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NEW ENHANCEMENTS TO SCALE FOR CRITICALITY SAFETY ANALYSIS

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ABSTRACT

As the speed, available memory, and reliability of computer hardware increases and the cost decreases, the complexity and usability of computer software will increase, taking advantage of the new hardware capabilities. Computer programs today must be more flexible and user friendly than those of the past. Within available resources, the SCALE staff at Oak Ridge National Laboratory (ORNL) is committed to upgrading its computer codes to keep pace with the current level of technology. This paper examines recent additions and enhancements to the criticality safety analysis sections of the SCALE code package [1]. These recent additions and enhancements made to SCALE can be divided into nine categories: (1) new analytical computer codes, (2) new cross-section libraries, (3) new criticality search sequences, (4) enhanced graphical capabilities, (5) additional KENO enhancements, (6) enhanced resonance processing capabilities, (7) enhanced material information processing capabilities, (8) portability of the SCALE code package, and (9) other minor enhancements, modifications, and corrections to SCALE. Each of these additions and enhancements to the criticality safety analysis capabilities of the SCALE code system are discussed below.

NEW ANALYTICAL COMPUTER CODES

A new version of the KENO series of Monte Carlo criticality safety computer codes called KENO-VI [2] has been added to the version 4.3 release of SCALE. A lengthy set of simple, easy-to-use geometric functions, similar to those provided in KENO-V.a [3], and the ability to build more complex geometric shapes (represented by sets of quadratic equations) are the heart of the geometry package in KENO-VI. The code's flexibility 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 translated to any position; and the use of an array boundary that intersects the array. Accompanying KENO-VI will be CSAS6, a new version of the SCALE Criticality Safety Analysis Sequence especially designed to automate the preparation of problem-dependent cross sections and analysis of problems with KENO-VI.

KENO-VI maintains all the flexibility and options of KENO-V.a plus a variety of new options. In KENO-VI, units can be constructed using both the simple geometric shapes provided and the tailored geometric shapes constructed using quadratic equations. KENO-VI and CSAS6 will include the new two-dimensional (2-D) color plotting capability that has been added to KENO-V.a as well as any new material information processing capabilities added to the existing criticality sequences. KENO-VI can be run stand-alone or as part of the SCALE Criticality Safety Analysis Sequence CSAS6.

Users should be aware that the added geometry features in KENO-VI can result in significantly longer run times than KENO-V.a. A KENO-VI problem that can be modeled with KENO-V.a will typically run twice as

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long as the same problem using KENO-V.a. Thus KENO-VI should not be viewed as a replacement for the existing KENO-V.a, but as an additional version for complex geometries that could not be modeled precisely in KENO-V.a.

NEW CROSS-SECTION LIBRARIES

New cross-section libraries released for use with SCALE-4.3 in 1995 include a 238-group library [4] and a 44-group library derivative from the 238-group library [5] containing approximately 300 sets of nuclide data processed from version 5 of the Evaluated Nuclear Data Files (ENDF/B-V). These two libraries will replace the 123-group GAM-THERMOS library and 218-group ENDF/B-IV library in SCALE-4.3. The 123GROUP and 218GROUP cross-section-library keywords were replaced with 44GROUP and 238GROUP keywords. The former libraries, which were the least used of the standard SCALE libraries, were removed as defaults so the new ENDF/B-V libraries, which give more accurate results, could be accessed directly via keyword input.

Several ENDF/B-VI nuclides including ^{16}O, ^{154}Eu, and ^{155}Eu were added to these libraries as the default. Analyses of benchmark critical experiments indicated a bias as a function of leakage that was mitigated using ENDF/B-VI ^{16}O data. The europium ENDF/B-VI data contain significant resonance structures not available in the ENDF/B-V data. Several nuclides also have multiple entries with different thermal-scattering law data. Data are available for hydrogen bound in water, polyethylene, benzene, and as a free gas. Deuterium is available bound in D_2O and as a free gas. Carbon is available using thermal graphite data and as a free gas. Thermal-scattering data for moderator materials such as hydrogen and graphite are available in these libraries at all temperatures available in ENDF/B-V.

The 238-group library was generated using AMPX-77 [6]. Resolved resonance parameters are included to account for the resolved resonance range. All resonance levels available in ENDF/B-V (s-, p-, and d-wave) are included in the library. Bondarenko shielding factors are included to account for the unresolved resonance range. Resonance structure in some light-to-intermediate mass nuclides such as ^{7}Li, ^{28}Si, ^{19}F, and ^{27}Al, and the Adler-Adler resonance data in ^{233}U and ^{241}Pu, are also accounted for using Bondarenko shielding factors. The resonance structure in these intermediate mass nuclides, as well as p-wave and d-wave resonances which were added, become important in problems where a large percentage of neutrons undergo fission in the intermediate energy range.

The 44-group library was collapsed from the 238-group library using a pressurized-water-reactor (PWR) fuel pin spectrum and was designed specifically for light-water-reactor (LWR) applications. This broad-group library has a similar group structure to the 27-group ENDF/B-IV library. Additional groups were added to accommodate two windows in the oxygen cross section and a window in the iron cross section, to add better definition for the Maxwellian thermal peak, and to provide structure across the broad 0.3-eV resonance in ^{239}Pu.

Another new library available for SCALE users is the VITAMIN-B6 199-group ENDF/B-VI library [7]. The group structure for this library has been enhanced from the VITAMIN-E 174-group ENDF/B-V library [8] to better cover the thermal range. Unfortunately ENDF/B-VI data cannot currently be processed using AMPX. NJOY [9], which uses the narrow resonance approximation, was used to produce multigroup cross sections for the nuclides. All resonance structures in the VITAMIN-B6 library are therefore represented using Bondarenko data. The VITAMIN-B6 library, which is linked to a 42-group gamma library, was produced for use with shielding codes. The narrow resonance approximation, which has proven satisfactory for shielding analysis, can produce unreliable results for criticality

calculations. Broad resonances such as those that occur in some nuclides near thermal energies are not satisfactorily represented using the narrow resonance approximation. Therefore, the use of the VITAMIN-B6 library is not recommended for criticality calculations without an extensive validation for the type of problems being analyzed.

NEW CRITICALITY SEARCH SEQUENCES

A new search feature has been added to the criticality search sequences in SCALE. Searches may now be done on the concentration of standard compositions in one or more mixtures in the problem. During a concentration search, if the search convergence criteria have not been met, the atom densities of the specified standard compositions are updated, problem-dependent resonance processing is performed using BONAMI, NITAWL, and applicable sections of the material information processor, and a new k_{eff} is calculated using KENO-V.a. Concentration searches cannot be performed on materials contained in cell-weighted mixtures.

In all search sequences (both geometry and concentration), problem-dependent resonance processing of the cross sections is now performed for each iteration prior to the execution of KENO. Heterogeneous effects, Dancoff factors, and self-shielding are now accounted for between iterations. Prior to the addition of concentration searches, a search sequence would update only the specified geometry, but not the cross sections, prior to calculating a new k_{eff} using KENO-V.a. Previously, to ensure the converged result was acceptable, the problem needed to be rerun with the converged geometry data. The recent changes to the search sequences eliminate the need to rerun a converged problem to account for changes in cross sections.

ENHANCED GRAPHICAL CAPABILITIES

The graphical display of KENO-V.a and KENO-VI geometry models has been dramatically improved by the new capability to produce high-resolution 2-D color plot files that can be viewed on-screen using appropriate viewer software or printed on a color printer. This new option is activated by using the parameter scr=yes in the KENO plot data. A plot file using up to 256 colors is generated. The plot data parameter "clr=" can be used to override the default color assignments. These plots can only be generated on UNIX workstations and MS-DOS-based personal computers (PC). When using this option, each individual fuel rod and water hole can be clearly seen in LWR fuel assemblies loaded in a cask (see Fig. 1).

In addition to the 2-D color plots, fractional values are now valid for the lpi= parameter in the plot data, which will make it easier to print circles on laser printers.

KENO-V.a ENHANCEMENTS

Enhancements to KENO-V.a fall into one of three categories: removed limitations, editing changes, or added capabilities.

Two independent limitations to KENO-V.a were removed. The first limitation involved HOLE boundaries touching other HOLE or adjacent geometry region boundaries. Significant errors in k_{eff} (as much as 1%) occurred when HOLE boundaries touched with no indication of a problem. HOLE boundaries may now touch other HOLE or adjacent geometry region boundaries.

The second limitation involved the number of scattering angles allowed. Although the parameter sct= (number of scattering angles) was limited to 13, no check was made to avoid overstoring data. Any number of scattering angles are now allowed.

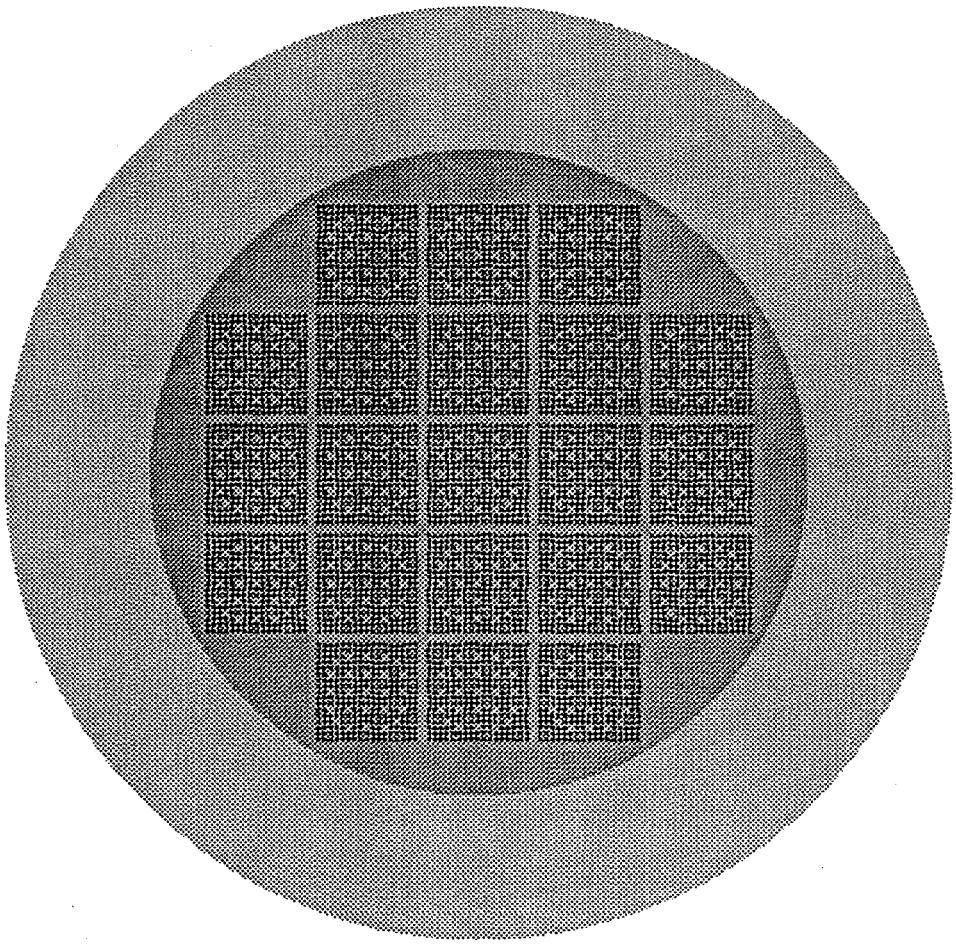

Figure 1. Spent fuel shipping cask

The mixing table edit has been changed to sort mixture data by mixture number. The mixture number and density make up the first line of the data for each mixture. The following lines, which represent the nuclides in the mixture, are sorted by nuclide number. Each line contains a nuclide number, atom density, weight fraction, ZA number, atomic weight, and nuclide title. This provides the user a concise table of the components that make up the mixtures used in the problem.

Three new capabilities were also added to KENO-V.a which provide the user with useful information for analyzing and checking the problem.

The energy corresponding to the average lethargy causing fission is now calculated and the printing of this information (i.e., NUB=YES) is now a default parameter. This is useful for determining trends in k_{eff} as a function of neutron energy to look for problem type biases.

System total fissions and absorptions by region are now calculated. A parameter to suppress printing fissions and absorptions by region for each group has been added. Set GAS=NO to print only the system totals by group. These values have several uses such as helping to verify proper problem sampling and determine region importance.

Finally, the total mass of each mixture in the problem is now calculated and printed. This can be used to help verify the geometry and material masses of the problem.

ENHANCED RESONANCE PROCESSING CAPABILITIES

In order to access the p-wave and d-wave resonance data in the ENDF/B-V libraries and improve the resonance processing in SCALE, major enhancements were made to the NITAWL-II code [10]. These enhancements included performing resonance calculations in double precision and modifications to the mesh generation over a resonance energy to better span higher energy resonances and to reduce excessive numbers of mesh points.

In addition, this new version of NITAWL-II is able to interpolate the available thermal-scattering matrices to obtain data for the temperature requested by user input (via direct input to NITAWL-II or via the SCALE Standard Composition data). Previously, NITAWL-II had no such capability and selected the thermal-scattering data that were closest to the requested temperature. Even with the new ENDF/B-V libraries, which have data at more temperatures, interpolation should better determine the effect that a change in a given temperature will have on the system multiplication factor.

The CSAS control module also has been modified via MIPLIB to provide two new parameters in the optional MORE DATA input:

MLV= maximum L value for which resonance calculation will be done (L = 0 is s-wave, L = 1 includes p-wave, L = 2 includes d-wave). The default value is L = 2.

MSH= maximum number of mesh points per resonance. The default value is 2001.

Note that if NITAWL-II is run stand-alone, the default values for MLV and MSH are 0 and 501, respectively.

ENHANCED MATERIAL INFORMATION PROCESSING CAPABILITIES

The Standard Composition Library has been expanded for compatibility with ENDF/B-VI cross-section libraries. In addition, the Material Information Processor Library (MIPLIB) has also been updated so that all the control modules can use ENDF/B-VI cross-section libraries via the new expanded Standard Composition Library. The changes were necessary because cross-section data for natural-element identifiers are not available in the ENDF/B-VI data. Most problems set up to use current cross-section libraries should now run without any changes using SCALE-formatted (e.g., the VITAMIN-B6 library) ENDF/B-VI libraries.

The changes to the Standard Composition Library were very extensive and fall into several categories. Additions were made so that nearly all the elements are given by both their full name and by their chemical symbol. The full-name elements are all given as naturally occurring abundance nuclides. Most chemical symbols, such as FE, also represent naturally occurring nuclides; however, a few represent the principal isotope. For instance, HYDROGEN would include trace amounts of deuterium, while H would be 100% ^{1}H. The isotopic distribution table in the Standard Composition Library was changed to include most of the natural elements as well as a few specially weighted elements in stainless steel and Inconel.

Naturally occurring elements will now be mixed if they are not explicitly contained in the library. The material information processor uses the following default procedure. If isotopic data are provided by the user in the material input, those data are always used. If isotopic data are not provided by input but data are provided in the library for the naturally occurring element, then that data will be used. Finally, if isotopic data are not specified and natural element data are not available in the library, a natural element will

be mixed using isotopic data from the Standard Composition Library.

Arbitrary materials may now contain more than one multiple-isotope nuclide and need not be the first nuclide listed in the arbitrary material. Also, although values for the multiple isotope indicator and resonance indicator must still be entered for arbitrary materials, these values are no longer used. Resonance processing is now set by MIPLIB via a check for resonance data on the cross-section library.

Atomic masses for isotopes were taken from ENDF/B-VI, if available. Atomic masses for naturally occurring elements were taken from ENDF/B-V, if available. Remaining atomic masses were taken from the GE Chart of the Nuclides [11] or the CRC Handbook of Chemistry and Physics [12].

PORTABILITY OF THE SCALE CODE PACKAGE

Due to the variety of workstations capable of using the SCALE code system, the source files in SCALE have been made less system-dependent to facilitate portability. When source differences are unavoidable due to system differences, the system-dependent aspects of the source are contained in special subroutines if possible. To facilitate the building and maintenance of version 4.3 of the SCALE system, MAKE files are now provided. The MAKE files contain all the commands needed to build and maintain the SCALE code system. Cross-section files are now being distributed as binary files that can be directly used on many workstations. Finally, the programming in SCALE is undergoing a slow migration to FORTRAN-90 as time and resources allow. SCALE has been successfully compiled with the FORTRAN-90 compiler on an IBM AIX workstation.

A MS-DOS PC-version of SCALE named SCALE-PC that contains all the capabilities of the workstation version is also available. Only the broad-group libraries will be made available at this time for SCALE-PC due to the length of these files. Currently, SCALE-PC is distributed on floppy disk but future plans are to distribute it on CD-ROM.

OTHER MINOR ENHANCEMENTS, MODIFICATIONS, AND CORRECTIONS TO SCALE

SCALE-4.2 Minor Modifications

Cross-Section Libraries: The atomic masses of several nuclides were modified to ensure all nuclide masses are in terms of neutron mass.

Standard Composition Library

1. Revised the resonance energy scattering and/or total cross sections for 197 materials based on the 44-group ENDF/B-V cross-section library. Consistent values were specified for both the natural elements and the individual isotopes of B, Zr, Eu, Hf, and W.

2. Added new composition name ZIRC2 for Zircaloy-2 to use with ENDF/B-V cross-section libraries. Cross-section data for Zircaloy-2 were available in ENDF/B-IV, but not in ENDF/B-V. This composition accesses the data for the individual nuclides.

MIPLIB, Material Information Processor

1. Added checks to avoid the use of negative number densities when solutions with physically unrealistic parameters are entered.

XSDRNPM

1. Modified to scale the weighting flux so that minimum value is 1E-20. This modification was made to reduce the likelihood that an underflow would occur when creating a weighted cross-section library for problems where there are large

variations in the flux (many orders of magnitude).

SUMMARY

The above-mentioned additions and enhancements represent the continuous effort at ORNL to provide the criticality safety community with state-of-the-art software. SCALE-4.3 is the latest in a series of upgrades to SCALE-4, which was released in 1990.

A geometry package capable of precisely modeling more complex modes has been added to SCALE via the CSAS6/KENO-VI analysis sequence. An option to search for the material concentration that yields a specified k_{eff} condition for a problem has been added to the existing CSAS/KENO-V.a sequence. The new concentration search and the previously available unit spacing search have been improved to modify the cross sections to represent the changing conditions during the search. Two-dimensional color plots of the KENO-V.a and KENO-VI geometries are available on-screen or via a color printer. Updated cross-section libraries and improvements in the automated, problem-dependent, cross-section processing in SCALE have expanded the versatility of the system to enable accurate analysis of problems where the complete resonance structure (resolved and unresolved) is important.

The criticality sequences within the SCALE system will continue to be improved. A prototype of a new sequence that has a new resonance-processing code called CENTRM is now being tested. CENTRM is a one-dimensional (1-D) deterministic code that calculates a pointwise flux in the resonance region for subsequent use in preparation of problem-dependent multigroup cross sections for a KENO-V.a calculation of k_{eff}. Work will begin in FY 1996 on development of a point cross-section version of KENO and a three-dimensional (3-D) graphics capability for visualization of geometry models.

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