SCALE Newsletter

Computational Physics and Engineering Division
Nuclear Engineering Applications Section
Oak Ridge National Laboratory
SCALE Web Site: http://www.cped.ornl.gov/scale

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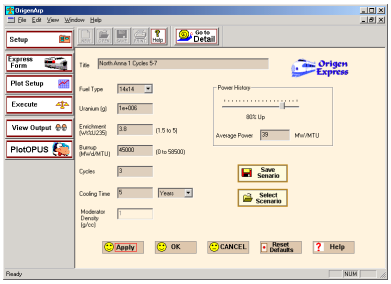
OrigenArp for Windows

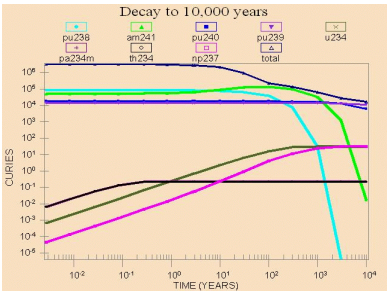
The new OrigenArp graphical user interface (GUI) is a Windows-based program that provides an easy-to-use method for setting up and executing the ORIGEN-ARP spent fuel characterization module in SCALE. ORIGEN-ARP is a sequence that serves as a faster alternative to the SAS2H sequence of the SCALE system to perform point-irradiation calculations with the ORIGEN-S code using problem-dependent cross sections. ARP (Automatic Rapid Processing) uses an algorithm that allows the generation of cross-section libraries for the ORIGEN-S code by interpolation over pre-generated SAS2H cross-section libraries. Interpolations are performed on burnup, enrichment, and optionally, water density.

The OrigenArp for Windows GUI replaces the MS-DOS menu program ORIGNARP and provides menus, toolbars, forms, and online help that assist the user in preparing a SCALE input file to execute ARP and ORIGEN-S. This new GUI contains several new features, including a simplified input form, referred to as Origen Express, that requires as few as four key input parameters. It also provides the capability to easily plot ORIGEN-S calculated results via the OPUS/PlotOPUS plotting utilities. A sample Origen Express input form and a plot from PlotOPUS are shown in the figures on this page.

OrigenArp for Windows and OPUS/PlotOPUS will be available to download from the SCALE web site in early February.



Sample Origen Express Input Form



Sample Plot From PlotOPUS

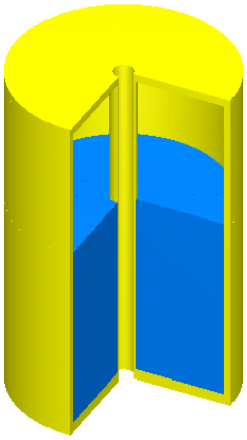
In This Issue ...

New Features in KENO3D Version 2.0 for KENO V.a and KENO-VI

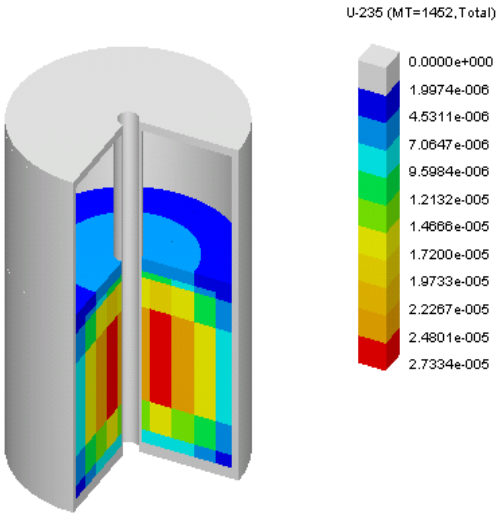
The extension of KENO3D to KENO-VI geometry models was accomplished in version 2.0 of KENO3D, which is compatible with both versions of KENO. An option to allow the plotting of activities and fluxes from the SCALE KMART post-processor for KENO V.a was added to KENO3D version 2.0. To plot KMART data, it is first necessary to run KENO V.a and KMART to generate the required KMART data file. This capability requires an updated version of KMART that is available on the SCALE Download web page. The two figures on this page show the KENO3D visualizations of the Sheba-II criticality experiment and the total neutron production in the experiment.

A hidden line removal algorithm for wireframe images has been implemented in KENO3D. Lines that would be occluded by solid bodies are removed. Previously, models that had a large number of edges were not very useful as wireframe images. However, by removing "hidden lines" the image becomes less cluttered. Hidden line removal only works with white or black backgrounds. A simpler procedure for editing mixture colors in KENO3D was implemented. Previously the color legend had to be presented in a separate view to allow color editing. Now the editing can occur in the same view as the model. The option to have the color legend in a separate view was eliminated. The axes option was modified to allow the user to place the axes at any specified coordinate. An option to allow the user to change the default wireframe color was added.

A KENO3D web site has been developed to provide users with a resource for timely information, software updates, and a mechanism for communicating with KENO3D developers. Included on the web site is a KENO3D Users Notebook for questions and answers regarding the use of KENO3D. The web site is located at www.cped.ornl.gov/scale/keno3d. A link also is available on the SCALE web site. KENO3D Version 2.0 for KENO V.a and KENO-VI was released by the Radiation Safety Information Computational Center (RSICC) in October.



Sheba-II Critical Experiment



Total Neutron Production in Sheba-II

SCALE Minor Modifications

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

MIPLIB: This library, which is used by the SCALE control modules, was updated to add an error message and terminate the problem if it contains elements whose isotopes do not sum to 100%. (MRR00-011)

KMART: An option was added to write a data file in format suitable for reading and plotting by KENO3D. Several other changes were made to compute statistics on activities and to compute activity densities instead of total volume activities. (MRR00-014)

KENO-VI Sample Problems: Sample problem no. 15 was updated to correct the enrichment data that did not sum to 100%. (DRR00-001)

New SCALE Cross-Section Libraries Report

A new report titled, *Experience With the SCALE Criticality Safety Cross-Section Libraries*, (NUREG/CR-6686), which was published in October, provides detailed information on the SCALE criticality safety cross-section libraries. Areas covered include the origins of the libraries, the data on which they are based, how they were generated, past experience and validations, and performance comparisons with measured critical experiments and numerical benchmarks. The report is available on the SCALE Validation / Benchmark Reports web page.

The performance of the SCALE criticality safety cross-section libraries on various types of fissile systems is examined in detail. Most of the performance areas are demonstrated by examining the performance of the libraries vs critical experiments to show general trends and weaknesses. In areas where directly applicable critical experiments do not exist, performance is examined based on the general knowledge of the strengths and weaknesses of the cross sections. In this case, experience in the use of the cross sections and comparisons with the results of other libraries on the same systems are relied on for establishing acceptability of application of a particular SCALE library to a particular fissile system.

This report should aid in establishing when a SCALE cross-section library would be expected to perform acceptably and where there are known or suspected deficiencies that would cause the calculations to be less reliable. To determine the acceptability of a library for a particular application, the calculational bias of the library should be established by directly applicable critical experiments.

Viewing Figures in Online SCALE Manual

A SCALE user reported that pages 195 and 196 in Sect. F17 (KENO-VI) of the online SCALE 4.4a Manual (PDF version) would not display in Adobe Acrobat. Some figures may appear as a series of horizontal lines, but they can be viewed by clicking on the zoom tool (magnifying glass icon) in Acrobat and then clicking on the figure to magnify it.

Bias in Monte Carlo k-eff Calculations

A KENO user recently inquired about the introduction of a slight negative bias in k_{eff} if too many generations are run. It has been known for some time that there is a small bias in the estimation of k_{eff} and its variance by conventional Monte Carlo programs. The bias is due to the repeated renormalization of the fission source by the eigenvalue so that the original number of starting neutrons is approximately maintained for each generation. The renormalization is necessary because the neutrons born in one generation are used as the starting points in the next generation. Because the number of neutrons born in a generation is not usually equal to the number started, starting neutrons must be produced each generation by renormalizing the source distribution from the previous generation.

A paper by A. M. Gelbard and A. G. Gu, "Biases in Monte Carlo Eigenvalue Calculations," *Nuclear Science and Engineering* (Vol. 117, 1994) shows an upper limit on the bias as a function of the number of histories per generation and the number of generations. Consequently, it has been shown that the eigenvalue bias under "normal" conditions (i.e., reasonable values for the number of neutron histories per generation and the number of generations) is smaller than the eigenvalue's standard deviation. The author states that to guarantee the bias is a small part of the standard deviation, it is better to limit the number of generations to not more than 400. The SCALE staff performed a test using an 1-D analytical benchmark with $k_{eff} = 1$. The results from a XSDRNPM discrete ordinates calculation were compared with several KENO Monte Carlo calculations of 100 million histories and standard deviations of less than 10^{-6}. The KENO cases employed a wide range of numbers of generations and neutrons per generation, up to an extreme of 100,000 generations with 1,000 neutrons per generation. In all cases, the bias for this simple problem was smaller than the 4 digits past the decimal printed in the KENO output for k_{eff}. For a KENO user running typical applications with reasonable numbers of generations, the bias should be negligible.

Automatic Mesh Generation in XSDRNPM

The CSAS1X, CSAS2X, and CSAS4X criticality safety sequences use the one-dimensional (1-D) XSDRNPM discrete ordinates code to cell weight, or homogenize, cross sections over a defined unit cell. The Material Information Processor automatically provides the mesh intervals used in XSDRNPM by the CSAS sequences and the SAS1, SAS1X, and SAS4 shielding sequences. (See Sect. M7.2.5.6 of the SCALE Manual for details about the automatic mesh generator.) The automatic mesh generator was designed primarily for lattice pin cell systems. For large 1-D systems, it has generally performed adequately, but problems have been reported with very large reflector regions that were important (e.g., beryllium or graphite).

To avoid such inadequacies, the XSDRNPM mesh generation algorithm used in these SCALE sequences was modified in SCALE 4.4a 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.

Although the new algorithm should provide reasonable results in most cases, the spatial mesh size (SZF) parameter in MORE DATA allows the user to alter the number of XSDRNPM mesh intervals provided by the Material Information Processor. The default value of SZF is 1. An absolute value of SZF less than 1 provides finer mesh and more mesh intervals, and a number greater than 1 yields coarser mesh and less mesh intervals. If SZF is positive, the interval spacing is generated as described in Sect. M7.2.5.6 of the SCALE Manual; if SZF is negative, the intervals are equally spaced in each zone. In addition, a new input option to manually override the automatic mesh generation was created in SCALE 4.4a. The user may specify the number of intervals in any zone by using INT(*iz*)=*x* in MORE DATA, where *iz* is the zone number and *x* is the number of intervals.

Don't Skip Body Numbers in QADS/QAD-CGGP

When using either QADS or QAD-CGGP in SCALE, number the bodies consecutively. The combinatorial geometry typically fails when a body number is skipped in the input file. It is permissible to have bodies that are not used in the zone data, but the bodies should always be numbered sequentially.

Cross-Section Interpolation Failure in ORIGEN-ARP

An ORIGEN-ARP user encountered an error in ARP, where it failed on a divide by zero, passing invalid data as cross sections to ORIGEN-S, which entered an infinite loop. The problem occurred in the power-interpolation scheme in ARP which was borrowed from BONAMI. The error is random and highly unlikely. If the interpolation point is changed by as little as 10^{-5}, the interpolation works. The problem occurs at points of inflection in the power fit values. The scheme linearly interpolates on the power from adjacent points. If the points are of opposite sign, the interpolated power can be less than 10^{-7} which causes underflows and a divide by zero in the scheme. If you encounter this problem, please contact the SCALE staff.

SCALE Training Course Schedule for 2001

The SCALE staff at Oak Ridge National Laboratory (ORNL) will be offering four training courses at ORNL in 2001. The courses will emphasize hands-on experience solving practical problems on PCs. There will be workgroups of two persons each. No prior experience in the use of SCALE is required to attend. The registration fee is $1800 for one course or $2700 for both spring or both fall courses **($300 discount if you register at least one month in advance)**. A copy of the SCALE software and manual on CD may be obtained for an additional fee of $310, and the KENO3D visualization tool on CD is available for $410 (single license). 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, bank transfer, or credit card (VISA or MasterCard only). The agenda and registration form are included on the following pages.

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 RSICC. **Foreign nationals must register at least eight weeks in advance to obtain security clearance.**

Date	Title	Description
April 23 – 27, 2001	SCALE Shielding & Source Terms Course	SCALE depletion/decay and shielding sequences (including new OrigenArp and PlotOPUS)
April 30 – May 4, 2001	SCALE KENO-VI Criticality Course	CSAS6/KENO-VI (including CSPAN and KENO3D)
October 15 – 19, 2001	SCALE Shielding & Source Terms Course	SCALE depletion/decay and shielding sequences (including new OrigenArp and PlotOPUS)
October 22 – 26, 2001	SCALE KENO V.a Criticality Course	CSAS/KENO V.a (including CSPAN and KENO3D)

SCALE Shielding and Source Terms Course

The SCALE Shielding and Source Terms Course emphasizes SAS2 and ORIGEN-ARP (depletion/source-term generation) and SAS4/ MORSE-SGC (3-D Monte Carlo neutron/gamma shielding). It also covers SAS1/XSDRNPM (1-D neutron/gamma shielding) and QADS/QAD-CGGP (3-D point kernel gamma shielding). The course will feature the use of the new SCALE Windows GUIs to be released in 2001: OrigenArp for Windows, ORIGEN-S plotting utility PlotOPUS, and ESPN shielding input processor for SAS4.

SCALE KENO-VI Criticality Course

The SCALE KENO-VI Criticality Course focuses on KENO-VI and the associated criticality analysis sequences in CSAS6. KENO-VI is the latest version of the KENO Monte Carlo criticality safety code. KENO-VI contains a much larger set of geometrical bodies than KENO V.a, including cuboids, cylinders, spheres, cones, dodecahedrons, elliptical cylinders, ellipsoids, hoppers, parallelpipeds, planes, rhomboids, and wedges. The flexibility of KENO-VI is increased by allowing the following features: intersecting geometry regions; hexagonal as well as cuboidal arrays; regions, holes, arrays, and units rotated to any angle and truncated to any position; and the use of an array boundary that intersects the array. Two-dimensional color plots of the geometry model can be generated in KENO, or the model may be viewed using the KENO3D visualization tool.

SCALE Shielding and Source Terms Course Agenda (April 23 – 27, 2001)

Monday
Overview of SCALE System
Introduction to SCALE Shielding Sequences
ORIGEN-ARP
Plotting ORIGEN Results with OPUS/PlotOPUS
OrigenArp / PlotOPUS Demonstration
ORIGEN-ARP Problem Definition
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
SAS1 1-D Shielding Sequences
SAS1X 1-D Combined Criticality/Shielding Sequences
SAS1 Problem Session

Thursday
SAS4 3-D Monte Carlo Shielding Analysis Sequences
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 Sequences
QADS Problem Definitions
QADS Problem Session
Shielding Course Wrap-up

The course will conclude with lunch on Friday. Attendees may stay for an optional afternoon problem session to work on problems they bring.

SCALE KENO-VI Course Agenda (April 30 – May 4, 2001)

Monday
Overview of SCALE System
Introduction to CSAS6
Standard Composition Library
Material Information Processor
Resonance Self-Shielding
Unit Cell / More Data
CSPAN Demo
Problem Session 1

Tuesday
Review of Problem Session 1
Geometry Data
Geometry Modification Data
Plot Data
Introduction to KENO-VI Output
Problem Session 2

Wednesday
Review of Problem Session 2
Parameter Data
Array Data
Content Data - Media/Hole/Array
KENO3D Tutorial
Problem Session 3

Thursday
Review of Problem Session 3
KENO-VI Output - How to Read It
Mixing Table Data
Start Data
Bias Data
Boundary Data
Problem Session 4

Friday
Review of Problem Session 4
Monte Carlo Uncertainties
Code and Data Validation Issues
Conclusion / Questions and Answers
The course will conclude with lunch on Friday.

SCALE Training Course Registration Form
Oak Ridge National Laboratory, Oak Ridge, Tennessee
SCALE Shielding & Source Terms Course
April 23–27, 2001
SCALE KENO-VI Criticality Course
April 30–May 4, 2001

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

I am registering for:			**Before March 23**	**After March 23**
☐ **Shielding and Source Terms Course**			Fee: $1,500	Fee: $1,800
☐ **KENO-VI Course**			Fee: 1,500	Fee: 1,800
☐ **Both Courses**			Fee: 2,400	Fee: 2,700
SCALE 4.4a on CD	☐ **Yes**	☐ **No**	Fee: 310	Fee: 310
KENO3D (single license)	☐ **Yes**	☐ **No**	Fee: 410	Fee: 410

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-VI	4	3	2	1	0
Other_____	4	3	2	1	0
Shielding	4	3	2	1	0
SAS1	4	3	2	1	0
SAS4	4	3	2	1	0
QADS/QAD-CGGP	4	3	2	1	0
Other_____	4	3	2	1	0
Source Terms/Depletion	4	3	2	1	0
SAS2	4	3	2	1	0
ORIGEN-S/ORIGEN-ARP	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: 815-327-6460
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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