SCALE-4: An Improved Computational System for Spent-Fuel Cask Analysis

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INTRODUCTION

Accurate criticality, shielding, and heat transfer analysis of shipping casks containing spent fuel or high-level waste (HLW) can be a challenging endeavor. In the 1960s and 1970s, this analysis experience was sometimes more frustrating than challenging. Accurate analysis typically mandated the use of large, complex computer codes that often required preprocessing of physics data, provided limited geometry modeling capabilities, and were designed for use by computational experts. The Transportation Branch of the U.S. Nuclear Regulatory Commission (NRC) recognized the need to obtain accurate results (for license evaluation) in a consistent manner, but could not justify the staff time required to become expert code users and remain such via routine use. Thus, the NRC staff requested Oak Ridge National Laboratory (ORNL) to develop a computational system that would (1) use well-established computer codes and data libraries, (2) have an input format designed for the occasional user and/or novice, (3) combine and automate analyses requiring multiple computer codes or calculations into standard analytic sequences, and (4) be well documented and publicly available.

With these goals in mind, the NRC and ORNL staff formulated the framework for a modular code system (SCALE) that would provide Standardized Computer Analyses for Licensing Evaluation. The major applications of interest to the NRC staff were nuclear facility and package designs. Since the initial release of SCALE in 1980, the code system has been heavily used by the NRC, Department of Energy contractors, and industry to perform criticality, shielding, and thermal analyses of transport package designs. The capabilities within the SCALE system (NUREG/CR-0200 1984) have also made it a favorite for use in a large number of other problem areas where criticality, shielding, or heat transfer analyses are required.

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The purpose of this paper is to provide specific information regarding the improvements available with Version 4.0 of the SCALE system and discuss the future of SCALE within the current computing and regulatory environment. The emphasis focuses on the improvements in SCALE-4 over that available in SCALE-3. A more detailed familiarization with the complete SCALE system can be found elsewhere (Parks 1987).

SYSTEM PORTABILITY

One of the more significant improvements made available by SCALE-4 is conversion of the FORTRAN to enable compilation with FORTRAN-77 compilers provided on the IBM-3033 and CRAY/X-MP at ORNL. Because of the additional functionality provided by these compilers, it was possible to replace many of the IBM assembler language routines provided in the system subroutine library with FORTRAN versions. In addition, the graphics codes have been updated to use Version 10.5 of the DISSPLA graphics package (*DISSPLA User's Manual* 1984/1985) rather than the outdated Version 8.2. Each module of the SCALE-4 system has been made operable on both the Cray and IBM computers at ORNL. These efforts should provide a software system that is more portable between different operating systems and computers.

FUNCTIONAL MODULES

The functional modules within SCALE are the individual codes selected or developed to provide the specific capabilities required to solve the problems of interest. One of the more noticeable changes in the SCALE-4 functional modules is the deletion of the Monte Carlo criticality code KENO IV and the geometry plotting module JUNEBUG. The functionality provided by KENO IV is available in the KENO V.a code that was also released with earlier versions of SCALE. The JUNEBUG package was deleted because of its inefficiencies coupled with the difficulties encountered in conversion to FORTRAN 77. The capabilities of the two new functional modules provided with SCALE-4 are briefly summarized below, together with the modules that have been improved significantly since the SCALE-3 release.

- ORIGEN-S performs point depletion and decay analyses to obtain isotopic concentrations, decay heat source terms, and radiation source spectra and strengths for use in subsequent system analyses. The SCALE-4 version of ORIGEN-S has been updated to provide the strength and spectra of neutrons from (α,n) reactions within borosilicate glass mixtures containing reprocessed HLW. The (α,n) component of the total source is less than 3% for five-year-cooled UO_2 fuel but rises to 35-40% for HLW in borosilicate glass.

- PLORIGEN is a new module that allows plots of ORIGEN-S output via the DISSPLA 10.5 graphics package. Isotopic concentrations, decay heat, and radiation source spectra can all be plotted in selected units and over selected decay time intervals.

- HEATING6.1 is an updated version of the HEATING6 finite-difference heat transfer code. The new version allows two- and three-dimensional (2-D and 3-D) radiation via the use of node-to-node connectors, 2- and 3-D spherical geometries, and a shared nodal location philosophy that allows full closure on cylindrical and spherical models (e.g., the same node can be used at 0° and 360°).

- OCULAR is a radiation exchange factor computer code compatible with the axisymmetric R-Z geometry of HEATING6.1. The code may be used to generate gray body exchange factors, as well as geometric configuration factors, which describe the radiative exchange in the cylindrical or annular enclosures that are characteristic of an axisymmetric cask geometry.

- NITAWL-II is an updated version of the NITAWL code that performs resonance self-shielding calculations using the Nordheim Integral Treatment. In NITAWL-II, the self-shielding is made with reference to infinite dilution values, a procedure that greatly

simplifies the base processing codes and allows one to make a Nordheim calculation that can be used with any input cross-section library containing the reference infinite dilution values. NITAWL-II also allows one to selectively pick which resonances or kinds of resonances are to be processed, without requiring the basic input library to be regenerated.

Many of the functional modules have been updated to fix inconsistencies or errors and/or enhance the user interface or calculational efficiency.

CONTROL MODULES

Although back-to-back execution of the individual functional modules is possible within SCALE, the overall goal of the developmental effort was to provide analysis sequences that automate the necessary data processing and manipulate the sequencing of individual module execution to accurately solve the problem of interest. The SCALE user is able to select (via a keyword) an analysis sequence characterized by the type of analysis (criticality, shielding, or heat transfer) to be performed and the geometric complexity of the system being analyzed. The user then prepares a single set of input for the control module corresponding to this analysis sequence. The control modules use this information to derive additional parameters and prepare the input for each of the functional modules in the analysis sequence.

Criticality Sequences

The CSAS4 control module provides all the criticality safety analysis sequences available in SCALE-4. The various analysis sequences within this control module are shown in Table 1 and have not changed from those provided with SCALE-3. Note that there are several sequences that generate processed cross-section data for subsequent use by individual functional modules. The only notable improvement in the sequences is that the search convergence for the CSAS4 and CSAS4X sequences have been significantly improved.

Shielding Sequences

Two new shielding analysis sequences are being provided with the SCALE-4 release. The SAS1 control module is a new module designed to enable general (not limited to spent-fuel cask applications) 1-D shielding analyses to be performed without requiring the user to be experienced in the use of each functional module. As with all the shielding and criticality control modules of SCALE, SAS1 uses the Material Information Processor to enable simplified input material specifications and automate the cross-section processing. Resonance self-shielding is performed by the Bondarenko factor method (BONAMI-S) or the Nordheim integral treatment (NITAWL-II). The XSDRNPM-S module may be used to optionally produce cell-weighted cross sections prior to simulation of the radiation transport through a slab, sphere, or cylindrical shield model. The XSDOSE functional module uses the surface flux from XSDRNPM-S to generate dose rates at points on or at some distance from a finite portion of the shield.

The SAS1 control module allows source spectra to be input from cards and/or an ORIGEN-S output file. The latter option was added to allow easy input of the neutron and gamma source spectra calculated by ORIGEN-S for spent-fuel assemblies and/or other radiation sources. Neutron, gamma, or coupled neutron-gamma libraries and sources may be used. Source spectra from cards or the ORIGEN-S output file can be specified for more than one material zone.

The second new shielding control module is called SAS4. The SAS3 sequence in SCALE provides automated data processing for subsequent execution of the Monte Carlo shielding code, MORSE-SGC. However, in Monte Carlo shielding analysis of a deep-penetration problem such as a spent-fuel cask, variance reduction techniques must be employed in order to calculate good results at an affordable cost. Generation of biasing parameters and application of the parameters to solve a particular problem are no trivial tasks. Nevertheless, a systematic approach has been developed

recently for automatically biasing a Monte Carlo transport calculation of a spent-fuel cask (Tang and Hoffman 1988). This approach uses adjoint fluxes from a 1-D discrete ordinates calculation with the XSDRNPM-S code to generate the biasing parameters for a Monte Carlo analysis by the MORSE-SGC/S code. The entire procedure for cross-section preparation, adjoint flux calculation, automatic generation of Monte Carlo biasing parameters, and a Monte Carlo calculation has been implemented in the new SAS4 control module. The module provides calculated radiation dose levels exterior to a multidimensional cask model. All necessary biasing parameters are derived from results of the adjoint XSDRNPM-S calculation. Then SAS4 automatically inputs the biasing parameters to MORSE-SGC/S so that the user is rid of this difficult input task.

A generic cask model has also been developed for SAS4 in order to implement the automated biasing procedure and a simplified cask geometry input option. The cask model is required to be symmetrical about the cask midplane. The cask model allows easy specification of the axial and radial shield zones, axial impact limiters, and the cask basket. By option, the SAS4 module allows specification of a homogenized source region or a detailed heterogeneous model. The source energy spectrum is provided to SAS4 either by direct input or is read from an ORIGEN-S output file.

Both the SAS1 and SAS4 control modules have been heavily tested and used at ORNL since 1985. In particular, work performed in support of an international comparison study (Parks et al. 1988) has demonstrated the validity of these sequences for cask applications.

Depletion Sequence

The SAS2 control module was originally developed for SCALE to provide a sequence that generated radiation source terms for spent fuel and subsequently utilized these sources within a 1-D shielding analysis of a shipping cask. Although the shielding portion of the sequence can still be accessed, the principal use of SAS2 over its history has been fuel depletion analysis to obtain radiation sources, decay heat, and spent-fuel isotopics for use in subsequent analyses. (Note: The sequence can be halted after the depletion/decay portion is complete.) When calculation of radiation sources was the prime objective, a unit fuel-pin cell could be used to obtain the burnup-dependent flux spectrum necessary to adjust the cross sections during the reactor depletion analysis. This simple procedure has been shown to produce conservative actinide inventories for pressurized-water reactor (PWR) spent fuel and does not provide the flexibility required for depletion of boiling-water reactor (BWR) fuel (Ryman et al. 1982). Thus, the original SAS2 sequence has been considerably enhanced to produce the SCALE-4 version which will be donated SAS2H.

For each time-dependent fuel composition, SAS2H performs 1-D neutron transport analysis (via XSDRNPM-S) of the reactor fuel assembly using a two-part procedure utilizing two separate unit-cell-lattice models. The first model is a unit fuel-pin cell from which cell-weighted cross sections are obtained. The second model represents a larger unit cell (e.g., an assembly) within an infinite lattice. Two examples of the larger unit cells are depicted in Figure 1. Diagram (A) applies to a PWR control rod assembly. Variations to diagram (B) (e.g., omitting the casing and channel moderator) would apply to different types of BWR or PWR assemblies. The essential rule in deriving the zone radii is to maintain the conservation of all zone-type volumes of the actual assembly.

The neutron flux obtained from the second (large) unit cell model is used to determine the appropriate nuclide cross sections for the specified burnup-dependent fuel composition. The cross sections derived in one burnup-dependent transport analysis are used in the depletion computation (via ORIGEN-S) that produces the next burnup-dependent fuel composition to be used in the next transport analysis. This sequence is repeated over the operating history of the reactor.

The validation of SAS2H performed to date has demonstrated good agreement with measured isotopic data (Parks 1987 and Parks 1989). Thus, the SAS2H method allows more accurate

isotopic results to be obtained for a wider variety of fuel assembly designs even though requiring only a small amount of additional input to that needed for previous SAS2 versions.

Heat Transfer Sequence

The HTAS1 control module was developed to generate the necessary HEATING input and automatically manipulate the module to perform a two-dimensional (R-Z) thermal analysis for a shipping cask during normal, fire, and post-fire conditions specified by the licensing regulation. With SCALE-4, the HTAS1 module has been updated to use HEATING6.1 and to incorporate multidimensional radiation in voided zones of the cask model.

DATA AND INFORMATION PROCESSING

The data base provided with the SCALE-4 release has been only slightly improved from that released with the earlier SCALE version. The major change of note is that the SCALE-4 cross-section libraries are consistent with NITAWL-II and will produce erroneous results when used with earlier NITAWL versions. Use of earlier SCALE libraries in NITAWL-II will generate an error message to the user. Minor corrections and additions to the Standard Composition Library data have also been made, and the code that creates this library (COMPOZ) has been altered to allow users to list the contents of the composition library that is being accessed.

Problem-dependent cross-section processing for all the criticality and shielding sequences is performed by accessing the Material Information Processor Library (MIPLIB). The function of MIPLIB is to read the input on material compositions and geometry pertinent to cross-section processing, access the Standard Composition Library to determine nuclide atom densities and resonance data, and establish the input and execution sequence for the required functional modules. The improvements made in MIPLIB are listed below.

- A corrected Dancoff factor used in resonance self-shielding was developed to more accurately account for the effect of "distant" lattice neighbors not included in the numerical integration technique. The effect of the correction can only be seen for problems where radiation transport to second and third neighbors in a lattice are of importance (Jordan et al. 1988).

- The procedure to generate nuclide number densities for solutions has been significantly improved.

- A library information table is printed by MIPLIB during each analysis sequence to identify the library(ies) accessed during the sequence.

- The density of a standard composition material can be input. This is a user convenience that eliminates the need to look up the theoretical density and calculate the correct volume fraction to input.

A new feature of SCALE-4 will be the inclusion of a special set of utility modules that will allow users to combine problem-dependent cross-section libraries or convert their non-SCALE cross-section libraries to obtain libraries with the format and nuclide identifiers required by the SCALE module. A utility module that will allow the contents of the library to be listed will also be provided.

DOCUMENTATION AND PUBLIC RELEASE

Due to extensive changes in the documentation, an entire new set of manuals is being prepared for the SCALE-4 release. Besides documentation on the new modules and document revisions for old modules, there will also be entirely new documentation for NITAWL-II, HEATING6.1, CSAS4, SAS2, MIPLIB, the cross-section and thermal properties data base, and the utility modules. The

documentation for the control modules and MIPLIB have sections that discuss the range of applicability and limitations of the sequences. These sections are an effort to provide additional guidance to the inexperienced user.

The current plans are for the SCALE-4 code to be provided to the Radiation Shielding Information Center (RSIC) at ORNL by October 1989. At this writing the code system is being assembled into a single production system, tested against verification problems, and brought under configuration control guidelines that will enable updates to be tracked in an accepted software quality assurance manner. Once the production system is verified, it will be provided to RSIC for preparation of the public code package.

FUTURE PLANS

With the release of SCALE-4, the analysis capabilities originally planned for the system ten years ago will be complete. However, there is interest at ORNL to (1) provide SCALE-compatible cross-section libraries that are based on ENDF/B-V or soon-to-be-released ENDF/B-VI data, (2) update the ORIGEN-S decay and fission yield data to ENDF/B-VI, (3) provide a "library" of verification and/or validation cases (Bryan et al. 1986) that allow users to easily verify and validate the particular SCALE package implemented on their system, and (4) develop a personal computer program that would allow input to the SCALE modules to be prepared in a user-friendly fashion with full-screen templates and interactive preliminary data checking. Initial work has also been performed on a three-dimensional heat transfer control module that evaluates fuel pin temperatures during the accident conditions specified by the NRC regulations (Wendel and Giles 1989).

It is not envisioned that any of the above work will significantly affect the SCALE-4 code package or documentation. The current thinking is to perform the above work and provide auxiliary packages to RSIC that can be obtained by users who desire updated cross sections, need guidance on verification and validation, and/or wish to use the template input screens.

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Table 1. Sequences provided in CSAS4 control module

Sequence keyword	Functional module sequence						Primary product
CSASN	BONAMI	NITAWL					Resonance-corrected cross sections
CSAS1X	BONAMI	NITAWL	XSDRNPM				1-D eigenvalue calculation
CSASI	BONAMI	NITAWL		ICE			Mixed, resonance-corrected cross sections
CSASIX	BONAMI	NITAWL	XSDRNPM	ICE			Mixed, cell-weighted cross sections
CSAS25	BONAMI	NITAWL			KENO V.a		k_{eff} value
CSAS2X	BONAMI	NITAWL	XSDRNPM		KENO V.a		k_{eff} value using homogenized cell
CSAS4	BONAMI	NITAWL			KENO V.a	MODIFY	Dimension alterations for optimum k_{eff}
CSAS4X	BONAMI	NITAWL	XSDRNPM		KENO V.a	MODIFY	Dimension alterations with homogenized cell

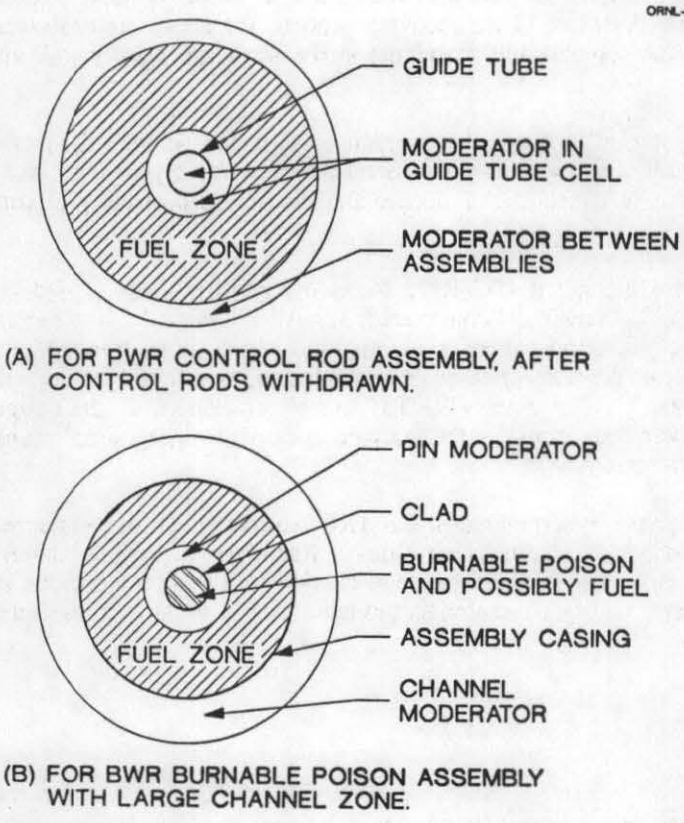

Figure 1. Unit cell models used in SAS2H depletion sequence.