Guide to Verification and Validation of the SCALE-4 Radiation Shielding Software

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Prepared for U.S. Nuclear Regulatory Commission



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Manuscript Completed: November 1996 Date Published: December 1996

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Prepared for Spent Fuel Project Office Office of Nuclear Material Safety and Safeguards U.S. Nuclear Regulatory Commission Washington, DC 20555-0001 NRC Job Code B0009



ABSTRACT

Whenever a decision is made to newly install the SCALE radiation shielding software on a computer system, the user should run a set of verification and validation (V&V) test cases to demonstrate that the software is properly installed and functioning correctly. This report is intended to serve as a guide for this V&V in that it specifies test cases to run and gives expected results. The report describes the V&V that has been performed for the radiation shielding software in a version of SCALE-4.¹

This report provides documentation of sample problems which are recommended for use in the V&V of the SCALE-4 system for all releases. The results reported in this document are from the SCALE-4.2P version which was run on an IBM RS/6000 workstation. These results verify that the SCALE-4 radiation shielding software has been correctly installed and is functioning properly. A set of problems for use by other shielding codes (e.g., MCNP,² TWOTRAN,³ MORSE⁴⁻⁶) performing similar V&V are discussed.

A validation has been performed for XSDRNPM⁷ and MORSE-SGC⁶ utilizing SAS1⁸ and SAS4⁹ shielding sequences and the SCALE 27-18 group (27N-18COUPLE) cross-section library for typical nuclear reactor spent fuel sources and a variety of transport package geometries. The experimental models used for the validation were taken from two previous applications of the SAS1 and SAS4 methods.

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1 INTRODUCTION

The purpose of this report is to present a guide on verification and validation (V&V) of the SCALE-4 radiation shielding software with the validation emphasis on spent fuel cask shielding. This report serves as documentation of the problems used in the V&V of the SCALE-4 system for all releases. The verification problems specified by code developers have been run, and the results compare well with those in the SCALE- 4.2 baseline.¹⁰ The SCALE V&V plan¹¹ describes the methods used for the baseline V&V.

Although there are many definitions of software V&V, the SCALE configuration management plan, SCALE-CMP-001,¹² specifies the following:

- Verification: Assurance that a computer code correctly performs the operations specified in a numerical model. This is usually accomplished by comparing results to a hand calculation or an analytical solution or approximation.
- Validation: Assurance that a model as embodied in a computer code is a correct representation of the process or system for which it is intended. This is usually accomplished by comparing code results to either physical data or a validated code designed to perform the same type of analysis.

These definitions apply in this document.

Verification and validation can be very similar in that both are exercising a code with input for which there is a known result. In some cases the same known system may be used in both the V&V. Verification and validation are different, however, because the end use of the results is different. Verification is intended to demonstrate that the software has been properly coded, installed on a computer, and performs the intended functions for a given set of input. Results of the verification are compared against documented results as specified in the verification plan. Validation is the process of demonstrating that the software predicts "correct" results for the "systems for which it is intended." The calculated results for systems with a known solution are used to establish the calculational bias. The establishment of the bias defines a range over which the result is acceptably correct. Experimental parameters and physical properties of these systems are used to determine the range of applicability of the validation and define the systems for which the bias applies.

In Sect. 2, the computer codes and data are briefly described; in Sect. 3, the results of the shielding code verification are presented; in Sect. 4, validation results are presented. The verification results in Sect. 3 have been subdivided into two categories. The first category is the installation verification. The results for the sample problems distributed with SCALE for each module are presented. These problems exercise many of the input options of the codes and are intended to demonstrate that the codes have been properly installed on the computer, are executing properly, and are properly interfacing with the system hardware configuration. The scripts used to execute the codes are also being tested during this phase. The installation verification represents a minimum set of problems that must be run each time the code is newly installed on a computer system. The second verification category is the functional verification. In this phase, the functionality of the codes is being tested. The codes are used to solve analytic problems for which the results are known. An intercode comparison between several shielding codes is also presented.

The validation presented in Sect. 4 is comprised of the analysis of several cask dose-rate experiments using both the SAS1 and SAS4 radiation shielding sequences. The validation experiments cover a fairly broad range of spent fuel burnups and two different cask material types. The SCALE 27N-18COUPLE ENDF/B-IV cross-section library was utilized throughout this work.

2 DESCRIPTION OF THE CODE PACKAGE

The following subsections give a brief description of the program modules which were verified and validated. Each module in SCALE has a version number which is updated whenever the code is revised. This version number is printed when the module is executed and is also indicated in the documentation distributed with each release. The version numbers of the program modules should be checked when calculations are performed to verify that the correct versions are being used. When a code version changes, the nature of the modifications should be reviewed and cases run should be checked to see if complete verification and/or validation is warranted.

2.1 BONAMI

BONAMI¹³ performs resonance shielding through the application of the Bondarenko shielding factor method. BONAMI reads an AMPX¹⁴ master format cross-section library and applies Bondarenko corrections to all nuclides that have Bondarenko data. Input to BONAMI, provided by the SAS1 and SAS4 control sequences, includes information relating to the physical characteristics (composition of material, size, geometry, temperature) of the system being calculated. BONAMI produces a Bondarenko-corrected master format library which is read by NITAWL-II.¹⁵ For SCALE libraries, the Bondarenko technique is used primarily to process unresolved region resonance data and to process resonance nuclides which were not prepared by XLACS¹⁶ (such as the SCALE 16-group Hansen-Roach library or ENDF/B-VI nuclides processed with NJOY¹⁷). For the 27N-18COUPLE master cross-section library used in this validation, the primary purpose of the BONAMI functional module is to select the required material cross sections and to create a problem-dependent AMPX master cross-section library to be processed by NITAWL-II. No data processing is performed in BONAMI for the 27N-18COUPLE cross-section library.

2.2 NITAWL-II

NITAWL-II applies the Nordheim Integral Treatment to perform neutron cross-section processing in the resolved resonance range for nuclides that have ENDF/B resonance parameter data. This technique involves the numerical integration of ENDF/B resonance parameters using a calculated flux distribution which is based on the collision density across each resonance and subsequent weighting of the cross section to the desired broad group structure. Input data to NITAWL-II, automatically provided by the SAS1 and SAS4 control sequences, include information relating to the physical and neutronic characteristics of the system being calculated. NITAWL-II uses these data to complete the processing of the problem-dependent master library from BONAMI. NITAWL-II assembles the group-to-group transfer arrays from the elastic and inelastic scattering components and performs other tasks to produce a problemdependent AMPX working format cross-section library which can be used by XSDRNPM and MORSE-SGC. The analyst specifies the resonance parameters based on the available options. The options include (1) a homogeneous medium treatment which treats the resonance region of the fissile mixture as if it were an infinite homogeneous media and (2) a finite lump treatment which treats the resonance region as if the fissile mixture were a discrete lump with a 1/E return flux at the boundary. This latter option is for problems where the system is substantially heterogeneous or where reflector effects are important. These options are automatically invoked in the SAS1 and SAS4 control sequences according to the keywords INFHOMMEDIUM, LATTICECELL, or MULTIREGION. The INFHOMMEDIUM option treats the various mixtures as an infinite homogeneous media. The LATTICECELL option utilizes an infinite lattice of repeated cells for the resonance self-shielding correction. With the MULTIREGION option, a single-cell resonance self-shielding calculation is made.

2.3 XSDRNPM

XSDRNPM is a general-purpose, one-dimensional (1-D), discrete-ordinates code used for several purposes in SCALE. In the SAS1X and SAS1 shielding sequences, XSDRNPM is used to solve the 1-D Boltzmann equation in slab, cylindrical, or spherical geometry. In the SAS4 shielding sequence XSDRNPM is used in the adjoint mode to produce 1-D importance fluxes which the control sequence then uses to generate automated biases for MORSE-SGC. As part of the SAS1X and SAS4 sequences, XSDRNPM is optionally used to solve the 1-D Boltzmann equation for a specified fissile system and then to produce spatially averaged cross sections for subsequent use in an XSDRNPM or MORSE-SGC calculation.

2.4 XSDOSE

XSDOSE is a computer program used in conjunction with XSDRNPM to compute the flux and the resulting dose at various points outside a finite cylinder or sphere. XSDOSE can also compute the flux and/or dose at various points due to a finite rectangular surface source or a circular disc. The code assumes that the outgoing angular flux distribution on the rectangle, cylinder, sphere, or disc is independent of position and that the surrounding media is a void. The numerical technique used in XSDOSE is suitable for points on, close to, or far away from the source.

2.5 SAS1 CONTROL MODULE

The SAS1 control module invokes the control sequences, SAS1 and SAS1X. These control sequences serve similar functions in that they read user-specified data, which includes the required cross-section library, specifications for mixtures, information for resonance region cross-section processing of nuclides (size, geometry, and temperature), and geometry models for XSDRNPM, and then prepare the input for the various functional modules, depending on which sequence is specified. Physical and neutronics information (such as theoretical density, molecular weights, average resonance region background cross sections, etc.) not supplied explicitly but required by the functional modules is supplied by the Standard Composition Library¹⁸ or calculated by the Materials Information Processor.¹⁹ The SAS1 and SAS4 control sequences were primarily used in the validation presented in Sect. 4. The SAS1 control sequence prepares the input for BONAMI, NITAWL-II, XSDRNPM, and XSDOSE.²⁰

2.6 MORSE-SGC

MORSE-SGC is a three-dimensional (3-D) multipurpose neutron and gamma-ray transport Monte Carlo code which is part of the SAS4 control sequence and also a stand-alone code in SCALE. The 3-D MARS geometry package used in MORSE allows modeling complicated structures such as spent fuel shipping casks. MORSE-SGC solves the 3-D Boltzmann equation in either forward or adjoint mode using multigroup cross-section libraries. A number of biasing options are available in MORSE-SGC; and when running MORSE-SGC as part of SAS4, the biasing parameters are provided by data from an adjoint XSDRNPM calculation.

2.7 SAS4 CONTROL MODULE

The SAS4 control module includes only a single control sequence, SAS4. This control sequence reads user-specified data, which include the required cross-section library, specifications for mixtures, information for resonance region

Description

cross-section processing of nuclides (size, geometry, and temperature), and geometry models for XSDRNPM and MORSE-SGC, and then prepares the input for the various functional modules, depending on which sequence is specified. Additional physical and neutronics information is supplied by the Standard Composition Library or calculated by the Materials Information Processor. The SAS1 and SAS4 control sequences were primarily used in the validation presented in Sect. 4. The SAS4 control sequence prepares the input for BONAMI, NITAWL-II, XSDRNPM, and MORSE-SGC.

2.8 THE 27-NEUTRON 18-GAMMA CROSS-SECTION LIBRARY

The 27 neutron-18 gamma group ENDF/B-IV AMPX master cross-section library in SCALE is activated in the SAS1 and SAS4 control sequences by specifying 27N-18COUPLE as the cross-section library name. The 27-group neutron library is the broad-group companion library to the 218-group Criticality Safety Reference Library. The Criticality Safety Reference Library master library, which is based on ENDF/B-IV data, was generated as a pseudo problem-independent fine-group structure library for use in general criticality safety analysis and shipping cask calculations. The 27-group library was collapsed from the 218-group library using a fission- $(1/E\sigma_t)$ -Maxwellian spectrum on a nuclide-by-nuclide basis. Explicit ENDF/B-IV resonance parameters are used by the NITAWL-II functional module in the CSAS,²¹ SAS1, and SAS4 control modules for calculating problem-dependent, self-shielded resonance region cross sections. The 18-group gamma library was generated directly from ENDF/B-IV data before being coupled with the 27-group neutron library.

The 27N-18COUPLE AMPX master format cross-section library was originally created in August 1981. With the release of SCALE-4.0, the original 27-group library was processed into the new AMPX master library format using CORECTOL.²² In addition, all the nuclides were processed with PERFUME,²² which adjusts moments to physically reasonable values. The cross sections distributed with versions of SCALE 4.0 or later are not compatible with previous versions of SCALE.

3 VERIFICATION

The purpose of this section is to present code verification results. Verification is accomplished by running the verification problems specified in the SCALE V&V plan and demonstrating that the codes perform consistently with the SCALE-4.2 baseline results. The verification has been subdivided into two categories: installation verification and functional verification. The installation verification input and output files are distributed along with the SCALE code package. Appendix A describes input files which are available (see the SCALE homepage on the World Wide Web (WWW) which can be accessed from http://www.cad.ornl.gov).

Included in Appendix B of Ref. 23 is a copy of the submit4.2p script which was used to execute the V&V problems. The scale4 script, which it references, is included in the SCALE distribution.

Included in Appendix B of this document is a listing of READX, a FORTRAN program which is used to collect the results from XSDRNPM, XSDOSE, and/or SAS1 calculations. Upon execution the user is prompted for the names of an index of the output files to be searched and the name of the output file to store the results. READX searches strings in the output and collects XSDRNPM and/or XSDOSE results.

3.1 INSTALLATION VERIFICATION

Installation verification consisted of running the sample problems normally distributed with the modules in the SCALE package and demonstrating that the results were consistent with those in the SCALE-4.2 baseline. The sample problems represent a minimum set of calculations which should be run when the codes are installed on a computer system.

Reference 23 contains results from the BONAMI, NITAWL-II, and XSDRNPM sample problems. The others are discussed in the following sections.

3.1.1 XSDOSE

XSDOSE sample problem results are presented in Table 1. Table 1 was generated using the FORTRAN utility code READX. The format of the output from READX consists of the results file name followed by a list of the output files scanned. If a string is identified as being from XSDRNPM, the first 20 characters of the title are printed followed by selected output from the module. The value of "lambda" from XSDRNPM is printed, if found, as is the message that the outer iteration limit was exceeded. Following the XSDRNPM results listing, the results from XSDOSE are listed. The format of the READX output gives the detector number followed by the neutron and gamma dose rates for each detector. A lambda of exactly 1.0000 generally means that the XSDRNPM problem was executed in the "fixed source" mode rather than in the "k-eff" mode. The results from each module are not identical but are consistent with the results presented in the SCALE-4.2 baseline. The results presented in Table 1 verify that XSDOSE is correctly installed.

3.1.2 MORSE-SGC

The MORSE-SGC sample problem results for eight sample problems are given in Tables 2 through 9. Monte Carlo calculations such as those performed in MORSE-SGC are particularly sensitive to changes in the random number sequence. Minor cross-section differences and differences in the random number generator between two different computers may lead to seemingly large changes in the results. The deviation of the results must be taken into consideration when comparing the code performance between different computer systems. The MORSE-SGC results are consistent with those presented in the SCALE-4.2 baseline. The results presented in Tables 2 through 9 verify that MORSE-SGC is correctly installed.

install.x1					
case					
title(20) xsdose[neutron dose	gamma dose]	xsdrn[lambda]
xsdose.out					
pb cask contain:	ing 15		1.00	000E+00	
detector # 1	2.80743E+00	3.26706E+01			
detector # 2	1.09850E+00	1.50380E+01			
detector # 3	5.98245E-01	8.82736E+00			
detector # 4	3.34328E-01	4.63837E+00			

Table 1. XSDOSE sample problem results

Table 2.Sample Problem 1 for MORSE-SGC

detector u	ncoll	fsd	total	fsd
r	esponse	uncoll	response	total
1 0.	0000E+00	.00000	2.6085E-02ª	.03735
2 0.	0000E+00	.00000	1.2185E-01	.03722
neutron deaths	numbe	r	weight	
killed by russian roul	ette 1304	1	.44505E+04	
escaped	1710	8	.12070E+05	
reached energy cutoff		0	.00000E+00	
reached time cutoff		0	.00000E+00	
number of scattering				
medium n	umber			
1 3	74266			
2 2	17580			
3 5	76359			

^aNeutrons/source neutron (upper axial leakage).

Table 3. Sample Problem 2 for MORSE-SGC

detector	uncoll response		fsd uncoll	t	total esponse	fs	sd al
1	0.0000E+00		.00000	2.0	6613E-02 ^a	.038	304
2	0.0000E+00		.00000	1.3	3410E-01	.036	549
neuutron deaths		number		weight			
killed by russian r	roulette	14275		.47119E+04			
escaped		15978		.12035E+05			
reached energy cuto	off	0		.00000E+00			
reached time cutoff		0		.00000E+00			
number of scatterin	ıg						
medium	number						
1	347450						
2	196900						
3	524253						

^aNeutrons/source neutron.

detector	uncoll		fsd	total	fsd
	response		uncoll	response	total
1	0.0000E+00		.00000	$2.5338E-02^{a}$.04462
2	0.0000E+00		.00000	7.4350E-02	.04235
neutron death	S	number		weight	
killed by rus	sian roulette	19423		.14790E+05	
escaped		9577		.12036E+05	
reached energy	y cutoff	0		.00000E+00	
reached time	cutoff	0		.00000E+00	
number of sca	ttering				
medium	number				
1	220109				
2	91026				
3	266583				
^a Neutrons/sc	ource neutron.				

Table 4.	Sample Problem	3 for MORSE-SGC

Table 5. S	Sample Problem 4 f	for MORSE-SGC
------------	--------------------	---------------

	4	ni r**2 neutron fl	lience	
detector	uncoll	fsd	total	fsd
4000001	response	uncoll	response	total
1	3.4192E = 01	.00659	1.8103E+00	.06953
2	1.2887E - 01	.01253	1.8715E+00	.05715
3	5.1554E = 02	.01822	1.6242E+00	.05508
4	4.1993E - 03	.03357	5.4490E-01	.06567
5	1.9259E-03	.03798	3.5945E-01	.10577
6	4.2804E-04	.04595	1.3052E-01	.07288
7	4.9218E-05	.05680	3.8628E-02	.20537
neutron deat	ths	number	weight	
killed by ru	ussian roulette	238	.16344E+01	
escaped		0	.00000E+00	
reached ener	rgy cutoff	1792	.14556E+04	
reached time	e cutoff	0	.00000E+00	
number of so	cattering			
medium	number			
1	37727			

	4 pi r**	2 neutron dose rate	(cm**2 rad/source)	
detector	uncoll	fsd	total	fsd
	response	uncoll	response	total
1	3.6315E-09	.00000	5.9368E-09	.03125
2	2.9621E-09	.00017	5.9944E-09	.02030
3	2.4162E-09	.00007	6.0837E-09	.01161
4	1.6076E-09	.00003	5.9268E-09	.03035
5	4.7353E-10	.00015	4.5111E-09	.01677
б	4.1084E-11	.00015	1.9427E-09	.06627
7	1.8188E-11	.00005	1.4891E-09	.04963
8	3.5645E-12	.00011	6.3351E-10	.05068
9	3.0927E-13	.00005	2.2177E-10	.19275
10	2.6832E-14	.00011	4.6922E-11	.06199
4 pi r**2 ga	amma dose rate			
		responses(detecto	r) (cm**2 rad/source)	
detector	uncoll	fsd	total	fsd
	response	uncoll	response	total
1	0.0000E+00	.00000	5.8971E-10	.07463
2	0.0000E+00	.00000	8.0956E-10	.05328
3	0.0000E+00	.00000	9.9445E-10	.04316
4	0.0000E+00	.00000	1.1589E-09	.02569
5	0.0000E+00	.00000	1.1439E-09	.02597
б	0.0000E+00	.00000	6.4773E-10	.02692
7	0.0000E+00	.00000	4.9373E-10	.03021
8	0.0000E+00	.00000	2.7453E-10	.03264
9	0.0000E+00	.00000	1.1823E-10	.06700
10	0.0000E+00	.00000	4.9335E-11	.08268
neutron deat	chs	number	weight	
killed by ru	ussian roulette	5472	.49019E+01	
escaped		0	.00000E+00	
reached ener	rgy cutoff	12534	.52371E+04	
reached time	e cutoff	0	.00000E+00	
number of so	cattering			
medium	number			
1	896906			

Table 6. Sample Problem 5 for MORSE-SGC

	4 pi r**2	2 gamma dose r	rate (cm**2 rad/sourc	e)
detector 1 2 3 4	uncoll response 1.3379E-09 1.2199E-09 1.1124E-09 9.2490E-10	fsd uncoll .00013 .00010 .00008 .00011	total response 1.4827E-09 1.4169E-09 1.3725E-09 1.2388E-09	fsd total .01092 .01102 .01082 .01386
5 6 7 8 9 10	5.3162E-10 1.7563E-10 1.2142E-10 5.8026E-11 1.9171E-11 6.3336E-12	.00015 .00010 .00002 .00007 .00007 .00010	8.9717E-10 4.0302E-10 3.0910E-10 1.7035E-10 7.0052E-11 2.7444E-11	.01824 .01778 .01254 .03963 .04644 .08996
neutron deaths	5	number	weight	
killed by russ escaped reached energy reached time o	sian roulette 7 cutoff cutoff	125 0 4953 0	.87152E-01 0 .38459E+04 0	
number of scat medium 1	terings number 88024			

Table 7. Sample Problem 6 for MORSE-SGC

4 pi r**2 group 1 fluence (neutrons/source)					
	responses(det	ector) sambo for 10) region air		
J		5 - 3	h - h -]	£	
detector	uncoll	ISO	total	ISQ	
1				LULAI 01E10	
1	2.9455E-UI 9.6761E 00	.00013	4.3051E-UI	.01510	
2	0.0701E-UZ	.00012	1.0051E-UI	.020/4	
3	2.5550E-02 2.2172E 02	.00017	1 24FOE 02	.05550	
4	2.2172E-03 6 5310E-04	.00013	1.2450E-02 5 9234E-03	.12140	
5	0.00000-04	.00004	5.9234E-03 6.9513E-01	.10555	
7	0.0000E+00	.00000	4 2041 E = 01	.02001	
7 Q	0.0000E+00	.00000	$1.7195\pi - 01$.02340	
9	0.0000E+00		7 1174 = 02	06968	
10	0.0000E+00	.00000	3 3579E-02	07235	
11	0.0000E+00		1 1566F = 02	15406	
12	0.0000E+00		4 6456E-03	17979	
13	0.0000E+00		2 4127 E - 03	26041	
14	0.0000E+00	.00000	$5,2260 \pi = 0.4$	48327	
11	0.0000100	:00000	J.2200E 04	. 10527	
	4 pi r**2	group 10 + 11 flu	ence (neutrons/source)		
	-				
	respon	ses(detector) samb	o for 10 region air		
.		C - 1	7	C 1	
detector	uncoll	ISO	total	ISd	
1	response	uncoll	response	total	
1	0.0000E+00	.00000	1.9688E-01	.08108	
2	0.0000E+00	.00000	1.9933E-01	.042/9	
3	0.0000E+00	.00000	1.7853E-01	.04141	
4	0.0000E+00	.00000	7.8431E-02	.07793	
5	0.0000E+00	.00000	4.2392E-02	.08443	
6	0.0000E+00	.00000	8.2689E-02	.09007	
/	0.0000E+00	.00000	1.8312E-01	.04964	
8	0.0000E+00	.00000	2.28/0E-01	.02822	
9	0.0000E+00	.00000	1.9442E-01	.03521	
10	0.0000E+00	.00000	1.3152E-01 8.0010E.02	.03500	
12	0.0000E+00	.00000	0.0919E-02	.00559	
12	0.0000E+00	.00000	4.0305E-02	.05019	
14	0.0000E+00	.00000	1 22825-02	.00810	
14	0.0000E+00	.00000	1.2202E-02	.09004	
	4 pi r**2	group 28 fluence	(gammas/source)		
	_		-		
	respon	ses(detector) samb	o for 10 region air		
.		C 1	7	C 1	
detector	uncoll	ISO	total	ISO	
1	response	uncoll	response	LOLAL	
1	0.0000E+00	.00000	8.0065E-02	.10309	
2	0.0000E+00	.00000	7.5910E-02	.08078	
3	0.0000E+00	.00000	5./9/UE-U2	.09354	
4	0.0000E+00	.00000	1.9154E-02	.1815/	
5	0.0000E+00	.00000	1.8556E-02	.25/45	
6	0.0000E+00	.00000	6.1707E-02	.18004	
7	0.0000E+00	.00000	8.5857E-02	.11901	
8	0.0000E+00	.00000	8.5908E-02	.08017	
9	0.0000E+00	.00000	6.6111E-02	.11662	
10	0.0000E+00	.00000	4.2590E-02	.11924	
11	0.0000E+00	.00000	2.3781E-02	.19755	
12	0.0000E+00	.00000	1.5793E-02	.17226	
13	0.0000E+00	.00000	9.2278E-03	.23568	
14	0.0000E+00	.00000	8.9564E-03	.25858	

Table 8. Sample Problem 7 for MORSE-SGC

	i pi i zi	ast neutron riuence	(incactions) boarce)	
	response	s(detector) sambo	for 10 region air	
detector	uncoll	fsd	total	fsd
	response	uncoll	response	total
1	2.9455E-01	.00013	1.6835E+00	.02388
2	8.6761E-02	.00012	2.1256E+00	.05465
3	2.5556E-02	.00017	1.8546E+00	.02068
4	2.2172E-03	.00013	1.0854E+00	.03122
5	6.5310E-04	.00004	7.2959E-01	.04364
6	0.0000E+00	.00000	1.3744E+00	.02288
7	0.0000E+00	.00000	1.7668E+00	.01937
8	0.0000E+00	.00000	2.0580E+00	.01549
9	0.0000E+00	.00000	1.8887E+00	.01778
10	0.0000E+00	.00000	1.5445E+00	.01641
11	0.0000E+00	.00000	1.0944E+00	.02624
12	0.0000E+00	.00000	6.9138E-01	.02952
13	0.0000E+00	.00000	3.2199E-01	.03716
14	0.0000E+00	.00000	2.2335E-01	.06414
14	0.0000E+00 4 pi r**2	.00000 gamma ray fluence	2.2335E-01 (gammas/source)	.06414
14	0.0000E+00 4 pi r**2 response	.00000 gamma ray fluence s(detector) sambo i	2.2335E-01 (gammas/source) for 10 region air	.06414
14 detector	0.0000E+00 4 pi r**2 response uncoll	.00000 gamma ray fluence s(detector) sambo i fsd	2.2335E-01 (gammas/source) for 10 region air total	.06414 fsd
14 detector	0.0000E+00 4 pi r**2 response uncoll response	.00000 gamma ray fluence s(detector) sambo i fsd uncoll	2.2335E-01 (gammas/source) for 10 region air total response	.06414 fsd total
14 detector 1	0.0000E+00 4 pi r**2 response uncoll response 0.0000E+00	.00000 gamma ray fluence s(detector) sambo i fsd uncoll .00000	2.2335E-01 (gammas/source) for 10 region air total response 1.8671E+00	.06414 fsd total .03590
14 detector 1 2	0.0000E+00 4 pi r**2 response uncoll response 0.0000E+00 0.0000E+00	.00000 gamma ray fluence s(detector) sambo i fsd uncoll .00000 .00000	2.2335E-01 (gammas/source) for 10 region air total response 1.8671E+00 2.3374E+00	.06414 fsd total .03590 .03844
14 detector 1 2 3	0.0000E+00 4 pi r**2 response 0.0000E+00 0.0000E+00 0.0000E+00	.00000 gamma ray fluence s(detector) sambo f fsd uncoll .00000 .00000 .00000	2.2335E-01 (gammas/source) for 10 region air total response 1.8671E+00 2.3374E+00 2.0659E+00	.06414 fsd total .03590 .03844 .03181
14 detector 1 2 3 4	0.0000E+00 4 pi r**2 response 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	.00000 gamma ray fluence s(detector) sambo f fsd uncoll .00000 .00000 .00000 .00000	2.2335E-01 (gammas/source) for 10 region air total response 1.8671E+00 2.3374E+00 2.0659E+00 1.0634E+00	fsd total .03590 .03844 .03181 .04872
14 detector 1 2 3 4 5	0.0000E+00 4 pi r**2 response 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	.00000 gamma ray fluence s(detector) sambo f fsd uncoll .00000 .00000 .00000 .00000 .00000	2.2335E-01 (gammas/source) for 10 region air total response 1.8671E+00 2.3374E+00 2.0659E+00 1.0634E+00 7.0830E-01	fsd total .03590 .03844 .03181 .04872 .06306
14 detector 1 2 3 4 5 6	0.0000E+00 4 pi r**2 response 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	.00000 gamma ray fluence s(detector) sambo : fsd uncoll .00000 .00000 .00000 .00000 .00000 .00000	2.2335E-01 (gammas/source) for 10 region air total response 1.8671E+00 2.3374E+00 2.0659E+00 1.0634E+00 7.0830E-01 1.0339E+00	fsd total .03590 .03844 .03181 .04872 .06306 .05670
14 detector 1 2 3 4 5 6 7	0.0000E+00 4 pi r**2 response 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	.00000 gamma ray fluence s(detector) sambo f fsd uncoll .00000 .00000 .00000 .00000 .00000 .00000 .00000	2.2335E-01 (gammas/source) for 10 region air total response 1.8671E+00 2.3374E+00 2.0659E+00 1.0634E+00 7.0830E-01 1.0339E+00 1.9054E+00	.06414 fsd total .03590 .03844 .03181 .04872 .06306 .05670 .03597
14 detector 1 2 3 4 5 6 7 8	0.0000E+00 4 pi r**2 response 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	.00000 gamma ray fluence s(detector) sambo f fsd uncoll .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000	2.2335E-01 (gammas/source) for 10 region air total response 1.8671E+00 2.0659E+00 1.0634E+00 7.0830E-01 1.0339E+00 1.9054E+00 2.4037E+00	.06414 fsd total .03590 .03844 .03181 .04872 .06306 .05670 .03597 .02618
14 detector 1 2 3 4 5 6 7 8 9	0.0000E+00 4 pi r**2 response 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	.00000 gamma ray fluence s(detector) sambo f fsd uncoll .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000	2.2335E-01 (gammas/source) for 10 region air total response 1.8671E+00 2.0659E+00 1.0634E+00 7.0830E-01 1.0339E+00 1.9054E+00 2.4037E+00 2.1083E+00	.06414 fsd total .03590 .03844 .03181 .04872 .06306 .05670 .03597 .02618 .02689
14 detector 1 2 3 4 5 6 7 8 9 10	0.0000E+00 4 pi r**2 response uncoll response 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	.00000 gamma ray fluence s(detector) sambo i fsd uncoll .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000	2.2335E-01 (gammas/source) for 10 region air total response 1.8671E+00 2.0659E+00 1.0634E+00 7.0830E-01 1.0339E+00 1.9054E+00 2.4037E+00 2.1083E+00 1.5378E+00	.06414 fsd total .03590 .03844 .03181 .04872 .06306 .05670 .03597 .02618 .02689 .02931
14 detector 1 2 3 4 5 6 7 8 9 10 11	0.0000E+00 4 pi r**2 response uncoll response 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	.00000 gamma ray fluence s(detector) sambo i fsd uncoll .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000	2.2335E-01 (gammas/source) for 10 region air total response 1.8671E+00 2.0659E+00 1.0634E+00 7.0830E-01 1.0339E+00 1.9054E+00 2.4037E+00 2.1083E+00 1.5378E+00 1.0625E+00	.06414 fsd total .03590 .03844 .03181 .04872 .06306 .05670 .03597 .02618 .02689 .02931 .04577
14 detector 1 2 3 4 5 6 7 8 9 10 11 12	0.0000E+00 4 pi r**2 response uncoll response 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	.00000 gamma ray fluence s(detector) sambo i fsd uncoll .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000	2.2335E-01 (gammas/source) for 10 region air total response 1.8671E+00 2.0659E+00 1.0634E+00 7.0830E-01 1.0339E+00 1.9054E+00 2.4037E+00 2.1083E+00 1.5378E+00 1.0625E+00 7.1153E-01	.06414 fsd total .03590 .03844 .03181 .04872 .06306 .05670 .03597 .02618 .02689 .02931 .04577 .04519
14 detector 1 2 3 4 5 6 7 8 9 10 11 12 13	0.0000E+00 4 pi r**2 response 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	.00000 gamma ray fluence s(detector) sambo f fsd uncoll .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000 .00000	2.2335E-01 (gammas/source) for 10 region air total response 1.8671E+00 2.0659E+00 1.0634E+00 7.0830E-01 1.0339E+00 1.9054E+00 2.4037E+00 1.5378E+00 1.5378E+00 1.0625E+00 7.1153E-01 3.7193E-01	.06414 fsd total .03590 .03844 .03181 .04872 .06306 .05670 .03597 .02618 .02689 .02931 .04577 .04519 .06360

Table 8 (continued)

detector	uncoll	fsd	total	fsd
	response	uncoll	response	total
1	0.0000E+00	.00000	2.6516E-02ª	.04292
2	0.0000E+00	.00000	8.3250E-02	.03898
neutron dea	ths	number	weight	
killed by r	ussian roulette	19458	.14465E+05	
escaped		9698	.11894E+05	
reached ener	rgy cutoff	0	.00000E+00	
reached time	e cutoff	0	.00000E+00	
number of s	catterings			
medium	number			
1	191134			
2	89668			
3	263639			
4	12739			

Table 9. Sample Problem 8 for MORSE-SGC

^aNeutrons/source neutron.

3.1.3 SAS1 Control Program

Sample problem results for the SAS1 and SAS1X control programs are presented in Table 10. Table 10 was generated using the FORTRAN utility code READX. The format of the output from READX consists of the results file name followed by a list of the output files scanned. If a string is identified as being from XSDRNPM, the first 20 characters of the title are printed followed by selected output from the module. The value of "lambda" from XSDRNPM is printed, if found, as is the message that the outer iteration limit was exceeded. Following the XSDRNPM results listing, the results from XSDOSE are listed. The format of the READX output gives the detector number followed by the neutron and gamma dose rates for each detector. A lambda of exactly 1.0000 generally means that the XSDRNPM problem was executed in the "fixed source" mode rather than in the "k-eff" mode. The results presented in Table 10 verify that SAS1 and SAS1X are correctly installed.

3.1.4 SAS4 Control Program

The SAS4 sample problem results for eight sample problems are given in Tables 11 through 18. Monte Carlo calculations such as those performed in SAS4 are particularly sensitive to changes in the random number sequence. Minor cross-section differences and differences in the random number generator between two different computers may lead to seemingly large changes in the results. The deviation of the results must be taken into consideration when comparing the code performance between different computer systems. The SAS4 results are consistent with those presented in the SCALE-4.2 baseline. The results presented in Tables 11 through 18 verify that SAS4 is correctly installed.

3.2 FUNCTIONAL VERIFICATION

Functional verification consists of running problems that have known results. These problems are not part of the sample problems and are normally only run for code verification. The problems include analytic problems for which the results are known and problems which test specific code capabilities for which there is a known code response. The functional verification of the shielding software included analysis of problems using BONAMI, NITAWL-II, XSDRNPM, DORT, MORSE, SAS1, and SAS4. The BONAMI and NITAWL problems are discussed in Ref. 23 which also contains the tabulated results. The calculations with the other codes are discussed in this report.

Both MORSE-SGC and XSDRNPM solve the Boltzmann transport equation: MORSE-SGC by use of the Monte Carlo method, and XSDRNPM by use of 1-D discrete ordinates. Both codes are used to calculate results for systems for which results are known. In addition, both codes are used to calculate systems for which published results with similar methods and codes are available. These problems provide additional verification that both MORSE-SGC and XSDRNPM yield the same result under appropriate circumstances and are properly solving the underlying equations.

3.2.1 XSDRNPM/DORT Comparison

The XSDRNPM and DORT codes use the discrete ordinates method to solve the Boltzmann transport equation in one and two dimensions, respectively. The codes were independently developed and utilize cross sections in entirely different formats. In order to verify that the XSDRNPM code was correctly solving the governing equations, the identical problem was solved using both XSDRNPM and DORT in one dimension. Both codes use the same spatial mesh intervals, but slightly different angular quadrature sets. The neutron and gamma dose rate results at the last three mesh intervals are presented in Table 19. Generally XSDRNPM results are about 3% higher than those of DORT.

Table 10. SAS1 and SAS1X	sample prob	olem results summary
--------------------------	-------------	----------------------

```
install.s1
        case
                  title(20 ...) xsdose[ neutron dose gamma dose ] xsdrn[ lambda ]
sasla.out
            cases 3 & 4 (prep) --
                                                                                                                                              6.33884E-01
            case 3 -- latticecell ***** outer iteration limit reached 1.00000E+00

      detector # 1
      9.82405E-03
      2.41848E-02

      detector # 2
      3.22216E-03
      8.57040E-03

      detector # 3
      1.88583E-03
      5.10295E-03

      detector # 4
      8.68795E-04
      2.46581E-03

      actector # 4
      8.08/95E-04
      2.46581E-03

      case 4 - latticecell
      ***** outer iteration limit reached
      1.00000E+00

      detector # 1
      9.83856E-03
      2.41754E-02

      detector # 2
      3.22694E-03
      8.56637E-03

      detector # 3
      1.88863E-03
      5.10036E-03

      detector # 4
      8.70083E-04
      2.46441E-03

sas1b.out
            case 9 -- infhommediu ***** outer iteration limit reached 1.00000E+00
            detector # 1
detector # 2
detector # 3
detector # 4
                                                                 9.81385E-03 2.42885E-02
3.21877E-03 8.60903E-03
                                                                 1.88385E-03 5.12646E-03
8.67895E-04 2.47758E-03
            case 10 - infhommediu ****** outer iteration limit reached 1.00000E+00

      detector # 1
      9.73054E-03
      2.44966E-02

      detector # 2
      3.17132E-03
      8.54545E-03

            detector # 3
detector # 4
                                                                  1.85065E-03 5.08756E-03
8.50298E-04 2.43972E-03
            case 11 - same as cas ****** outer iteration limit reached 1.00000E+00

      detector # 1
      9.10375E-03
      2.36866E-02

      detector # 2
      2.96884E-03
      8.29292E-03

      detector # 3
      1.73286E-03
      4.94473E-03

      detector # 4
      7.96503E-04
      2.37761E-03

            case 12 - same as cas ****** outer iteration limit reached 1.00000E+00

      detector # 1
      1.00380E-02
      2.43368E-02

      detector # 2
      3.27123E-03
      8.47387E-03

      detector # 3
      1.90889E-03
      5.04147E-03

      detector # 4
      8.76983E-04
      2.41494E-03

            case 13 - infhommediu ****** outer iteration limit reached 1.00000E+00

      detector # 1
      2.73115E-01
      2.96196E-02

      detector # 2
      8.94215E-02
      1.11937E-02

      detector # 3
      5.07223E-02
      6.83115E-03

      detector # 4
      2.19531E-02
      3.43786E-03

            case 14 - infhommediu ****** outer iteration limit reached 1.00000E+00

      detector # 1
      2.72761E-01
      2.99700E-02

      detector # 2
      8.82572E-02
      1.11507E-02

      detector # 3
      5.00984E-02
      6.78880E-03

      detector # 4
      2.17143E-02
      3.38100E-03

sas1c.out
            case 15 -- multiregio ****** outer iteration limit reached 1.00000E+00
                                                              1.54147E-02 1.25561E-02
6.17558E-03 7.05051E-03
2.26585E-03 3.25708E-03
6.25971E-04 9.42758E-04
            detector # 1
            detector # 2
detector # 3
detector # 4
            case 16 -- same as ca ****** outer iteration limit reached 1.00000E+00
            detector # 1
                                                              1.54516E-02 1.25232E-02
6.19041E-03 7.03092E-03
2.27130E-03 3.24787E-03
6.27477E-04 9.40083E-04
            detector # 2
detector # 3
detector # 4
            case 17 -- multiregio ****** outer iteration limit reached 1.00000E+00
            detector # 1
detector # 2
detector # 3
detector # 4
                                                             1.44879E-01 1.93552E-02
4.12009E-02 1.16621E-02
1.39100E-02 5.45496E-03
            detector # 4 3.78104E-03 1.58178E-03
case 18 -- multiregio ***** outer iteration limit reached 1.00000E+00
```

Table 10 (continued)

detector # 1	1.33735E-01 3.21465E-02	
detector # 2	4.91246E-02 1.26236E-02	
detector # 3	1.75721E-02 5.41498E-03	
detector # 4	4.83020E-03 1.54816E-03	
case 19 multiregio *	***** outer iteration limit reached	1.00000E+00
detector # 1	9.24033E-01 2.47464E-02	
detector # 2	2.55059E-01 1.44049E-02	
detector # 3	8.52278E-02 6.65262E-03	
detector # 4	2.31159E-02 1.92462E-03	
sas1d.out		
case 20 infhommedi *	***** outer iteration limit reached	1.00000E+00
detector # 1	1.54788E-02 1.24866E-02	
detector # 2	6.19804E-03 7.02130E-03	
detector # 3	2.27381E-03 3.24492E-03	
detector # 4	6.28157E-04 9.39295E-04	
case 21 infhommedi *	***** outer iteration limit reached	1.00000E+00
detector # 1	1.44879E-01 1.93552E-02	
detector # 2	4.12008E-02 1.16621E-02	
detector # 3	1.39099E-02 5.45496E-03	
detector # 4	3.78103E-03 1.58178E-03	
sasle.out		
case 26homogeneous		9.99879E-01
storage pool dose *	***** outer iteration limit reached	1.0000E+00
detector # 1	1.32799E-30 $1.12234E-18$	1.000002.00
detector # 2	7.40496E-31 7.27625E-19	
detector # 3	5.09708E - 31 $5.09396E - 19$	
detector # 4	2.90596E - 31 $3.01732E - 19$	

 Table 11.
 Sample Problem 1 for SAS4 Control Program

	ansi	standard neutron	dose rate (rem/h)	
		1	responses(detector)	
detector 1 2 3 4 5 6	uncoll response 0.0000E+00 0.0000E+00 0.0000E+00 1.2403E-12 6.3184E-13	fsd uncol .00000 .00000 .00000 .00000 .62620 .55792	total 11 response 0 5.0977E-1 0 1.1512E-1 0 5.6202E-1 0 3.3520E-1 0 1.3686E-1 2 6.5279E-2	fsd total 0 .05764 0 .04691 11 .04861 11 .05675 10 .08528 11 .06175
7 neutron de killed by escaped reached en reached t:	1.0591E-14 eaths russian roulette nergy cutoff ime cutoff	.6550 number 4142 1683 0 0	5 2.1518E-1 weight .36872E+04 .64581E+03 .00000E+00 .00000E+00	.36382
number of medium 1 2 3 4 5 6 7 8	scattering number 0 0 6222 16287 0 7451 0			

	ansi	standard neutron dose	rate (rem/h)	
		responses(detect	cor)	
detector	uncoll	fsd	total	fsd
1	0 0000E+00	00000	2 0379E-10	0544?
2	0.0000E+00	. 00000	1.7071E - 11	.04965
3	0.0000E+00	.00000	8.1208E-12	.05807
4	0.0000E+00	.00000	4.5910E-12	.06727
5	3.3598E-13	.46921	3.5100E-11	.04792
6	1.3791E-13	.45931	1.0970E-11	.04809
7	2.0959E-14	.57403	1.8855E-11	.26072
neutron death	S	number	weight	
killed by rus	sian roulette	23045	.88214E+04	
escaped		8100	.64672E+04	
reached energ	y cutoff	0	.00000E+00	
reached time	cutoff	0	.00000E+00	
number of sca	ttering			
medium	number			
1	0			
2	0			
3	0			
4	52158			
5	164036			
6	U			
./	83033			
8	U			

Table 12. Sample Problem 2 for SAS4 Control Program

Table 13. Sample Problem 3 for SAS4 Cont	trol Program
--	--------------

	ans	i standard neu	tron dose	rate (rem/h)	
		respon	ises(detec	tor)	
datactor	ungoll	fa	4	totol	fad
detector		15	5u	LOLAI	ISU
1	response	unc	2011	response	LOLAI
1	0.0000E+00	.00	0000	8.5443E-UI	.02393
2	0.0000E+00	.00	1000	1.9623E-01	.02489
3	0.0000E+00	.00	000	9.5887E-02	.02583
4	0.0000E+00	.00	000	5.7205E-02	.02685
5	1.6666E-03	. 25	815	2.4720E-01	.04622
6	8.1507E-04	.19	686	1.2520E-01	.03753
7	1.6833E-05	.40	624	2.5079E-02	.15401
	le				
lieutron deat	agion reulette	20712	1	WEIGHL	
KIIIEd by Iu	ISSIAII IOUIELLE	20715	• 1	02375+03	
escaped		/01/	. 2	9500E+04	
reached ener	gy cutoil	0	.0	00008+00	
reached time	cutoll	0	.0	00008+00	
number of	scattering				
medium	number				
1	32429				
2	4246				
2	4240				
3	20966				
4 5	50900 70157				
5	78134				

	ansi s	tandard neutron dose responses(detec	rate (rem/h) tor)	
detector 1 2 3 4 5 6 7	uncoll response 0.0000E+00 0.0000E+00 0.0000E+00 3.5484E-04 1.6084E-04 2.2304E-05	fsd uncoll .00000 .00000 .00000 .00000 .44472 .43437 45225	total response 3.4678E-01 2.7689E-02 1.0488E-02 6.1214E-03 6.0587E-02 1.8578E-02 2.1615E-02	fsd total .06997 .07676 .07307 .07693 .05800 .05596 13740
neutron dea killed by n escaped reached ene reached tin	aths russian roulette ergy cutoff me cutoff	number 11710 3741 0 0	weight .37690E+04 .28423E+04 .0000E+00 .00000E+00	
number of s medium 1 2 3 4 5	scattering number 32801 4264 0 24426 77178			

Table 14. Sample Problem 4 for SAS4 Control Program

Table 15. Sample Problem 5 for SAS4 Control Program

_

	ansi	standard neutron do	se rate (rem/h)	
		responses(de	tector)	
detector	uncoll	fsd	total	fsd
	response	uncoll	response	total
1	0.00 ⁰ 0E+00	.00000	9.1253E-01	.06407
2	0.0000E+00	.00000	2.0025E-01	.07217
3	0.0000E+00	.00000	9.5534E-02	.06761
4	0.0000E+00	.00000	5.7084E-02	.06997
5	1.5079E-03	.47052	2.4518E-01	.08546
6	8.0343E-04	.49767	1.2011E-01	.06812
7	1.7637E-06	.85348	2.7856E-02	.25911
neutron death killed by rus escaped reached energ reached time	s sian roulette y cutoff cutoff	number 4002 1602 0 0	weight .33840E+04 .57589E+03 .00000E+00 .00000E+00	
number of sca medium 1 2 3 4 5	ttering			

	ansi	. standard gamma dose r	rate (rem/h)	
		respo	onses(detector)	
detector	uncoll response	fsd uncoll	total response	fsd total
2 3 4	0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00	.00000 .00000 .00000	5.1757E-02 3.9470E-02 2.9917E-02	.12247 .13672 .14923
5 6 7	4.5852E-02 1.6601E-02 1.9754E-04	.33905 .34418 .33777	1.3909E-01 5.0124E-02 5.9966E-03	.15904 .14633 .12898
neutron de killed by escaped reached en reached ti	aths russian roulette ergy cutoff me cutoff	number 52599 4523 0 0	weight .51265E+03 .15740E-02 .00000E+00 .00000E+00	
number of medium 1 2 3 4 5 6 7 8	scattering number 0 0 8280 13947 0 51780 0			

Table 16. Sample Problem 6 for SAS4 Control Program

Table 17. Sample Problem 7 for SAS4 Control Program

	alist st	responses(detecto	or)	
detector	uncoll	fsd	total	fsd
	response	uncoll	response	total
1	0.0000E+00	.00000	3.7352E-03	.12894
2	0.0000E+00	.00000	1.0607E-03	.16911
3	0.0000E+00	.00000	7.2748E-04	.17576
4	0.0000E+00	.00000	5.1467E-04	.18527
5	1.6372E-04	.13276	5.5669E-03	.23292
6	9.8695E-05	.11514	2.1551E-03	.13922
7	5.7168E-05	.11241	1.1494E-03	.13516
8	3.6187E-05	.11175	6.8521E-04	.13755
neutron dea killed by r escaped reached ene reached tim	ths ussian roulette rgy cutoff e cutoff	number 111278 62066 0 0	weight .11518E+04 .89183E-03 .00000E+00 .00000E+00	
number of s medium 1 2 3 4 5	cattering 186830 0 352402 241437 26594			

	ansi	standard gamma responses(d	dose rate (rem/h) etector)	
detector 1 2 3 4 5 6 7 8	uncoll response 0.0000E+00 0.0000E+00 0.0000E+00 3.1385E-17 1.7221E-17 9.2813E-18 5.6178E-18	fsd unco .0000 .0000 .0000 .1285 .1101 .1081 .1073	total ll response 0 3.5464E-16 0 8.0261E-17 0 5.5821E-17 0 3.9181E-17 7 4.4863E-16 4 1.9219E-16 0 9.1164E-17 9 5.2837E-17	fsd total .03234 .03170 .03362 .03548 .04251 .04716 .05177 .05283
neutron death killed by rus escaped reached energ reached time	s sian roulette y cutoff cutoff	number 78343 35381 0 0	weight .11039E+06 .10993E+02 .00000E+00 .00000E+00	
number of sca medium 1 2 3 4 5	ttering number 5882 0 80529 45978 53826			

Table 18.	Sample Problem	8 for SAS4	Control Program	n
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Table 19. Dose rates (mrem/h) of OECD Problem 1acalculated by XSDRNPM and DORT

	Radial	Ne	eutron	Ga	amma
Interval No.	midpoint (cm)	DORT	XSDRNPM	DORT	XSDRNPM
134	77.01	95.51	98.47	59.36	60.48
135	77.41	81.64	84.38	51.96	53.05
136	77.80	66.49	68.31	44.44	45.45

The problem solved in this exercise was OECD problem 1a which will be further discussed in Sect. 3.2.3. These results verify that the XSDRNPM code is correctly solving the basic discrete ordinates equations.

3.2.2 MORSE-SGC/MORSE-CGA Comparison

Eight MORSE-SGC sample problems were summarized in Sect. 3.1.2. Sample problems 4-7 were previously analyzed²⁴ with the MORSE-CGA code. Although both MORSE-CGA and MORSE-SGC are based on the same parent code, some 16 years of independent development have given rise to two largely independent codes. Tables 20 through 23 compare the results of MORSE-CGA and MORSE-SGC for sample problems 4 through 7, respectively. Since both codes use Monte Carlo methods with their associated standard deviations, the two sets of results are consistent with each other. Thus the version of MORSE-SGC is verified to be functioning as intended.

3.2.3 SAS1/SAS4 Comparison

As an additional means of verifying both the underlying computer codes, XSDRNPM and MORSE-SGC, and the shielding analysis sequences, SAS1 and SAS4, this section presents the application of these code packages to OECD problem 1a. This problem is a simple model of a typical spent fuel cask. The cask consists of a dry cavity of 80 cm diameter and 450 cm height, surrounded by a 38-cm-thick cast iron side shield and bottom, and 42 cm of steel for the cask lid. The source spectrum and magnitude are fixed to determine a computational benchmark problem in which only the cross-section set and computational methodology are allowed to vary.

The SAS1 and SAS4 solutions to the OECD problem set have been previously published elsewhere.^{25,26} The results from the verification plan are presented in Table 24 as the reference set along with the verification results performed in this study. The reference results are given at the cask side surface and 1, 2, and 10 m away from the cask side surface. Reference results are given for the SAS1 and SAS4 codes followed by the results for both the DORT²⁷ and MCNP codes. The DORT results (a 2-D discrete-ordinates method) and the MCNP results (a point Monte Carlo method) generally agree to within 10% of the SAS1 and SAS4 results. This provides a good indicator of the appropriateness of the individual solution methodologies for this particular problem set.

Table 24 also compares the verification results of the radial dose rates calculated by SAS1 and SAS4 with the reference results. SAS1 results for the reference and verification cases are in agreement to within 5% for all cases. Similarly, for the SAS4 results, after accounting for the standard deviations in the Monte Carlo calculations, the reference and verification results are in general agreement. These results verify that the SAS1 and SAS4 control programs are functioning as intended for this series of problems.

			fsd total	.08982	.08924	.08768	.19685	.10183	.08854	ht	3+01 3+04		6
		S	total response	2.1246E+0 2.2012E+0	1.8050E+0	6.8964E-01	4.6693E-01	1.8961E-01	3.1405E-02	weig	0.141901 0 0.157011 0	No.	3846
nple problem 4	4 pi r**2 fluence	RISC 6000 CGA Results	fsd uncoll.	0.00559 0.01011	0.01437	0.02710	0.03110	0.03842	0.04787	No.	212 0 1826 0		
GA results for san		IBM	uncoll. response	3.3862E-01 1.2691E-01	5.0596E-02	4.1025E-03	1.8808E-03	4.1824E-04	4.8231E-05	leaths	y Russian roulette energy cutoff time cutoff	of scatterings	1
1ORSE-C			detector No.	1	i m	4	5	9	Г	neutron d	killed by escaped reached reached	number o	medium
E-SGC and N			fsd total	.06953	.05508	.06567	.10577	.07288	.20537				
parison of MORS	ce	C results	total response	1.8103E+0 1.8715E+0	1.6242E+0	5.4490E-01	3.5945E-01	1.3052E-01	3.8628E-02	weight	0.16344E+01 0 0.14556E+04 0	No.	37727
able 20. Com	4 pi r**2 fluen	RISC 6000 SGG	fsd uncoll.	0.00659 0.01253	0.01822	0.03357	0.03798	0.04595	0.05680	No.	238 0 1792 0		
T		IBM	uncoll. response	3.4192E-01 1.2887E-01	5.1554E-02	4.1993E-03	1.9259E-03	4.2804E-04	4.9218E-05	S	issian roulette rgy cutoff e cutoff	atterings	
			detector No.	1 7	ι m	4	5	9	7	neutron death	killed by Ru escaped reached ener reached time	number of sci	medium 1

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		Table 21. (Comparison of N	MORSE-SGC ar	nd MORSE	CGA results f	or sample probl	lem 5	ļ
	4 pi r**2 r	reutron dose rate ((cm**2 rad/source)			4 pi r**2 neutroi	n dose rate (cm**2 ra	d/source)	
	IBM	RISC 6000 work:	station results			IBM RI	ISC 6000 CGA results		
detector	uncoll. response	fsd uncoll.	total response	fsd total	detector	uncoll. response	total response	fsd total	
- c	3.6315E-09	0	5.9368E-09	0.03125	- c	3.6315E-09	5.9163E-09 6.0001E.00	0.02028	
νm	2.4162E-09	0.00007	5.9944E-09 6.0837E-09	0.01161	4 m	2.4162E-09	0.0001E-09 6.2945E-09	0.02065	
4	1.6076E-09	0.00003	5.9268E-09	0.03035	4	1.6076E-09	6.2306E-09	0.02886	
S.	4.7353E-10	0.00015	4.5111E-09	0.01677	5	4.7353E-10	4.5683E-09	0.03747	
1 9	4.1084E-11	0.00015	1.9427E-09	0.06627	1 0	4.1084E-11	2.0395E-09	0.04118	
- ~	1.0100E-11 3 5645E-12	5000000 110000	1.4691E-09 6 3351E-10	0.05068	~ ~	1.0100E-11 3 5645E-12	1.4/33E-U9 7 3367E-10	0.04506	
6	3.0927E-13	0.00005	2.2177E-10	0.19275	6	3.0927E-13	2.2097E-10	0.07137	
10	2.6832E-14	0.00011	4.6922E-11	0.06199	10	2.6832E-14	5.3047E-11	0.10338	
	4 pi r**2 {	gamma dose rate (cm**2 rad/source)			4 pi r**2 gamm	a dose rate (cm**2 ra	d/source)	
	total	fsd				total		fsd	
detector	response	total			detector	response		total	
1	5.8971E-10	0.07463			1	6.2053E-10		0.05940	
2	8.0956E-10	0.05328			2	7.9292E-10		0.04630	
ŝ	9.9445E-10	0.04316			ŝ	8.9389E-09		0.04430	
4	1.1589E-09	0.02569			4	1.1208E-09		0.03807	
5	1.1439E-09	0.02597			5	1.1601E-09		0.01990	
9	6.4773E-10	0.02692			9	6.2287E-10		0.02411	
L	4.9373E-10	0.03021			7	5.2094E-10		0.05266	
8	2.7453E-10	0.03264			8	2.8975E-10		0.04473	
9 10	1.1823E-10 4.9335E-11	0.06700 0.08268			9 10	1.1284E-10 4.8233E-11		0.05760 0.06660	
			;						
neutron death:	s		No.	weight	neutron dea	ths	No.	weight	
killed by Rus	ssian roulette		5472 0	0.49019E+01	killed by R	ussian roulette	5544 0	0.49674E+01 0	
reached ener reached time	gy cutoff cutoff		0 12534 0	$0 \\ 0.52371E+04 \\ 0$	escaped reached en reached tin	ergy cutoff 1e cutoff	0 12385 0	0.51508E+040	
number of sca	tterings			No.	number of s	catterings		No.	
medium 1			š	36906	medium 1			897968	
									I

4 pi r**2 gamma dose rate	Its IBM RISC 6000 CGA Results	fsd uncoll. total fsd	total response response total	.01092 1.3379E-09 1.5019E-09 .01452	.01102 1.2199E-09 1.4329E-09 .01268	.01082 1.1124E-09 1.3619E-09 .01473	.01386 9.2489E-10 1.2291E-09 .00820	.01824 5.3162E-10 9.1015E-10 .01161	.01778 1.7564E-10 4.1029E-10 .03192	.01254 1.2142E-10 3.0769E-10 .02416	.03963 5.8027E-11 1.6890E-10 .03055	.04644 1.9171E-11 7.0728E-11 .03502	.08996 6.3337E-12 2.6522E-11 .06400	ht mumber weight	3-01 106 .70327E-01	0 0	3+04 4976 .38996E+04	0 0		number	00444
	Г	uncoll.	response	1.3379Е-09	1.2199Е-09	1.1124E-09	9.2489E-10	5.3162E-10	1.7564E-10	1.2142E-10	5.8027E-11	1.9171E-11	6.3337E-12		106	0	4976	0			
a	ults	fsd	total	.01092	.01102	.01082	.01386	.01824	.01778	.01254	.03963	.04644	.08996	ght	2E-01)E+04				
gamma dose rat	SC 6000 SGC Res	total	response	1.4827E-09	1.4169Е-09	1.3725E-09	1.2388E-09	8.9717E-10	4.0302E-10	3.0910E-10	1.7035E-10	7.0052E-11	2.7444E-11	er wei	.87152		.38459				
4 pi r**2	IBM RI	fsd	uncoll	.00013	.00010	.00008	.00011	.00015	.00010	.00002	.00007	.00007	.00010	dmun	tte 125	0	4953	0		er.	#
		uncoll	response	1.3379Е-09	1.2199Е-09	1.1124E-09	9.2490E-10	5.3162E-10	1.7563E-10	1.2142E-10	5.8026E-11	1.9171E-11	6.3336Е-12	leaths	russian roule		nergy cutoff	ime cutoff	scatterings	oquinu	7000
		detector		1	2	e	4	D	9	7	8	6	10	neutron d	killed by	escaped	reached e	reached t	number of	medium	-

Table 22. Comparison of MORSE-SGC and MORSE-CGA results for sample problem 6

		Table 23. Com	parison of MORS.	E-SGC and M(DRSE-CGA	results for sample f	oroblem 7	
	4 pi r**2 fast	neutron fluenc€	e (neutrons/sourc	(ə:	4 p	i r**2 fast neutro	in fluence (neutro:	ns/source)
	IBM RIS	C 6000 workstat	ion results			IBM RISC (6000 CGA results	
detector	uncoll. response	fsd uncoll.	total response	fsd total	detector	uncoll. response	total response	fsd total
	2.9455E-01	0.00013	1.6835E+0	0.02388	н (2.9455E-01	1.6928E+0	0.03639
01 0	8.6761E-02 2 ессер-02	0.00012	2.1256E+0 1 0516F+0	0.05465	01 0	8.6761E-02 р бебер-0р	2.0253E+0 1 00405+0	0.02228
0 4	2.2172E-02	0.00013	1.0854E+0	0.03122	4	2.2172E-03	1.1060E+0	0.03684
5	6.5310E-04	0.00004	7.2959Е-01	0.04364	5	6.5310E-04	6.9022E-01	0.03722
9	0	0	1.3744E+0	0.02288	9	0	1.3909E+0	0.02295
7	0	0	1.7668E+0	0.01937	7	0	1.8074E+0	0.02169
œ	0	0	2.0580E+0	0.01549	80	0	2.0747E+0	0.01526
6	0	0	1.8887E+0	0.01778	თ	0	1.9017E+0	0.01680
10	0 0	0 0	1.5445E+0	0.01641	10	0 0	1.4803E+0	0.01718
1 T F		5 0	L.U944E+U с 01205 01	U.U2624 0 00060			L.U./64E+U	0.02700
1 1 1			3.2199E-01	0.03716	1 1 1		3.4195E-01	0.04300
14	0 0	0 0	2.2335E-01	0.06414	14	0	2.0063E-01	0.05856
	4 pi r**2	gamma fluence (gammas/source)			4 pi r**2 gamma f	fluence (gammas/sc	ource)
		total		fsd			total	fsd
detector		response		total	-	detector	response	total
·						·		
-1 C		1.8671E+U		08350.0 19350 0		-1 C	1.7018E+0 2 2248E+0	05850.0
4 m		2.0659E+0		0.03181		4 (**	2.0450E+0	0.03551
- 4		1.0634E+0		0.04872		- 4	1.1018E+0	0.04874
ъ		7.0830E-01		0.06306		Ð	6.7627E-01	0.04220
9		1.0339E+0		0.05670		9	9.3182E-01	0.05875
7		1.9054E+0		0.03597		7	1.8204E+0	0.03318
ω (2.4037E+0		0.02618		ω α	2.2993E+0	0.02376
ר ע כ		Z.IU83E+0 1 5378F+0		0.02089		- م ح	Z.IO/3E+U 1 5650E+0	0.02942 0 03954
11		1.0625E+0		0.04577		11	1.0783E+0	0.04665
12		7.1153E-01		0.04519		12	6.9116E-01	0.03681
13		3.7193E-01		0.06360		13	З.7549Е-01	0.05538
14		4.1743E-01		0.08860		14	4.0906E-01	0.08352
neutron de	aths	No.	weight		neutron d€	eaths	No.	weight
killed by	Russian	4107	0.38345E+01		killed by	Russian roulette	4112	0.38410E+01
roulette					escaped			
escaped reached en reached ti	ergy cutoff me cutoff	0467	0.42919E+04 0		reached ei reached ti	nergy cutoff ime cutoff	0 0 108	0.42438E+04 0
number of	scatterings				number of	scatterings		
medium 1		778625			medium 1		776337	

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]	Reference results			Verification r	esults
	Neutron	Primary gamma	Secondary gamma	Neutron	Primary gamma	Secondary gamma
Surface SAS1	62.0	41.7	0.41	59.5 (-4%) ^b	41.4 (-1%)	0.42 (2%)
SAS4-avg.	58.0 (0.02) ^a	37.0 (0.04)	0.35 (0.07)	55.7 (0.02)	39.3 (0.05)	0.36 (0.04) (3%)
DORT-avg.	57.4	36.3	0.38	(-4%)	(0%)	
MCNP-avg.	64.1 (0.02)	34.1 (0.07)	0.46 (0.08)			
1 meter SAS1	19.2	16.0	0.13	18.4 (-4%)	15.9 (1%)	0.14 (<8%)
SAS4	18.8 (0.02)	20.0 (0.20)	0.11 (0.25)	17.7	14.4	0.12 (0.05) (9%)
DORT	18.3	15.5	0.13	(-6%)	(0.14) (-28%)	
MCNP	20.8 (0.02)	13.5 (0.10)	0.14 (0.06)			
2 meters SAS1	10.7	9.7	0.08			0.08 (0%)
SAS4	10.0 (0.02)	11.9 (0.30)	0.04 (0.08)	10.2 (-5%)	9.6 (-1%)	0.06 (0.04) (<50%)
DORT	9.5	8.7	0.07	(0.02)	(0.09)	
MCNP	11.1 (0.02)	7.7 (0.07)	0.08 (0.05)	(-0%)	(-38%)	
10 meters SAS1	0.95	1.17	0.007			0.007 (0%)
SAS4	0.80 (0.18)	1.03 (0.13)	0.005 (0.19)	0.91 (-4%)	1.16 (-1%)	0.005 (0.04) (0%)
DORT	0.78	0.95	0.006	0.78	1.21	
MCNP	0.91 (0.02)	0.85 (0.06)	0.006 (0.04)	(-3%)	(17%)	

Table 24. Radial dose rate (mrem/h) comparison for OECD Problem 1a

^aFractional standard deviation in Monte Carlo calculations.

^bPercent difference between the verification and reference results.

4 VALIDATION

4.1 INTRODUCTION

The purpose of this section is to present the results of a radiation shielding validation of SAS1/XSDRNPM and MORSE-SGC using the 27N-18COUPLE SCALE cross-section library. Results using XSDRNPM via the SAS1 sequence are presented for only a few of the cases since most of the experimental configurations are multidimensional in nature.

The experimental models used for the validation were taken from previously documented studies.²⁸ The experiments modeled cover a fairly broad range of cask-type systems and spent fuel enrichments and cooling times. No descriptions or discussions of the experiments will be given in this report; however, the availability of the calculational models is discussed in Appendix A.

Unlike the criticality safety validation study, where a large number of benchmark quality experiments are available to provide good coverage for most practical applications, radiation shielding applications largely depend on a few tailored experiments very specific to each particular area. For radiation shielding analyses of spent fuel transportation/storage cask applications, the required number of experiments to completely envelop all situations would indeed be large. For example, currently there are several gamma shield materials; iron, lead, depleted uranium, and concrete; several neutron shielding materials; epoxy resins, water, ethylene glycol, polyethylene; a wide range of fuel enrichments from about 2.0 to 5.0 wt % ²³⁵U; spent fuel burnups ranging from 20 to 60 GWd/MTU; and spent fuel cooling times ranging from 6 months to 15 years. Each of these parameter ranges would need experimental coverage for the validation results to be completely general. Therefore, a general validation for spent fuel cask applications is impractical, since the required number of benchmark measurements is not available. The regulatory approach to this problem has been to require a measurement to be performed prior to each shipment of spent fuel. This approach tends to decrease the regulatory requirements for radiation shielding computational validation. However, this does not completely solve the problem from a practical standpoint when optimal, cost-effective radioactive material packaging is desired. The use of simple but conservative approximations can lead to overly conservative and hence, non-cost-effective designs.

Recent trends in package development have concentrated on cost-effective, optimal designs where multidimensional analysis techniques become necessary. The use of better computational methods and the corresponding decrease in conservatism has the effect of increasing the level of validation required. This validation has taken a dual approach to assuring the quality of the radiation shielding applications to spent fuel cask analysis and design. The first step involves the analysis of simple shielding benchmarks consisting of the attenuation of both neutron and gamma-ray point sources through standard cask materials of varying thicknesses. These benchmark problems primarily allow the performance of the cross sections through varying thicknesses of shielding materials to be validated. This is particularly useful since the solution methodology and geometry modeling aspects of the code have already largely been validated through the code verification procedures (see Sect. 3).

In order for these simple benchmarks to be truly realistic, the point sources used must be typical of those seen for spent fuel. The neutron source spectrum from spent fuel is largely a fission spectrum and thus changes little with burnup or cooling time. The ²⁵²Cf spontaneous fission point source is therefore representative of nearly all neutron sources from spent fuel. The neutron experiments have been performed with iron, polyethylene, graphite, and a number of other shielding materials. For completeness, further experiments are needed on lead and depleted uranium shield materials. The gamma-ray source spectrum for spent fuel results from the decay gamma rays for a number of individual fission products. Over the first 100-year period of decay after the end of irradiation, some 8 to 10 fission-product and activation isotopes dominate the contribution to the gamma-ray dose rates from spent fuel. These isotopes have very different decay times and characteristic gamma-ray spectra. Thus, gamma-ray benchmark experiments need to be

Validation

performed for most or all of these isotopes. At present, only a ⁶⁰Co source has been applied in these benchmark experiments.

In the absence of complete benchmark information for attenuation characteristics of various neutron and gamma-ray spectra, the second step for validation includes the analysis of actual spent fuel cask measurements. Due to the complexity and expense of these measurements the number of available experiments is rather small. However, these experiments allow a good overall representation of the expected accuracies of actual spent fuel cask dose-rate analyses to be evaluated.

In Sect. 4.2 the sources of the simple benchmark and cask experiment models are given. The calculational results and analysis of the data are presented in Sect. 4.3.

4.2 PROBLEM DESCRIPTION

The simple benchmark and cask experiment validation models were taken from a previous study²⁸ which included application of SAS1 and SAS4 sequences. The models were obtained from the authors of the report and were used unaltered.

The simple benchmark problems executed for this validation study included 18 neutron dose-rate calculations and 6 gamma-ray dose-rate calculations. The neutron dose measurements were performed using a 252 Cf source while the photon measurements utilized a 60 Co source. The measurement configuration consisted of a point source followed by 0 to 35 cm of steel, graphite, or polyethylene for the neutron measurements and 0 to 25 cm of steel for the gamma-ray measurements. The shielding material consisted of 80- × 80-cm slabs located approximately 1 m from the source. These problems can be approximately modeled in one dimension; however, a paraffin source collimator cannot be modeled effectively in one dimension and represents a source of approximation.

The storage casks included in this analysis were the Ventilated Storage Cask (VSC), a reinforced concrete cask loaded with 17 consolidated fuel canisters, the TN-24P forged steel storage cask loaded with 24 unconsolidated pressurized-water-reactor (PWR) spent fuel assemblies and with 24 consolidated fuel canisters, the Westinghouse MC-10 forged steel storage cask with 24 PWR spent fuel assemblies, and the CASTOR-V/21 nodular cast-iron storage cask loaded with 21 PWR spent fuel assemblies. The spent fuel burnup ranged from 24 to 36 GWd/MTU, with enrichments from 1.9 to 3.2 wt % ²³⁵U, and cooling times from 2 to 14 years. The fuel assemblies were Westinghouse 15 × 15 PWR assemblies irradiated from 1973 to 1983 in the Surry-2 reactor, or from 1974 to 1977 in the Turkey Point reactor.

4.3 RESULTS AND DISCUSSION

The simple benchmarks described in the previous section were analyzed with both SAS1 and SAS4. The neutron results are given in Tables 25 through 27 for graphite, iron, and polyethylene shields, respectively. The maximum deviations for the SAS4 3-D results from the measured results are 15%, 17%, and 27% for the three shields. Most of the 3-D results for these benchmark problems are overestimates. The SAS1 1-D neutron results show similar trends to the 3-D results with the exception of the zero-thickness cases. Here the backscatter from the paraffin collimator is not accounted for, resulting in an underprediction for these cases. Once any appreciable attenuation occurs, the neutron backscatter becomes relatively unimportant. The maximum deviations for the 1-D results are 39%, 45%, and 24%, which are generally larger than those of the 3-D results due to the geometry approximations.

		Dose equiv	valent rate (µ	Sv/h)	
Thickness (cm)	Experiment	SAS1 calculation	C/E	SAS4 calculation	C/E
0	176.2	133.4	0.76	203.3(1%)	1.15
5	131.3	131.4	1.00	146.8(2%)	1.12
15	66.4	74.8	1.13	75.4(3%)	1.14
20	45.5	52.7	1.16	-	
25	30.8	36.9	1.20	34.8(4%)	1.13
35	13.5	18.8	1.39	15.3(6%)	1.13

 Table 25. Comparison of measured and calculated neutron dose rates for graphite slabs

Table 26. Comparison of measured and calculated neutrondose rates for iron slabs

		Dose equiv	valent rate (µ	Sv/h)	
Thickness (cm)	Experiment	SAS1 calculation	C/E	SAS4 calculation	C/E
0	165.3	123.5	0.75	184.5(1%)	1.12
5	118.2	123.4	1.04	136.9(2%)	1.16
15	62.5	79.2	1.27	69.2(5%)	1.11
20	46.3	60.9	1.32	-	
25	34.6	46.6	1.35	33.2(5%)	0.96
35	19.0	27.5	1.45	15.8(7%)	0.83

Validation

	do	se rates for polyet Dose equ	uivalent rate	s e (µSv/h)	
Thickness (cm)	Experiment	SAS1 calculation	C/E	SAS4 calculation	C/E
0	683.0	517.1	0.76	779.0(1%)	1.14
5	288.0	258.8	0.90	354.0(3%)	1.23
15	42.6	42.1	0.99	54.2(6%)	1.27
20	18.3	17.7	0.97	-	
25	8.3	7.7	0.93	10.2(6%)	1.23
35	2.25	1.7	0.76	2.15(9%)	0.96

 Table 27. Comparison of measured and calculated neutron dose rates for polyethylene slabs

Table 28. Comparison of measured and calculated photondose rates for iron slabs

		Dose ec	quivalent rate	(µSv/h)	
Thickness (cm)	Experiment	SAS1 calculation	C/E	SAS4 calculation	C/E
0	1020.0	769.1	0.75	980.0(1%)	0.96
5	255.0	220.6	0.87	-	
10	60.0	45.2	0.75	-	
15	9.62	8.24	0.87	10.4(7%)	1.08
20	1.67	1.41	0.84	1.54(5%)	0.92
25	0.34	0.24	0.71	0.29(6%)	0.85

The gamma-ray results for the simple geometry benchmarks are given in Table 28 for shield thicknesses from 0 to 25 cm of iron. The results generally agree reasonably well with the measurements for both the 1- and 3-D cases, with maximum deviations of 29% and 15%, respectively.

These benchmark results are useful since they give the expected cross-section performance as a function of the shield thickness. Other uncertainties must of course be considered for actual cask calculations, such as the source and material concentration uncertainties. Typically the material concentrations are chosen to give conservative results. Additional benchmark experiments of this type are needed to provide complete coverage for the various cask materials (i.e., lead, depleted uranium, as well as additional gamma sources ¹³⁷Cs, ¹⁵⁴Eu, ¹³⁴Cs, ¹⁴⁴Pr, etc.). In the absence of additional benchmark quality simple experiments, individual cask measurements for a variety of cask types are useful to study common trends in the calculated versus measured results. These results can also be used to demonstrate the overall validity of the calculational procedures.

The cask results included in this validation work are largely due to the work included in the verification plan. To ensure consistency with the published results, selected cask problems were transferred to the validation computer and reanalyzed to ensure consistency. In all cases the results were consistent within the Monte Carlo statistical uncertainties of the two sets of results.

The complete cask results using the standard SCALE 27N-18COUPLE library are given in Table 29. For the neutron and photon results in Table 29, a number of trends are noted. With the exception of the three cask side measurements below 4 mrem/h, the neutron doses agree with measurements to within 30%. It appears that the three measurements below 4 mrem/h have significant uncertainties. For gamma-ray doses on the cask side, an overprediction of the measured results by over a factor of 2 is seen. Some of the causes of this overprediction will be discussed later. The gamma dose trends for the cask lid and bottom are reasonably consistent (agreement to within 30%), with several exceptions. The low predicted gamma dose rate for the VSC lid appears to be due to the presence of thermocouple penetrations in the lid that were not modeled. The overprediction of the TN-24P bottom measurements for consolidated fuel are reasonably consistent with the trend seen for gamma doses on the cask side. This was somewhat expected since the bottom endfittings were removed in the consolidation process, and hence only the active fuel contributes to the bottom doses.

In an effort to determine the causes of the overprediction of gamma doses on the cask side, revised calculations were performed at selected detector locations for all cask configurations. Revisions included the use of a 44-gamma-group library for the gamma-ray transport, a newly generated 44-neutron-group library²⁹ for the source-term predictions, and an approximate representation of the cooling fins for the TN-24P cask. The 44-neutron-group library was used in the source-generation calculation to predict the spectra at various stages of burnup. This library is primarily based on ENDF/B-V but contains ENDF/B-VI cross section for ¹⁵⁴Eu and ¹⁵⁵Eu. These Eu isotopes are important for both spent fuel source terms and burnup credit application, and major updates were made in the ENDF/B-VI evaluation. The effect of these cross-section changes was enhanced ¹⁵⁴Eu capture and, hence, decreases of some 30 to 40% in the ¹⁵⁴Eu inventories in the spent fuel. Gamma rays from ¹⁵⁴Eu are a major contributor to the total doses along the cask side surfaces.

The updated gamma dose-rate results indicate little effect along the cask lid and bottom as expected since the dominant contributor in these areas, ⁶⁰Co, was unchanged from the previous calculations. The gamma side doses show significant reductions for all cask configurations. These doses continue to exhibit similar trends for both iron and concrete gamma shields. The gamma side dose-rate predictions are still higher than the experimental values by an average factor of about 1.6. The fact that all of these casks have similar calculated to experimental ratios indicates a common or similar source of the overpredictions. Due to the large amount of attenuation (about 5 orders of magnitude) as little as a 4% increase in the iron or concrete cross sections or densities could account for this overprediction.

Validation

		Neutron (mrem/h)		Gamma (mrem/h)			
		Calc.	Meas.	Ratio (c/m) ^c	Calc.	Meas.	Ratio (c/m) ^c
Side	MC-10 (91.5) ^a	$21.6(2)^{d}$	19.6	1.10	$45.9(2)^{d}$	21.4	2.15
	Castor (91.5)	8.5(2)	11.4	0.75	76.4(4)	30.2	2.53
	TN-24 (91.5)	1.3(2)	2.8	0.47	33.4(1)	12.3	2.71
	TN-24 con. (91.5)	1.7(1)	4.0	0.43	13.9(2)	5.8	2.40
	VSC (91.5)	1.9(1)	1	1.90	44.5(2)	20	2.22
Lid	MC-10 (80×80) ^b	58.0(2)	56.7	1.02	21.8(1)	14.6	1.49
	Castor (40.0)	50.6(4)	51.5	0.98	25.8(3)	38.4	0.67
	TN-24 (58.2)	31.0(4)	28.5	1.09	39.9(1)	37.9	1.05
	TN-24 con.(58.2)	32.2(3)	31.7	1.02	9.2(1)	12.7	0.72
	VSC (58.2)	7.7(2)	10	0.77	3.4(3)	10	0.34
Bottom	MC-10 (80×80)	6.0(3)	4.6	1.30	52.5(1)	62.0	0.85
	Castor (40.0)	54.9(3)	51.3	1.07	29.3(3)	24.5	1.20
	TN-24 (58.2)	75.6(3)	57.9	1.30	129.1(1)	117.0	1.10
	TN-24 con.(58.2)	79.2(2)	75.8	1.05	10.1(2)	3	3.36

Table 29. Summary of SAS4 3-D dose-rate results

^aRadii or heights of surface detectors in cm.

^bMC-10 axial surface detectors are 80 cm by 80 cm.

^cCalculated/measured.

^dPercent standard deviations.

4.4 CONCLUSIONS

The general trends seen in this work are agreement with 30% or better with the measurements for neutron dose rates along the cask side, lid, and bottom. The gamma-ray dose rates with substantial contributions from the top endfitting, plenum, and bottom endfitting regions are also in good agreement. Based on the SCALE 27N-18COUPLE library, gamma-ray dose-rate calculations with major contributions due to the active fuel show over a factor of 2 overprediction of the measured quantities for casks with iron and concrete shields. Significant uncertainties exist in the quantification of ⁵⁹Co concentrations in the endfitting hardware materials. The results shown here support the accuracy of source generation and dose estimation methods in these regions given accurate impurity characterizations. Thus it is felt that the practice of using upper bounds for ⁵⁹Co initial concentrations should assure conservative cask calculations.

Fortunately the gamma-ray dose discrepancies seen along the cask sides for both the iron and concrete shield surfaces are overpredictions. While these overpredictions are not totally understood, the trends observed, combined with the other verification and validation results, should allow confidence to be placed in the shielding results for a shipping/storage package.

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APPENDIX A

VERIFICATION/VALIDATION INPUT

In order for users to perform the verification and/or validation described in this report, the input files for the problems must be available. This appendix contains two tables that correlate input files with the results presented in this document. Table A.1 provides information on the verification problems; Table A.2 does likewise for the validation problems. Users should refer to the SCALE homepage on the World Wide Web which can be accessed from http://www.cad.ornl.gov for additional information on accessing these input files.

Appendix A

Table A.1 Input files for SCALE shielding code verification

File Names

Description

BONAMI.INP	BONAMI Sample Problems
NITAWL.INP	NITAWL Sample Problems
XSDRN.INP	XSDRNPM Sample Problems
XSDOSE.INP	XSDOSE Sample Problems
MORSE1.INP-MORSE8.INP	MORSE Sample Problems
SAS1A.INP-SAS1FX.INP	SAS1 Sample Problems
SAS4A.INP-SAS4H.INP	SAS4 Sample Problems
XSDRN.S1	XSDRN Cases for Table 19
DORTN.IN, DORTG.IN	DORT Cases for Table 19
INA.S1	SAS1 Cases for Table 24
INA*.S4	SAS4 Cases for Table 24
DORT1NEA, DORT1GEA	DORT Cases for Table 24

File Names	Description
UEKI1.S4 - UEKI5.S4	SAS4 Cases for Table 25
UEKI11.S4 - UEKI15.S4	SAS4 Cases for Table 26
UEKI31.S4 - UEKI35.S4	SAS4 Cases for Table 27
UEKI21.S4, UEKI24.S4-UEKI26.S4	SAS4 Cases for Table 28
UEKIGPH.S1	SAS1 Cases for Table 25
UEKICST.S1	SAS1 Cases for Table 26
UEKIPLY.S1	SAS1 Cases for Table 27
UEKIGAM.S1	SAS1 Cases for Table 28
MCTOPxx.INP	MC-10 Cask Top Cases - Table 29
MCBTMxx.INP	MC-10 Cask Bottom Cases
MCRADxx.INP	MC-10 Cask Radial Cases
C21Txx.INP	CASTOR Cask Top Cases - Table 29
C21Bxx.INP	CASTOR Cask Bottom Cases
C21Rxx.INP	CASTOR Cask Radial Cases
INPUTxx.T24	TN-24P Cask Cases - Table 29
INPUTxx.C24	TN-24P Consolidated Fuel Cases
INPUTxx.VSC	VSC Cask Cases

Table A.2 Input files for SCALE shielding code validation

Appendix A

APPENDIX B

UTILITY CODE LISTINGS

Attached is a list of the computer program READX used to process outputs for XSDOSE and SAS1 programs.

```
program readx
    character iline*132,iline0*132,icase*12,aeg*11,keff*6,sigma*6
    character index*12, results*40, plots*40, title*21, lambda*11
    character stats*12,error*36,lib*3,grps*3,neutron*19,gamma*19
    logical iflag
    integer ipt*1
cwcj
   This program scans the file list in the INDEX file for certain
с
   xsdose and xsdrn output. The findings are edited into several
с
   output files.
с
cwcj
с
c 'INDEX' has a list of output files that are to be scanned
   (max length filename = 12).
с
с
    write(*, (1x,a))') 'enter the index file name ---> '
    read(*, '(a)') index
с
c 'RESULTS' contains an edit of the casename, title, and xsdose or xsdrn
   results only if a string is found to contain a search string.
с
с
    write(*, (1x,a))) 'enter the results file name ---> '
    read(*, '(a)') results
с
       is =1
    open(7, file = index)
    open(8,file=results)
    write(8, '(1x,a,/)') results
    write(8,2000)
2000 format(5x, 'case', /, t11, 'title(20 ...)', 2x, 'xsdose[', 1x, 'neutron',
   * ' dose',2x, 'gamma dose',1x,']',2x, 'xsdrn[',3x, 'lambda',2x,']',/)
с
   ik and ix are counters to help in editing files with multiple outputs.
с
с
    ik
          = 0
         = 0
    ix
c outer control loop
  10 continue
     read(7, '(a12)', end = 40) icase
     ilib = 0
     neut = 0
     title = ' '
     error = ' '
     aeg = ' '
     keff = ' '
     sigma = ' '
```

NUREG/CR-6484

```
lambda = ' '
     iline = ' '
     iline0 = ' '
     neutron = ' '
     gamma = ' '
     write(*, '(1x,a)') icase
     inquire(file=icase,exist=iflag)
     if(iflag) then
       write(8, (1x,a)) icase
       open(10, file = icase, err = 41)
  20
       iline0 = iline
       read(10, '(a)', end = 42) iline
c check for xsdrn stuff
       if(iline(21:26).eq.'lambda') then
  we found some xsdrn stuff
с
        lambda = iline(29:39)
   now get the title
с
        read(10, '(a)') iline
   check iteration limit
с
        if(iline(10:14).eq.'outer') then
          error = iline(3:39)
          write(*, '(1x,a)') error
          read(10, '(a)') iline
        end if
        read(10, '(a)') iline
        title = iline(24:44)
  go ahead and print it and skip the counter check
с
        write(8, '(t8,a,t30,a,t69,a)') title,error,lambda
        title = ' '
        error = ' '
        lambda = ' '
        neut = 0
        goto 20
       end if
с
     look for xsdose information
с
    if(iline(54:60).eq.'(total)') then
    neut = neut + 1
    if(mod(neut,2).eq.0) then
    gamma = iline(40:50)
    ndet = int(neut/2)
    write(8, '(t8,10hdetector #,i3,t34,a,t48,a)') ndet, neutron, gamma
     neutron = ' '
     gamma = ' '
    goto 20
    endif
    neutron = iline(40:50)
    goto 20
    endif
    goto 20
    endif
```

Appendix B

goto 10 41 write(*, '(1x,a)') 'file not found' goto 10 42 write(*, '(1x,a)') 'EOF in output' close(10) goto 10 40 write(*, '(1x,a)') 'EOF in index' close(8) close(9) close(10) if(is.eq.1) then write(11,1002) ik 1002 format(/,t2,'#of_obs = ',i3) close(11) end if stop 40 end

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NRC FORM 335 (2-89) NRCM 1102 3201, 3202 2. TITLE AND SUBTITLE	C FORM 335 39) C M 1102 11, 3202 TITLE AND SUBTITLE Guide to Verification and Validation of the SCALE-4 Radiation Shielding Software		REPORT NUMBER Assigned by NRC, Add Vol., Supp., Rev., and Addendum Numbers, if any.) NUREG/CR-6484 ORNL/TM-13277			
Guide to Verification an Radiation Shielding Soft						
		3. M		VEAD		
		De	cember	1996		
		4. FIN	or grant ni B00	UMBER 109		
5. AUTHOR(S)		6. TYPE OF REPORT				
B. L. Broadhead, M. B.	B. L. Broadhead, M. B. Emmett, J. S. Tang			Technical		
			7. PERIOD COVERED (Inclusive Dates)			
 PERFORMING ORGANIZATION — NAME AND ADDRESS (If NRC, provide Division, Office or Region, U.S. Nuclear Regulatory Commission, and mailing address; if contractor, provide name and mailing address.) Oak Ridge National Laboratory Managed by Lockheed Martin Energy Research Corporation P.O. Box 2008 Oak Ridge, TN 37831-6370 						
 9. SPONSORING ORGANIZATION — NAME AND ADDRESS (If NRC, type "Same as above"; if contractor, provide NRC Division, Office or Region, U.S. Regulatory Commission, and mailing address.) Spent Fuel Project Office Office of Nuclear Material Safety and Safeguards U.S. Nuclear Regulatory Commission Washington, DC 20555-0001 						
10. SUPPLEMENTARY NOTES C. J. Withee, NRC Project	ot Manager (Revised 2/18/2000)					
11. ABSTRACT (200 words or less) Whenever a decision is made to newly install the SCALE radiation shielding software on a computer system, the user should run a set of verification and validation (V&V) test cases to demonstrate that the software is properly installed and functioning correctly. This report is intended to serve as a guide for this V&V in that it specifies test cases to run and gives expected results. The report describes the V&V that has been performed for the radiation shielding software in a version of SCALE-4.1 This report provides documentation of sample problems which are recommended for use in the V&V of the SCALE-4 system for all releases. The results reported in this document are from the SCALE-4.2P version which was run on an IBM RS/6000 workstation. These results verify that the SCALE-4 radiation shielding software has been correctly installed and is functioning properly. A set of problems for use by other shielding codes (e.g., MCNP, ² TWOTRAN, ³ MORSE ⁴⁻⁶) performing similar V&V are discussed. A validation has been performed for XSDRNPM ⁷ and MORSE-SGC ⁶ utilizing SAS1 ⁸ and SAS4 ⁹ shielding sequences and the SCALE 27-18 group (27N-18 COUPLE) cross-section library for typical nuclear spent fuel sources and a variety of transport package geometries. The experimental models used for the validation were taken from two previous applications of the SAS1 and SAS4 methods.						
12. KEY WORDS/DESCRIPTORS (I	List words or phrases that will assist researchers in locating the report.)		13. AVAILABILITY STATEMENT			
SCALE, criticality safety, radiation shielding, verification, validation		-	14. SECURITY	CLASSIFICATION		
			(This Page)	unclassified		
			(This Report)	unclassified		
			15. NUMBER O	F PAGES		
		-				
		1	16. PRICE			