SCALE Newsletter

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

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SCALE Newsletter Going All Electronic

This last issue of the SCALE Newsletter will be the final issue that will arrive in your mailbox. Future issues of the SCALE Newsletter will be published and distributed in electronic format only. Beginning with the previous issue (July 1999), the newsletter is published on the Web in a PDF file that is identical to the hard copy that is mailed to our subscribers. By eliminating the distribution by U.S. mail of about 700 copies, we can save significant costs for personnel time to print, package and mail them. Current and past issues of the SCALE Newsletter can be found on the Web at **http://www.cped.ornl.gov/scale/scale_news.html**. You may receive notification by e-mail of new issues of the SCALE Newsletter available on the Web by clicking on the **"Join List"** button there.

SCALE 4.4a is coming soon! See page 3 for more information.

SCALE Training Course Schedule

The SCALE staff at ORNL will be offering several training courses in 2000. The courses will emphasize hands-on experience solving practical problems on PCs. There will be workgroups of two persons each for the ORNL courses. No prior experience in the use of SCALE is required to attend. The registration fee is $1,800 ($300 discount if you register at least one month before the course). A copy of the SCALE software and manual on CD may be obtained for an additional fee of $310. Registrations will be accepted on a first-come basis. Registration forms submitted directly from the Web are preferred. Registration via FAX or e-mail is also acceptable. The registration fee must be paid by check, travelers checks, or credit card (VISA or MasterCard only). The agenda and registration form for the April KENO-VI course are included later in this issue. **Foreign nationals must register at least six weeks in advance.**

In This Issue ...

Date	Title	Location
April 10–14	SCALE KENO-VI Criticality Course	ORNL
May 15–19	SCALE KENO-VI Criticality Course	Paris, France; contact Enrico Sartori (e-mail sartori@nea.fr)
October 16–20	SCALE KENO V.a Criticality Course	ORNL
October 23–27	SCALE Shielding/Source Terms Course	ORNL

For further information, contact Kay Lichtenwalter, x4s@ornl.gov , 865-574-9213.

SCALE Web Updates

Note that the address of the SCALE Web site has changed. The new address is (www.cped.ornl.gov/scale). Please update the bookmark in your Web browser. Users are encouraged to visit the site often for current information and updates on SCALE. Listed below are highlights of the latest updates.

- Information and registration for the SCALE Training Courses for 2000 were placed on the Training page.
- Announcement of the availability of KENO3D from the Radiation Safety Information Computational Center (RSICC) was posted on the Home page.
- SCALE shielding verification and validation (V&V) input files from NUREG/CR-6484, with Acrobat PDF files that explain how to combine case results for comparison with results reported in NUREG/CR-6484, were added to the Download page.

QAD-CGGP Sample Problem on Sun Workstations

In testing of SCALE 4.4a on a Sun workstation at ORNL, some of the input numbers in the QAD-CGGP sample problem had to be edited by hand for the input to be read correctly. Several of the numbers had exponents without an "E" as part of the exponent. Sun complained that they were illegal real numbers. An "E" was added to each number that had an exponent without an "E" and the sample problem ran correctly. We believe there is an error in the Sun Fortran library, and that the original input is legal. Sun users may need to make the same modification on their installations.

Reflector Biasing in KENO with Low-Density Reflectors

KENO users are warned not to use reflector biasing with low-density reflector materials. A problem was recently reported by a user where a KENO input file was originally set up for a system with a nominal density water reflector using reflector biasing to reduce computational time. Later, the density of the reflector region was reduced to investigate the effects of low-density water. The calculated k_{eff} values varied widely due to high-weight neutrons from the outer reflector region re-entering the fissile material.

Users who have attended one of our SCALE/KENO training courses should be aware of the danger of mismatched reflector regions where high-importance reflector regions are placed near low-importance reflector regions. Similarly, the use of reflector bias data generated for nominal density reflector materials with reflector regions containing low-density reflector materials causes a mismatch between the bias data and materials. This mismatch can result in high-weight neutrons from the outer reflector region returning to the fissile material. To avoid this problem, turn off reflector biasing if the reflector material is not nominal density.

What's New in SCALE 4.4a?

A significant number of updates have been made to SCALE in the past year since the release of SCALE 4.4. Most of these updates were minor corrections or enhancements. Because some of these updates could be important to SCALE users, this interim release of SCALE 4.4a is being made available.

Shielding Modules
SAS4 and PICTURE were enhanced to allow the generation of two-dimensional (2-D) plots when the "PARM=CHECK" option is used. This option is similar to the plotting option in the CSAS criticality sequences. Another innovation was the addition of an option that allows users to specify an X-Y, X-Z, or Y-Z plot and have the code automatically calculate the cosines used for the plot.

A discrepancy in scoring boundary crossings of surface detectors was corrected in MORSE. Contributions to user-specified surface detectors in MORSE in SCALE 4.4 could have been underestimated because of a failure to determine which surface detector to score. This failure was due to the comparison of a single-precision variable to a double-precision variable. Most affected cases would have a zero result for the surface detector, indicating that no particles have crossed the surface detector boundary. Detector location coordinates of four digits or less would not be expected to experience this problem. MORSE was updated to correct a problem in determining the correct day of the week for dates after December 31, 1999.

A coding error introduced in QAD-CGGP in SCALE 4.4 has been identified and corrected. Because of inconsistent array dimensions, if more than a very limited number of bodies are input in one zone, the additional zone data are lost or stored incorrectly. This situation typically causes the code to fail. Though extremely unlikely, it might be possible for a case like this to run if the incorrectly stored geometry happened to be valid. SCALE 4.4 users should check under the "input zone data" header in the QAD-CGGP output to verify that the zone data agree with their input.

Depletion Modules
SAS2 was corrected to fix an error introduced in SCALE 4.4 that caused the PARM=OLDSAS2 option to fail. Another discrepancy introduced in SCALE 4.4 caused spent fuel isotopic data written to file FT72F001 to be incorrect in certain cases. This error, which has been corrected, occurred in cases where burnable poison rods or other inserts are removed from or inserted into the fuel assembly between fuel cycles. SAS2 can now correctly handle multiple fuel zones in the path B model. A minor discrepancy was corrected where invalid characters were being written to title records in the ORIGEN-S binary library. Some text editors could not read the SAS2 output file when invalid characters were present.

Criticality Modules
KENO-VI 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. Several corrections were made to KENO-VI to prevent a particle from becoming lost and causing the code to enter an infinite loop.

A large number of enhancements were made to XSDRNPM. The Fortran source for XSDRNPM was converted to Fortran 90 free format. The input/output units were all moved to the 0$ array. The energy of the average lethargy causing fission was added to the balance tables. The output files from the balance tables and the activities were modified and converted to ASCII files. A new ASCII file was created that contains the input and derived data from a problem. The coarse mesh generation algorithm used in rebalancing the inner iterations was modified to correct a problem that prevented convergence for a very small class of problems. The code was modified to recycle if the final iteration performed after convergence failed the convergence test. For group-banding cases, convergence is now reset after initial convergence to an order of magnitude less than overall convergence to prevent looping through iterations and never converging. The default value for flux convergence tolerance, PTC, was reduced from 10^{-4} to 10^{-5}. The calculation of activities by interval, an option that was available many years ago, was reintroduced in the code.

The XSDRNPM mesh generation algorithm in MIPLIB 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 highly absorbing regions. New input options to override the automatic mesh generation were added. Although this enhancement was designed primarily for CSAS1X, it potentially affects all control modules that use XSDRNPM, except SAS2H.

SCALE 4.4a will be available soon from RSICC. Check the SCALE web site for the announcement of the release.

CSPAN Included in SCALE 4.4a

CSPAN (**C**riticality **S**afety Input **P**rocessor for **An**alysis) is the Windows GUI replacement for the CSASIN input processor for the CSAS criticality sequences in SCALE. CSASIN was an MS-DOS program developed in 1990-91 to assist new and occasional SCALE users. Because CSASIN is incompatible with Pentium II and later PCs, a new easier-to-use and more powerful Windows program has been developed. CSPAN can be used to read and modify an existing SCALE input file or to create a new input file. CSPAN can call SCALE to execute CSAS using the input file it creates. The SCALE Standard Composition library and the selected SCALE cross-section library are read by CSPAN, and the user is only allowed access to those compositions available on the selected cross-section library. The program handles the entry of basic standard compositions, solutions, and arbitrary materials, unit cell data, optional parameter data, and KENO V.a input data. CSPAN can call SCALE to execute any CSAS case. CSPAN runs under Windows 95, 98, or NT. Checks for errors are included throughout the program to verify that the input is valid. The initial version distributed with SCALE 4.4a is considered a beta test version. Help files have not been developed yet.

Visual Heating Included in SCALE 4.4a

The initial version of a Windows-based GUI for HEATING named Visual Heating is also included in the SCALE 4.4a release. Visual Heating assists the user in preparing a HEATING input file and includes a 3-D graphics display of HEATING geometry models using OpenGL. Visual HEATING can execute the HEATING case in SCALE and display the output file in a text editor. It includes an HTML Help system similar to many commercial Windows programs. The help system is accessible both from the main menu bar and by pressing the F1 key. Most of the information in the HEATING User's Manual (Sect. F10 of the SCALE Manual) is included in the help system along with explanations of Visual HEATING input screens.

SCALE Minor Modifications

The following minor corrections and updates have been made since last July. These modifications are included in the public release of SCALE 4.4a.

HEATING: The code was updated, including Fortran 90 dynamic memory allocation, to improve portability on both workstation and PC platforms. (MRR 99-027)

SAS2: The following modifications were made:
(1) The calculation of the light-element concentrations in ORIGEN-S was corrected when multiple fuel zones (MX=500) are used in the PATH B model. The code previously assumed only one fuel zone was present and did not sum the zone volumes when multiple zones were present, resulting in erroneous light-element concentrations in the ORIGEN-S depletion calculations. (2) The depletion of light-element nuclides with mixture numbers 50 through 59 is now permitted. (3) The use of 1$ data for MXT (input level 3) when reading a second working library in NITAWL is now permitted. (MRR 99-025)

UNIXLIB: Subroutine JSTIME was modified to return time to the precision supplied by the system. (MRR99-028)

These modifications are **not** included in version 4.4a.

KENO-VI: (1) Three options were added to read from input or calculate approximately the correct geometry volumes so the fluxes and fission densities would be appropriately normalized. (2) A problem was corrected that caused a particle to go into an infinite loop due to a round-off error when trying to exit an array. (3) A problem was corrected where a particle could go into an infinite loop when a unit shares an outer boundary with a chord and is in an array. (MRRs 99-026, 30, 37)

C5TOC6: This utility was also updated to add volumes to the CSAS6/KENO-VI input file that is created. In addition, the default array size was increased. (MRR99-036)

K5TOK6: This utility was updated to print the correct code title in the output banner and to add volumes to the KENO-VI input. (MRR99-035)

CSAS6 and KENO-VI sample problems: Input data for the sample problems were changed to illustrate the new volume calculation options. Each of the options is used. (DRR99-006)

MIPLIB: Subroutine EPSIG was corrected to prevent calculation of the square root of a negative number when a material with a very low number density was used in a problem with a curvilinear coordinate system. (MRR99-031)

PERFUME: Fixed dimension arrays were removed from the common block Common_angle, and automatic arrays were created to pass through argument lists. (MRR99-034)

PERFUME Sample Problem: A FIDO array type was updated for reading EPS. (DRR99-008)

WAX: Limits on the maximum number of input nuclides were removed. Fixed dimension arrays were replaced with flexibly dimensioned arrays. (MRR99-029)

SCALE KENO-VI Training Course Agenda

(April 10–14, 2000)
The course will conclude at noon on Friday.

Monday
Overview of SCALE
Introduction to CSAS6
Standard Composition Library
Material Information Processor Input
Resonance Self-Shielding
Unit Cell Geometry - Lattice Cell / Multiregion
Optional Parameter Data
Problem Session 1

Tuesday
Review of Problem Session 1
KENO-VI Parameters
KENO-VI Geometry
KENO-VI Plot Data
Problem Session 2

Wednesday
Review of Problem Session 2
KENO-VI Output - How to Read It
Holes
Arrays
Chords and Origins
KENO3D
Problem Session 3

Thursday
Review of Problem Session 3
Start Data
Bias Data
Boundary Data
Mixing Table
Problem Session 4

Friday
Review of Problem Session 4
Monte Carlo Uncertainties
Code and Data Validation Issues
Conclusion / Questions and Answers

SCALE KENO -VI Training Course Registration Form

Oak Ridge National Laboratory, Oak Ridge, Tennessee

April 10–14, 2000

Please use the Web registration form if possible (**http://www.cped.ornl.gov/scale/scale_course_reg.html**)

I am registering (check one):

☐ **Before March 10** Fee: $1,500

☐ **After March 10** Fee: $1,800

Do you want to receive a copy of SCALE on CD ($310 extra)? ☐ **Yes** ☐ **No** Fee: $ 310

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
CSAS6/KENO-VI	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: 865-576-3513
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.

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