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

Number 24 **July 2001**

New ORIGEN-ARP Package Is Available from RSICC

The SCALE staff at ORNL has created a new isotope generation and depletion code system to satisfy a need for an easy-to-use standardized method of isotope depletion/decay analysis for spent nuclear fuel (SNF), fissile material, and other radioactive material. It can be used to solve for isotopic inventory, radiation source terms, and decay heat. ORIGEN-ARP features the Origen Express form that enables a user to setup and run a calculation (including plots) in less than one minute. It is available from the Radiation Safety Information Computational Center (RSICC) as code package CCC-702.

ORIGEN-ARP is an automated system to perform isotopic depletion/decay calculations using the ARP (Automated Rapid Processing) and ORIGEN-S codes of the SCALE system. The package includes the OrigenArp Windows graphical user interface (GUI) that prepares input for ARP and ORIGEN-S. ARP automatically interpolates cross sections for the ORIGEN-S depletion analysis using enrichment, burnup, and optionally moderator density, from libraries generated with the SCALE SAS2 depletion sequence. Library sets for four LWR fuel assembly designs (BWR 8x8, PWR 14×14, 15×15, 17×17) are included. The libraries span enrichments from 1.5 to 5 wt % U-235 and burnups of 0 to 60,000 MWD/MTU. Other libraries (e.g., DLC-210 for CANDU fuel) are available from RSICC. SCALE users can generate their own libraries for other fuel assembly designs using the tools in SCALE 4.4a. The interpolated cross sections from ARP are passed to ORIGEN-S to perform the depletion/decay calculations. The ORIGEN-ARP package includes the post-processing utility module OPUS to generate ASCII plot data files and the PlotOPUS Windows GUI to plot the data. For more information on the OrigenArp Windows GUI, OPUS, and PlotOPUS, refer to the January 2001 issue of the *SCALE Newsletter*.

This package is intended for users who do not need the additional criticality safety and radiation shielding capabilities of SCALE. It runs on Pentium PCs with 32 MB RAM under Windows 95/NT or later. SCALE users can download the components that are not distributed in SCALE 4.4a (OrigenArp GUI, OPUS, and PlotOPUS) from the SCALE Download web page. **Note that the RSICC source CCC-371/ORIGEN2.1 has not been updated since 1991, and all new ORIGEN users are advised to request the ORIGEN-ARP package.** The ORIGEN-ARP package has its own web site and user notebook. Users can access it from the SCALE website or go directly to www.cped.ornl.gov/origen-arp.

New users are encouraged to attend the SCALE Source Terms and Shielding Course, October 22–26, at ORNL. Information and a registration form are included in this newsletter.

In This Issue ...

ORIGEN-ARP Libraries for CANDU Fuel Available from RSICC

RSICC data package DLC-210 from Atomic Energy of Canada Limited (AECL) contains burnup-dependent ORIGEN-S cross-section libraries for CANDU reactor fuel characterization. The updated cross sections were generated using the WIMS-AECL lattice code and ENDF/B-V and -VI based data. The libraries in this data collection are designed for characterizing spent fuel from CANDU pressurized heavy water reactors. Two libraries are provided: one for the 28-element fuel bundle design, the other for the 37-element fuel bundle design. The libraries may be used with the ORIGEN-ARP sequence in SCALE. For more information check the RSICC abstract for DLC-210.

STARBUCS: A New SCALE Sequence for Burnup Credit

STARBUCS (**St**andardized **A**nalysis of **R**eactivity for **Bu**rnup **C**redit using **S**CALE) is a new sequence to perform criticality calculations for spent fuel systems employing burnup credit. STARBUCS automates the coupling of the depletion and criticality aspects of the calculation, thereby eliminating the need to manually process spent fuel isotopic compositions from a burnup calculation into the units and formats required by criticality codes. STARBUCS automatically prepares the input for all codes in the analysis sequence, executes the codes through the SCALE driver, and performs all module interface and data management functions for the user.

STARBUCS uses the ORIGEN-ARP methodology to perform the burnup analysis for each spatially-varying burnup region of a fuel assembly. The final spent fuel compositions are used to generate macroscopic fuel cross sections using the CSAS Criticality Safety Analysis Sequence. Finally, the KENO V.a code (or optionally KENO-VI) is used to perform a 3-D criticality calculation.

Options are provided to allow simulation of many of the dominant burnup credit phenomena. An arbitrary axial and/or horizontal burnup profile may be specified. Default "built-in" profiles are also available. The user may select the specific actinides and fission products to be used in the criticality calculation and optionally specify isotopic correction factors to account for bias and uncertainty in the calculated inventories. The user may also specify any irradiation and cooling time history. The input format is fashioned around the existing depletion (SAS2H) and criticality (CSAS) sequences of SCALE. Only a minimal amount of input beyond that typically required for a fresh-fuel calculation is needed to perform a burnup credit calculation using STARBUCS.

A search capability is also being developed for STARBUCS. This feature generates cask loading curves that define acceptable spent fuel enrichment and burnup combinations in an automated manner. The search performs multiple STARBUCS calculations, adjusting a fuel parameter (e.g., enrichment) until a desired k_{eff} value is obtained. The CPU time required on current generation workstations is about 1 hour for a typical cask calculation. A loading curve of 10 points, requiring approximately 5 iterations per point, can be generated in roughly 2 days of continuous computing.

STARBUCS is designed to assist in the analysis and review of criticality calculations involving burnup credit casks. However, the program is sufficiently general to allow virtually any configuration of spent fuel (e.g., a storage pool) to be simulated. Any KENO geometry model may be used in the burnup credit calculation. Options to generate MCNP formatted composition data are currently being considered.

Results using STARBUCS for a generic cask design will be presented at the 2001 ANS NCSD Embedded Topical Meeting in Reno. STARBUCS will be released with SCALE 5 in 2002.

SCALE Website Updates

Several files have been added or updated in the SCALE Download Directory on the web this year.

- KENO-VI - Some significant corrections and enhancements have been made to the code since its release in SCALE.4.4a. **All KENO-VI users are advised to obtain this update.**

  1) The code was modified to allow a unit in an array to contain a hole as its only region. **Prior to this fix, the code might run and give erroneous results.** A media record that assigns a material to the region is still recommended.

  2) An error was corrected where several identical fuel assemblies, all represented by the same unit number were loaded into an array. **The k-eff for this case was approximately 25% low**. If each assembly in the array was represented by a unique unit number (each unit was identical), the correct calculated k-eff value was obtained.

  3) Three options were added to read from input or calculate approximately the geometry volumes so the fluxes and fission densities would be appropriately normalized.

  4) An error was corrected that caused a particle to go into an infinite loop due to a round-off error when trying to exit an array.

  5) An error 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.

  6) The code was corrected for a fatal error that occurred when the option to collect matrix information by array number at the highest array nesting level (HAL=YES) is activated.

- KMART - An option to plot activities and fluxes from the SCALE KMART post-processor for KENO V.a was included in KENO3D version 2.0. This capability requires an updated version of KMART for SCALE 4.4 or 4.4a that is now available to download.

- OrigenArp for Windows - Several corrections and improvements have been made to this new GUI. The version on the website is identical to the one released in the RSICC ORIGEN-ARP package.

- OPUS and PlotOPUS - Several corrections have also been made to these ORIGEN post-processing and plotting codes. The versions on the website are identical to those in the RSICC ORIGEN-ARP package.

- Updated files for SCALE on Windows PCs - These updated files allow SCALE 4.4 or 4.4a to run correctly on Windows 2000 and Millennium Edition (ME) platforms. They also include the new OPUS utility to generate ORIGEN-S plot data files and updated files for all versions of Windows to automatically copy ORIGEN-S plot data files generated by OPUS and color GIF plot files generated by PICTURE to the user's directory.

One report has been added to the SCALE Validation web page

- *Verification and Validation of the ORIGEN-S Code and Nuclear Data Libraries* (RC-1429, COG-I-95-150) - Atomic Energy of Canada Limited (AECL) has approved posting of this document on the Oak Ridge National Laboratory SCALE website with the understanding that it has not been edited for wide publication.

SCALE Training Courses

The SCALE staff is offering both criticality safety and radiation source terms/shielding training courses at ORNL in October 2001. The courses emphasize hands-on experience solving practical problems on PCs. No prior experience in the use of SCALE is required to attend. The registration fee is $1800 for one course or $3000 for both courses ($300 discount if you register by September 21, 2001). A copy of the SCALE software and manual on CD may be obtained for an additional fee of $450. 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 may be paid by check, electronic bank transfer, or credit card (Visa or MasterCard only). The agenda and registration form are included in this issue.

Words to the Wise...

Correct Temperature Data Are Important

In a recent SCALE training course, participants running one of the SAS2 class problems obtained good agreement on the gamma source, but the neutron source was approximately 35 % high. After a thorough review, our staff read a warning message in the output that helped identify the problem:

MP-21 ***WARNING* Standard composition card number 12 implies that mixture number 3 has a temperature of 550 degrees Kelvin, whereas standard composition specification card 13 implies that mixture number 3 has a temperature of 900 degrees Kelvin. (One of these may have been the value specified by default.) The code will assume the higher of the two and proceed. If this is not satisfactory, the user should enter the correct temperature on each of the standard composition specification cards indicated.**

The users had put a trace quantity of Co-59 in the water (a recommended practice), along with boron (500 ppm). The temperature of Co-59 was inadvertently entered with the **fuel temperature** instead of the **water temperature**. As a result, the code increased the temperature of the boron and water to that of the fuel and ran the case. The increased temperature of the hydrogen scattering kernel hardened the spectrum considerably and resulted in a higher neutron source.

Note that this same type of error could occur in other SCALE modules, such as CSAS. The lessons here are hopefully obvious: (1) carefully check your input for consistency in temperature data for compositions that are part of the same mixture, and (2) carefully check your output for warning messages.

SCALE on Windows 2000 and Millennium Edition (ME) PC's

SCALE 4.4a was released prior to Microsoft Windows Millennium Edition (ME), and SCALE 4.4 was released prior to Windows 2000 and ME. SCALE 4.4 and 4.4a users can download updated files for SCALE on all versions of Windows from the SCALE Download web page. See the "SCALE Website Updates" article for more information.

SAS2 Error Messages

If a SAS2 case contains a downtime of zero at the end of a cycle, the following message may appear in the ORIGEN-S output:

Error in input, delta t is negative, m = *x*

The message occurs because the final downtime is zero, and SAS2 incorrectly applies a negative value of 10^{-19} days. In most instances, the calculation will continue normally and the results should be correct. However, other cases may fail. This error has been corrected in SCALE 5. A workaround for this error is to specify a very small positive downtime (e.g., DOWN=0.001) in the SAS2 input.

A SAS2 error message that routinely appears in the output is

Warning, error in lib. on unit *xx*
for id. no. 999
za no. (id(xx)) is 0.
Its number density is not updated.

This message can be ignored. It is not an error. The message is written during conversion of excited state nuclide IDs from the SCALE cross-section library to ORIGEN-S nuclide IDs. It assumes all nuclides have valid ZA numbers. The pseudo nuclide 1/VABSORBER with an ID of 999 is identified as an invalid nuclide. SAS2 has been corrected to skip the message for this pseudo nuclide in SCALE 5.

SAS4 Minor Errors

SAS4 users should be aware of two minor errors that have been recently identified. These errors will be corrected in SCALE5.

The first error occurs if the user fails to input a value for TMAX (maximum CPU time). The program fails to initialize TMAX, and the job typically terminates immediately because TMAX=0. The workaround for this problem is to always specify a value for TMAX in the input.

The second error is in SUBROUTINE IMPREG where an undefined unit number is passed to an error subroutine for use in printing an error message. The common block LUNIT is missing. The fix for this discrepancy is to add the following statement to SUBROUTINE IMPREG.

COMMON /LUNIT/ INN, IOUT, N12(14)

SCALE Minor Modifications

The following minor modifications have been made to SCALE this year.

ORIGEN-S: The code was updated to (1) improve the calculation of concentrations of nuclides following the removal of short-lived nuclides to make a reduced transition matrix and (2) correct the determination of the matrix norm. The value of the matrix norm is used in the determination of which short-lived nuclides are removed from the matrix, and in establishing the number of exponential terms required for series convergence. (3) FIDO and debugging printout were redirected to a temporary file named _fido000 to reduce and clean up the output. (4) The precision in the printed output was increased from three to four digits. (5) The number of expansion terms in the matrix solution was increased by one to eliminate messages in the output that the maximum error in the matrix exceeded 0.1%. This change is consistent with ORIGEN2. (6) Calls to an internal subroutine named EXIT were removed to avoid conflicts with the SCALE subroutine library. (7) A "STOP" was added for cases where the change in time between timesteps is negative. These modifications have been incorporated in the verison of ORIGEN-S included in the new RSICC ORIGEN-ARP package.
(MRRs 00-003, 01-001)

OPUS: This new SCALE utility module is designed to read ORIGEN-S generated data and produce output data tables in a format that is easily read by the plotting program PlotOPUS. The plot and print file formats have been modified to accommodate cases with large numbers of timesteps.
(MRRs 00-015, 01-003)

ARP: The code was updated to correct a divide-by-zero error in the burnup interpolation algorithm that could occur in very rare circumstances. (MRR 01-002)

GENWGTS/GWAS: The code was updated for compatibility with the current version of XSDRNPM. Changes made to XSDRNPM in MRR98-065 required changes to read the XSDRNPM data needed to generate biasing weights for KENO. (MRRs 99-032, 99-033)

OPUS sample problems: Ten sample problems for the ORIGEN-S post-processing utility OPUS were added to SCALE. (DRR 01-001)

Upcoming Professional Meetings

- **Nuclear Criticality Safety Division Topical Meeting (November 11–15, 2001)**

  The Nuclear Criticality Safety Division of the American Nuclear Society invites you to attend its 6th topical meeting to be held in Reno, Nevada in November 2001. The meeting will be an embedded topical held along with the ANS Winter Meeting. The theme of the meeting will be **Practical Implementation of Nuclear Criticality Safety**. The meeting will focus on the challenges and changes that are taking place within the field of criticality safety and how these will be implemented in the design of new facilities, the operation of existing processes, and in technical areas such as burnup credit, decommissioning, and waste storage. The purpose of the meeting is to provide a forum to exchange information on current developments in nuclear criticality safety. It will provide an opportunity for the industry and the regulators to exchange views and experiences. For more information, visit the meeting website at http://ncsd.ans.org/topical.

- **Radiation Protection and Shielding Topical Meeting (April 14–17, 2002)**

  The 12th Biennial Topical Meeting of the Radiation Protection and Shielding Division of the American Nuclear Society (ANS) will be held in Santa Fe, New Mexico, on April 14–17, 2002. This meeting is hosted by the ANS Trinity Section and cosponsored by the Health Physics Society (HPS), OECD/AEN, and RSICC. Abstracts of 250 words are due by October 1, 2001. For more information, visit the meeting website at http://www.lanl.gov/RPSD2002.

SCALE 2001 Training Course Registration Form

Oak Ridge National Laboratory, Oak Ridge, Tennessee

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

I am registering for:			**Before Sept. 21**	**After Sept. 21**
☐ **Source Terms and Shielding Course (Oct. 15–19)**			Fee: $1,500	Fee: $1,800
☐ **KENO V.a Course (Oct. 22–26)**			Fee: 1,500	Fee: 1,800
☐ **Both Courses**			Fee: 2,700	Fee: 3,000
SCALE 4.4a on CD	☐ **Yes**	☐ **No**	Fee: 450	Fee: 450
KENO3D (single license)	☐ **Yes**	☐ **No**	Fee: 550	Fee: 550

Total Fee $ _____

Name _____

Citizenship _____

Organization _____

Mailing address _____

_____

_____

E-mail _____ **Telephone** _____ **Fax** _____

Your level of experience (circle one)	Very High	High	Medium	Low	None
Criticality					
CSAS/KENO V.a	4	3	2	1	0
Other_____	4	3	2	1	0
Source Terms/Depletion					
SAS2	4	3	2	1	0
ORIGEN-ARP/ ORIGEN-S	4	3	2	1	0
Other_____	4	3	2	1	0
Shielding					
SAS1	4	3	2	1	0
SAS3/SAS4/MORSE	4	3	2	1	0
QADS/QAD-CGGP	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 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: scalehelp@ornl.gov

Classes may be canceled if minimum enrollment is not obtained.

Course fees are refundable up to one month before each class.

Foreign Nationals must register at least 8 weeks in advance.

SCALE Source Terms and Shielding Course Agenda

(October 15–19, 2001)

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

Thursday
SAS4 3-D Shielding Sequence
SAS4 Variance Reduction Techniques
SAS4 MARS Geometry Option
SAS4 Validation/Limitations
SAS4/ESPN Demonstration
SAS4 Problem Definitions
SAS4 Problem Session

Friday
QADS 3-D Point Kernel Shielding Analysis Sequence
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 that they bring.

SCALE KENO V.a Course Agenda

(October 22–26, 2001)

Monday
Overview of SCALE System
Introduction to CSAS
Standard Composition Library
Material Information Processor Library
Resonance Self-Shielding
Unit Cell Geometry - Lattice Cell/Multiregion
CSPAN Demo
Problem Session 1

Tuesday
Review of Problem Session 1
KENO V.a Parameters
KENO V.a Geometry
KENO V.a Plot Data
Problem Session 2

Wednesday
Review of Problem Session 2
Introduction to KENO V.a Output
KENO3D Tutorial
HOLEs
Arrays
Problem Session 3

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

Friday
Review of Problem Session 4
Monte Carlo Uncertainties
Code and Data Validation Issues
KENO V.a Course Wrap-up

The course will conclude with lunch on Friday.

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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.

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Managed by UT-Battelle, LLC, for the U.S. Department of Energy under contract DE-AC05-00OR22725.