ridge National Laboratory and sponsored by the Spent Fuel Project Office of the U.S. Nuclear Regulatory Commission and the U.S. Department of Energy Package Approval and Safety Program.

Managed by Lockheed Martin Energy Research Corporation, for the U.S. Department of Energy under contract DE-AC05-96OR22464.