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SCALE-PC SHIELDING ANALYSIS SEQUENCES

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ABSTRACT

The SCALE computational system is a modular code system for analyses of nuclear fuel facility and package designs. With the release of SCALE-PC Version 4.3, the radiation shielding analysis community now has the capability to execute the SCALE shielding analysis sequences contained in the control modules SAS1, SAS2, SAS3, and SAS4 on a MS-DOS personal computer (PC). In addition, SCALE-PC includes two new sequences, QADS and ORIGEN-ARP. The capabilities of each sequence are presented, along with example applications.

I. INTRODUCTION

The SCALE computational system[1] (Standardized Computer Analyses for Licensing Evaluation) is a modular code system developed at Oak Ridge National Laboratory (ORNL) for analyses of nuclear fuel facility and package designs. SCALE includes modules for performing criticality safety, shielding, depletion/decay, and heat transfer analyses. The system uses well-established computer codes referred to as functional modules that can be executed within standard analytic sequences contained in control modules. These sequences utilize an easy-to-use input format designed for the occasional or novice user and automate the data processing and coupling between functional modules.

With the release of SCALE-PC Version 4.3, the radiation shielding analysis community now has the capability to execute the SCALE shielding analysis sequences contained in the control modules SAS1, SAS2, SAS3, and SAS4 on a MS-DOS personal computer (PC). The prior release of SCALE-PC contained only the criticality safety analysis sequences. The PC version of SCALE is specifically designed for ease of installation and use on a PC platform. The package includes the program executables and binary versions of the cross-section libraries so the user does not have to compile any program or run any setup cases prior to using SCALE-PC; however, the FORTRAN source and complete makefiles are also included. The installation procedure is a simple batch file that creates the directory structure on the user's PC and installs all the necessary files by uncompressing them from self-extracting executables. The primary

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distribution media will be CD-ROM due to the size of the system, approximately 300 megabytes (MB). The minimum operating system requirements are a 386 PC with 8 MB RAM and MS-DOS 5.0 or later.

The shielding control modules of SCALE use 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) and/or the Nordheim integral treatment (NITAWL-II). In the SCALE system, a set of flux-to-dose-rate conversion values is provided in most of the SCALE cross-section libraries. The default dose factors used in the SCALE shielding sequences are the ANSI standard (ANSI/ANS-6.1.1-1977) neutron and gamma flux-to-dose-rate factors. Other dose factors can be specified. Sequences for radiation source generation and shielding are contained in the SCALE control modules Shielding Analysis Sequences 1 through 4 (SAS1, SAS2, SAS3, and SAS4). In addition, SCALE-PC includes two new sequences, QADS and ORIGEN-ARP. The ORIGEN-ARP sequence is available only in the PC version. The capabilities of each sequence will be presented, along with examples of their use.

II. SAS1, 1-D SHIELDING ANALYSIS

The SAS1 control module is designed to perform general one-dimensional (1-D) shielding analyses. The XSDRNPM module is a 1-D discrete-ordinates radiation transport code that can perform criticality or shielding calculations. In SAS1, it may be used optionally to produce cell-weighted cross sections prior to calculation of the radiation transport through a slab, sphere, or cylindrical shield model. The XSDOSE functional module uses the surface flux from XSDRNPM to generate dose rates at points on or at some distance from a finite portion of the shield.

The SAS1 control module can read the neutron and gamma source spectra directly from the input file 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 (using SAS2 or ORIGEN-ARP) for spent fuel assemblies and/or other radiation sources. Neutron, gamma, or coupled neutron-gamma libraries and sources may be used. Source spectra can be specified for more than one material zone. In addition to the dose rates available from the XSDOSE output of SAS1, the dose rates internal to the shield are always provided in the activity tables at the end of the XSDRNPM-S output.

SAS1 also provides a sequence where a leakage spectrum from a 1-D criticality calculation is used as a boundary source for a 1-D shielding analysis. This feature is useful for analysis of simple geometry criticality alarm systems or simulated criticality accidents, where a simple critical system can be modeled, and the resulting leakage automatically used as a source in a subsequent shielding calculation.

III. SAS2, SPENT FUEL DEPLETION/DECAY SOURCE TERM GENERATION

The SAS2 sequence, also referred to as SAS2H, performs nuclear fuel depletion/decay analysis. The principal uses of the sequence are to obtain radiation sources, decay heat, and spent fuel isotopics for use in subsequent shielding or criticality analyses. In addition, SAS2 can optionally use the radiation sources it calculates to perform a 1-D radial shielding analysis of a shipping cask using XSDRNPM and XSDOSE. Problem-dependent resonance processing of neutron cross sections is performed by SAS2 using the BONAMI and NITAWL-II modules. The XSDRNPM module is used to produce weighted and collapsed cross sections for the fuel-depletion calculations. Data from the weighted cross-section library and spectra

produced by XSDRNPM are used by the COUPLE module to update an ORIGEN-S nuclear data library and modify the ORIGEN-S spectral parameters. Any master AMPX cross-section library[2] with SCALE nuclide identifiers can be used by the SAS2 module. A new library available in SCALE-PC is the 44-group ENDF/B-V library which contains cross sections for all nuclides in ENDF/B-V. The ORIGEN-S data libraries (Sect. M7 of ref. 1) contain the half-lives, decay constants, fission yields, and Q-values, based on ENDF/B-VI data.

The ORIGEN-S module is a point-depletion code used for the depletion/decay portion of SAS2. It computes the time-dependent concentrations and source terms for a large number of isotopes that are simultaneously generated or depleted through neutronic transmutation, fission, radioactive decay, input feed rates, and physical or chemical removal rates. The time dependence of the nuclide concentrations is solved by using the matrix exponential expansion technique. A generalized form of the Bateman equation is used to solve for concentrations of short-lived nuclides to ensure better accuracy. One of the outstanding features of ORIGEN-S is its capability to generate neutron and/or gamma sources in any group structure.

SAS2 utilizes two separate 1-D models in each pass through the neutronic analysis. The first model, path A, is a fuel-pin cell from which cell-weighted fuel cross sections are obtained for the second model, path B. The path B model can be specified to approximately represent the neutronic features of an assembly, including water holes and absorber rods, within an infinite lattice. The flux and weighted cross sections obtained from the fuel region of the path B model are used to determine the cross sections and spectral parameters for the ORIGEN-S point-depletion analysis. Each ORIGEN-S case produces the burnup-dependent fuel composition for the next pass through the neutronics analysis. The analysis proceeds with each succeeding library and corresponding assembly power and time interval. Ultimately, the nuclide inventory (actinides, fission products, and light elements) is computed at the burnup corresponding to the discharge of the assembly from the reactor. Finally, a decay-only subcase is computed for the requested spent fuel cooling time. These calculated compositions are applied in both the determination of radiation sources and heat generation rates and are available for use in the optional shielding analysis.

IV. ORIGEN-ARP, FAST MENU-DRIVEN ISOTOPIC DEPLETION/DECAY SOURCE-TERM GENERATION

ORIGEN-ARP is an easy-to-use interface for performing light-water-reactor (LWR) spent fuel analyses on a PC. In addition, ORIGEN-ARP can perform decay-only calculations to generate radiation sources for any radioactive material, such as nuclear waste. Its purpose is similar to the SAS2 sequence because it uses ORIGEN-S to generate radiation source spectra and other spent fuel data. For generating neutron and gamma source spectra for standard LWR fuel designs or other radioactive sources, it offers two distinct advantages. First, ORIGEN-ARP is much easier to use than SAS2 because it provides a sophisticated pull-down menu program with data entry screens featuring context-sensitive help messages, multiple-choice menus, and extensive error checking. This program automatically prepares the input for the Automated Rapid Processing (ARP) code and ORIGEN-S and executes these codes at the click of a button. Second, it is much faster than SAS2. The ARP code interpolates cross sections on burnup and enrichment using a set of libraries for four LWR fuel assembly designs (BWR 8 × 8, PWR 14 × 14, 15 × 15, 17 × 17) that span enrichments from 1–5 wt % ^{235}U and burnups of 0–60,000 MWD/MTU. The interpolated cross sections are passed to ORIGEN-S to perform the calculations. Comparisons of ORIGEN-ARP and SAS2 have shown very good agreement.[3] Note that the run time for a typical SAS2 case was 43.5 min. on a 75-MHZ Pentium PC compared to less than 1 min. for the corresponding ORIGEN-ARP case.

V. SAS3 AND SAS4, 3-D MONTE CARLO SHIELDING ANALYSIS SEQUENCES

The SAS3 sequence in SCALE provides automated data processing via BONAMI, NITAWL-II, and XSDRNPM for subsequent execution of the Monte Carlo shielding code, MORSE-SGC. However, in a 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 in reasonable run times. The SAS4 sequence employs such a technique by using adjoint fluxes from a 1-D discrete-ordinates calculation with the XSDRNPM code to generate the biasing parameters for a Monte Carlo analysis by the MORSE-SGC code. The SAS4 module provides calculated radiation dose levels exterior to a multidimensional cask model. Most of the standard biasing options in the MORSE-SGC code, including source biasing, splitting, Russian roulette, path-length stretching, and collision energy biasing, are invoked. All the required biasing parameters in SAS4 are derived from results of the adjoint XSDRNPM calculation and automatically input to MORSE-SGC. Like SAS1, the source energy spectrum is read either directly from the input file or an ORIGEN-S output file.

A great deal of consideration has been given to the development of the SAS4 geometry model options. A generic cask model has been developed for SAS4 in order to implement the automated biasing procedure and the simplified geometry input option. The simplified input is used to generate geometry input for the MORSE-SGC module. The cask model has most of the features commonly found in shipping and storage casks. However, SAS4 is not limited to cask geometries. An option is provided for the user to supply detailed MORSE/MARS geometry input directly to SAS4. This option allows users to model other types of shielding problems that can benefit from the automated generation of 1-D biasing parameters.

Surface and point detectors are used in the Monte Carlo calculation. The surface detectors are analog detectors that calculate averaged responses based on particles crossing the detector surfaces. The accuracy and precision of the responses depend on the number of particles and their respective weights crossing the detector surfaces. Four surface detectors are automatically implemented in SAS4, on the outermost surface of the cask and 1, 2, and 3 m from this surface. The point detectors are input by the user. It is important that the positions of the point detectors (radial or axial) are consistent with the direction of the transport calculation. Because of the automated biasing procedure in SAS4, neutron and gamma doses are computed in separate calculations. In a radial biasing calculation, next-event estimations are made from all collision and source points to the point detectors. In an axial biasing calculation, next-event estimations are made only from points that lie in the half (top or bottom) of the cask nearest to the detectors. This procedure assumes that for an axial calculation, the contributions from collision and source points in the other half of the cask are negligible. In a next-event estimation, tracking is made from a source or collision point to point detectors that are many mean-free paths away. Since tracking is the most time-consuming portion of Monte Carlo transport analysis, next-event estimation to point detectors will significantly add
to the time of a calculation. Flux-to-dose-rate conversion factors for surface and point detectors can be selected from those provided in SCALE.

VI. QADS, 3-D POINT-KERNEL SHIELDING ANALYSIS

QADS[4] is a new control module available in SCALE. QADS performs multidimensional point-kernel estimation of gamma transport through practically any type of shielding materials using a simplified input scheme that follows the general input philosophy of the other SCALE shielding sequences. Although QADS has been used by the ORNL staff for several years, Version 4.3 of SCALE-PC marks the initial

release of QADS for public use. QADS was designed to capture the flexibility and power of the QAD technique[5] for problems amenable to point-kernel solution while allowing for an efficient and user-friendly input interface. QADS preprocesses the actual input for the QAD-CGGP code[5] and then calls and executes QAD-CGGP automatically. The SCALE Material Information Processor is used to allow simplified input of materials. QADS can read the source spectra from the input file or an ORIGEN-S file. The geometry is read using the well-known MORSE combinatorial geometry package. Finally, the dose portion of the input follows similarly the XSDOSE input data in SAS1. The combined use of the SCALE standard compositions and free-form input with the multidimensional geometry capabilities and generally short running time of point-kernel techniques produces a very powerful procedure for shielding analysis of a wide variety of problems.

VII. APPLICATIONS OF SCALE-PC

SAS2 and SAS4 were used in a recent EPRI study[6] to perform 3-D dose-rate analyses of five spent fuel storage cask configurations for comparison with measured shielding results. The analysis and results for one of these casks, the Westinghouse MC-10, is described here. The MC-10 is a forged-steel cask designed to hold 24 PWR spent fuel assemblies. In this case, the assemblies were Westinghouse 15 × 15 assemblies irradiated in the Virginia Power Surry-2 reactor, with enrichments form 1.9 to 3.2 wt % ^{235}U, burnups of 24,000 to 35,000 MWD/MTU, and cooling times of 4 to 10 years.

The cask calculations were primarily performed with SAS4 utilizing the SCALE 27-neutron/18-gamma-group cross-section library and ANSI/ANS 6.1.1-1977 flux-to-dose conversion factors. Previous work has shown that, for neutron doses, the SCALE 27/18 library produces good agreement (within approximately 3%) with point-cross-section libraries.[7] The SAS2 sequence was used to generate neutron and gamma-ray source spectra for average burnups of various assembly "types." These assembly types were groupings of spent fuel with similar burnup, initial enrichment, and cooling histories. In most cases, each cask was loaded with two to three assembly types. The gamma-ray source variations due to fuel burnup in the axial direction were accounted for by inclusion of burnup peaking factors from typical Surry fuel. Based on previous experience, scale factors consisting of the burnup peaking factors raised to the fourth power were used to estimate the neutron source axial variations.

The calculational results shown in Table 1 are surface-averaged results obtained by SAS4 using boundary-crossing estimators. For the side doses, the averaging surface is the outside cask surface with an extent corresponding to the middle half of the cavity height, H (i.e., ± H/2 from the axial midplane). For the lid and bottom doses, the averaging surface was 80 × 80 cm. The measured values shown in Table 1 are similarly averaged over the corresponding surfaces if sufficient dose-rate measurement locations were reported. The neutron doses agree with measurements to within 30%. For gamma-ray doses on the cask side, an overprediction of the measured results by greater than a factor of 2 is seen. The cause of this overprediction is not clearly understood, particularly in view of the good agreement achieved for neutrons. The gamma dose for the cask lid was 50% high.

In an initial effort to investigate the cause of the discrepancies seen in the photon results, the MC-10 cask was analyzed with the MCNP Monte Carlo code.[8] MCNP uses a continuous-energy cross-section representation that should measure the adequacy of the SAS4 groupwise cross-section representation. The radial results obtained for the MC-10 cask are given in Table 1 and show generally good agreement (within 20% for neutrons and 5% for gammas) between SAS4 and MCNP for this problem. Further investigation

into the gamma-ray discrepancies revealed shortcomings in the 18-gamma-group structure as well as capture cross sections for some of the important fission-product materials. Therefore, revised calculations were performed for the cask side that used a fine-group 44-gamma-group library for the gamma-ray transport and the SCALE 44-neutron-group ENDF/B-V library for the source-term predictions. The 44-group neutron library was used in the source-generation calculation to predict the spectra at various stages of burnup. Although this library is based on ENDF/B-V, it contains ENDF/B-VI cross sections for ^{154}Eu and ^{155}Eu. These Eu isotopes are important for both spent fuel source terms and burnup credit applications, and major updates were made in the ENDF/B-VI evaluation.[9] The effect of these cross-section changes was enhanced ^{154}Eu capture and, hence, decreases of some 30 to 40% in the ^{154}Eu inventories in the spent fuel. Gamma rays from ^{154}Eu are a major contributor to the total doses along the cask side surfaces.

The updated gamma dose-rate results are shown in Table 1. The lid and bottom dose rates were not recalculated since the dominant contributor in these areas, ^{60}Co, was unchanged from the previous calculations. The gamma side dose-rate predictions are still higher than the experimental values by about 50%. Because of the large amount of attenuation (~5 orders of magnitude), as little as a 4% increase in the iron cross sections could account for this overprediction.

A sample application of QADS and SAS1 is the evaluation of proposed design concepts that would provide acceptable doses following a dropped-fuel-bundle accident in an advanced boiling-water-reactor (BWR) conceptual plant design. QADS was selected for this analysis because the problem is a gamma-only scoping evaluation that requires three-dimensional (3-D) modeling. Doses were calculated in the upper drywell of the reactor for two proposed designs of the biological shield region of the upper drywell.

The reactor cavity and upper drywell area modeled in the calculations are illustrated in Fig. 1. The first design evaluated included a 17.78-cm (7-in.)-thick lip consisting of 15.24 cm (6 in.) of concrete on a 2.54-cm (1-in.)-thick steel plate located immediately above the biological shield, as shown in Fig. 3. The second design is a similar concrete and steel lip that is significantly thicker. This thick lip extends 306.82 cm (1.2 ft) toward the vessel from the drywell ceiling wall, is 51.1 cm (1.7 ft) in height, and consists of 46.7 cm (18.4 in.) of concrete resting on a 5.08-cm (2-in.) steel plate that extends 60.2 cm (2 ft) into the upper drywell. The bundle was assumed to be lying horizontally on the bellows tangential to the reactor vessel. Dose calculations were performed for detector locations in the upper drywell 1 cm outside the biological shield. Five different elevations were selected at each radial incrementing order to bracket the maximum dose point for that radius.

Two additional calculations were performed with SAS1 to confirm the QADS results. In order to model the problem in one dimension, trigonometric calculations were performed by hand to determine the thickness of each material on a straight-line trajectory from the fuel bundle to the detector location of maximum dose. These dimensions were then used in a 1-D cylindrical model. The resulting peak dose rates obtained were 7208 rem/h for the thin concrete/steel lip and 24 rem/h for the thick concrete/steel lip. These results confirmed the QADS results of 6976 and 24 rem/h, respectively.

VII. CONCLUSION

The release of SCALE-PC Version 4.3 provides for the first time the automated radiation shielding analysis sequences of SCALE for PC users. Included in this version are two new SCALE sequences, QADS and ORIGEN-ARP. The availability of these powerful and easy-to-use analytical tools on the PC

now makes it possible for any analyst to perform a wide range of shielding calculations on his desktop computer.

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TABLE 1
SAS4 results for MC-10 cask dose rates

		Neutron			Gamma		
Location	Code	Calculated	Measured	Ratio/cm[a]	Calculated	Measured	Ratio (c/m)
Side	SAS4	21.6(2)[b]	19.6	1.10	45.9(2)	21.4	2.15
	MCNP	25.5(3)	19.6	1.30	48.4(3)	21.4	2.26
	SAS4 revised[c]	–			32.6(1)	21.4	1.52
Lid	SAS4	58.0(2)	56.7	1.02	21.8(1)	14.6	1.49
Bottom	SAS4	6.0(3)	4.6	1.30	52.5(1)	62.0	0.85

[a]Calculated/measured.
[b]Percentage standard deviation.
[c]SCALE 44-neutron-group ENDF/B-V library and 44-gamma-group library.

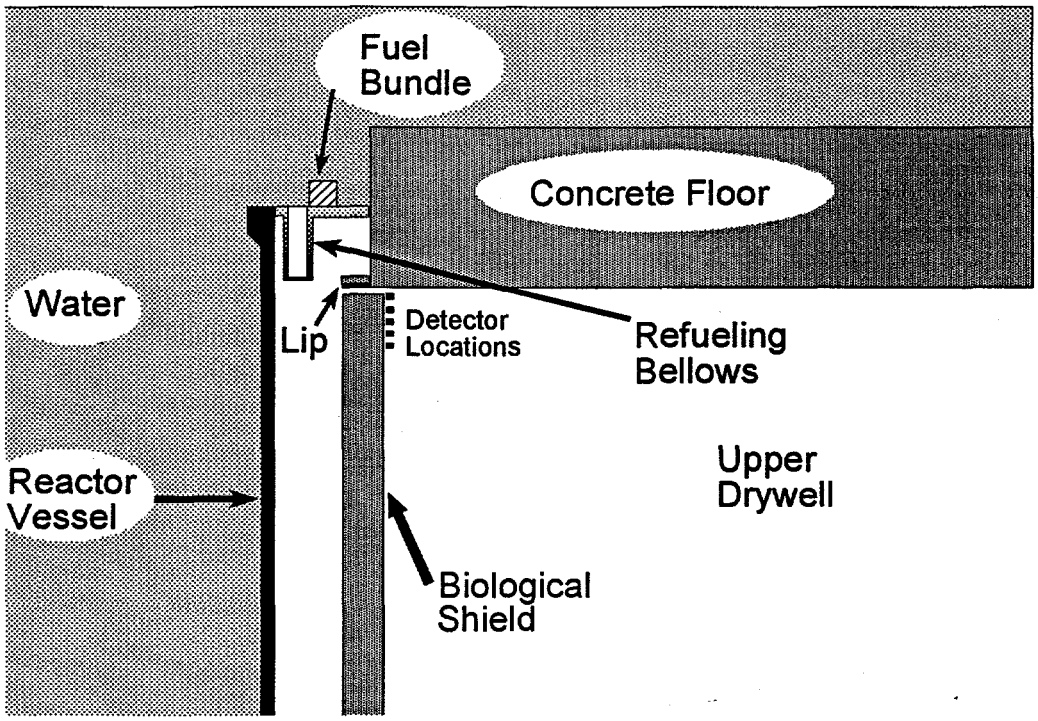

Figure 1. Advanced BWR upper drywell conceptual design.

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