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SCALE Radiation Shielding V&V Package

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Abstract

Verification and validation (V&V) are essential elements of software quality assurance (QA) for computer codes that are used for scientific calculations. The sponsors of the SCALE code system have required a QA plan and a V&V plan. For purposes of validating and verifying the SCALE shielding codes, a set of problems has been assembled and tested.

INTRODUCTION

Verification and validation (V&V) are essential elements of software quality assurance (QA) for computer codes that are used for performing scientific calculations, since it ensures the reliability and accuracy of such software. As part of the SCALE QA [1] and V&V[2] plans, a general V&V package for the SCALE radiation shielding codes has been assembled, tested and documented.[3] The SCALE radiation shielding V&V package is being made available to SCALE[4] users through the Radiation Safety Information Computational Center (RSICC) to assist them in performing adequate V&V for their SCALE applications. This radiation shielding software V&V package consists of a set of verification problems specified by the code developers and a set of validation problems for typical nuclear reactor spent fuel sources and a variety of transport package geometries. Although the V&V problems were originally run with SCALE 4.2, the results reported here are from SCALE 4.3.

VERIFICATION

The verification problems for the SCALE shielding software are divided into two categories: installation and functional. The installation problems are the standard sample problems for BONAMI, NITAWL-II, XSDRNPM, XSDOSE, SAS1, SAS4, and MORSE-SGC as distributed by RSICC with the SCALE package. These problems exercise many of the options of the codes and are intended to demonstrate that the codes are properly installed on the computer, are executing properly and are properly interfacing with the system hardware configuration. This verification represents the minimum set of problems that must be run each time the code is newly installed on a computer system.

Functional verification problems test the functionality of the codes by solving problems which have known solutions. These problems include analytic problems that have known results and problems which test specific code capabilities. The functional verification of the shielding software included comparison of results from XSDRNPM and DORT, MORSE-SGC and MORSE-CGA, and SAS1 and SAS4.

The SCALE V&V plan specifies that verification of SAS1 and SAS4 must include the benchmark configuration (denoted as OECD Problem 1a) defined by the Organization for Economic Cooperation and Development's Nuclear Energy Agency's (OECD/NEA) working group on shielding assessment of transportation packages. Problem 1a is a simple model of a typical spent fuel cask. The cask consists of a dry cavity of 40 cm radius and 450-cm height, surrounded by a 38-cm-thick cylindrical-shaped cast-iron side shield and bottom, and 42 cm of steel for the cask lid. The source spectrum and magnitude are fixed to define a computational benchmark problem in which only the cross section set and computational methodology are allowed to vary. The reference results are given at the cask side surface, and 1, 2, and 10 m away from the cask side surface. SAS1 and SAS4 solutions to the OECD problem have been previously published[5,6]. These results are presented in Table 1 as the reference set along with the results from the current study. Reference results from SAS1 and SAS4 are compared

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

	Reference results			Verification results		
	Neutron	Primary gamma	Secondary gamma	Neutron	Primary gamma	Secondary gamma
Surface						
SAS1	62.0	41.7	0.41	61.9 (-0.1%)[b]	41.7 (0%)	0.41 (0%)
SAS4-avg.[c]	58.0 (0.02)[a]	37.0 (0.04)	0.35 (0.07)	57.2 (0.02) (-0.3%)	39.3 (0.02) (8%)	0.37 (0.03) (-3%)
DORT-avg.	57.4	36.3	0.38	-	-	-
MCNP-avg.	64.1 (0.02)	34.1 (0.07)	0.46 (0.08)	-	-	-
1 meter						
SAS1	19.2	16.0	0.13	19.2 (0%)	16.0 (0%)	0.13 (0%)
SAS4[c]	18.8 (0.02)	20.0 (0.20)	0.11 (0.25)	18.5 (0.02) (1%)	14.5 (0.11) (-9%)	0.12 (0.05) (-9%)
DORT	18.3	15.5	0.13	-	-	-
MCNP	20.8 (0.02)	13.5 (0.10)	0.14 (0.06)	-	-	-
2 meters						
SAS1	10.7	9.7	0.08	10.6 (-0.1%)	9.7 (0%)	0.08 (0%)
SAS4[c]	10.0 (0.02)	11.9 (0.30)	0.04 (0.08)	9.76 (0.02) (3%)	9.09 (0.10) (4%)	0.06 (0.04) (-15%)
DORT	9.5	8.7	0.07	-	-	-
MCNP	11.1 (0.02)	7.7 (0.07)	0.08 (0.05)	-	-	-
10 meters						
SAS1	0.95	1.17	0.007	0.95 (0%)	1.17 (0%)	0.007 (0%)
SAS4[c]	0.80 (0.18)	1.03 (0.13)	0.005 (0.19)	0.78 (0.02) (0%)	0.96 (0.06) (1%)	0.005 (0.03) (-20%)
DORT	0.78	0.95	0.006	-	-	-
MCNP	0.91 (0.02)	0.85 (0.06)	0.006 (0.04)	-	-	-

[a]Fractional standard deviation in Monte Carlo calculations.
[b]Percent difference between the verification and reference results.
[c]The percentage differences for SAS-4 are comparisons with the DORT results due to the large fractional standard deviations on the reference SAS4 results.

with those from DORT (a two-dimensional discrete ordinates method) and MCNP (a point Monte Carlo method). The DORT and MCNP results which are also shown in Table 1 generally agree to within 10% of the SAS1 and

SAS4 reference results. This is a good indication of the appropriateness of the individual solution methodologies for this problem. SAS1 results for the reference and verification cases are in agreement too within 1% for all cases. Similarly, the verification results for the SAS4 Monte Carlo cases are in general agreement with the reference results from the DORT discrete ordinates cases. A comparison with the SAS4 reference results is not included because the reference cases did not process enough particles to give meaningful standard deviations. Overall these results verify that SAS1 and SAS4 are functioning as intended for the OECD problem.

Functional verification also includes comparison of results from sample problems four through seven of the MORSE-SGC code package as run by MORSE-CGA and MORSE-SGC. Although both of these codes are based on the same parent code, more than 16 years of independent development have resulted in two largely independent codes. Results for all four of these problems are presented elsewhere, but only Sample Problem 5 will be discussed in this paper. Sample problem five is a combined neutron-gamma case which calculates the secondary gamma-ray dose due to neutrons of energies greater than 0.011 MeV at several radial distances from a point, isotropic, 12.2 to 15 MeV source in an infinite medium of air. Table 2 compares the results of MORSE-SGC and MORSE-CGA for this problem. The uncollided neutron response from the two codes is identical. Since both codes use the Monte Carlo method with its associated standard deviations, the total response results are also consistent with each other. Thus, the version of MORSE-SGC used by SAS4 is verified as functioning in the intended manner.

VALIDATION

Validation problems usually involve calculation of experiments. For the SCALE shielding software validation, the emphasis is on spent fuel cask shielding. The experimental models used for the validation were taken from previously documented studies.[7] The experiments cover a fairly broad range of cask type systems and spent fuel enrichments and cooling times. This validation takes a dual approach to assuring the quality of the radiation shielding applications to spent fuel analysis and design. The first step involves analysis of simple shielding benchmarks consisting of the attenuation of both neutron and gamma-ray point sources through standard cask materials of varying thicknesses. The problem geometry consists of an 80 × 80-cm slab located approximately one from the source. The neutron dose measurements utilize a ^{252}Cf source; the gamma dose measurements, a ^{60}Co source. Several slab thicknesses were analyzed with both SAS1 and SAS4. For the neutron calculations, the shielding materials used were graphite, polyethylene, and steel; for gammas, the shielding material was steel. Table 3 contains the results for the neutron calculation with a steel slab of 0, 5, 15, 20, 25, and 35 cm thicknesses. Results of the other cases are reported in Ref. 3.

Comparison of the SAS1 results with the earlier calculations that used SCALE 4.2 indicated significant differences for thicknesses greater than 5 cm. Further analysis revealed that the earlier cases had used the SCALE standard composition CARBON STEEL for the steel while the current case had used the actual steel composition. A second case was run using the CARBON STEEL and these results were consistent with the earlier cases. Results from both compositions are reported in Table 3. The SAS4 cases all used the actual steel composition. The maximum deviation for the SAS4 3-D results from the measured results is 13% for the steel slab. The 3-D results for this benchmark tend to be overestimated. The SAS1 1-D results show similar trends to the 3-D results with the exception of the zero-thickness case. Here the backscatter from the paraffin collimator is not accounted for, resulting in under prediction. Once any appreciable attenuation occurs, the neutron backscatter becomes relatively insignificant. The maximum deviation for the 1-D results is 83% for the actual steel composition and 52% for the CARBON STEEL, which are larger than those of the 3-D results due to the geometry approximations.

The second step of the validation includes analysis of actual spent fuel cask measurements. Because of the complexity and expense of these measurements the number of available experiments is quite small, but those that do exist allow a good overall representation of the dose-rate analyses to be evaluated. Several spent fuel storage casks were used, including the Ventilated Storage Cask (VSC), a reinforced concrete cask loaded with 17 consolidated fuel canisters; the CASTOR- V/21 nodular cast-iron storage cask with 21 pressurized-water-reactor (PWR) spent fuel assemblies; the Westinghouse MC-10 forged steel storage cask with 24 PWR spent fuel assemblies; and the TN-24P forged steel cask loaded with 24 unconsolidated PWR spent fuel assemblies and with 24 consolidated fuel canisters. The spent fuel burnup ranged from 24-36 GWd/MTU, with enrichments from 1.9 to 3.2 wt. % ^{235}U and cooling times from two to 14 years. Comparison of calculated versus measured neutron and gamma ray results for these five casks is given in Table 4 for cases at the side, bottom and top of each cask.

Table 2. Comparison of MORSE-SGC and MORSE CGA results for sample problem 5

4 pi r2 neutron dose rate (cm**2 rad/source)**
IBM RISC 6000 workstation results

detector	uncoll. response	fsd uncoll.	total response	fsd total
1	3.6315E-09	0	5.9368E-09	0.03125
2	2.9621E-09	0.00017	5.9944E-09	0.02030
3	2.4162E-09	0.00007	6.0837E-09	0.01161
4	1.6076E-09	0.00003	5.9268E-09	0.03035
5	4.7353E-10	0.00015	4.5111E-09	0.01677
6	4.1084E-11	0.00015	1.9427E-09	0.06627
7	1.8188E-11	0.00005	1.4891E-09	0.04963
8	3.5645E-12	0.00011	6.3351E-10	0.05068
9	3.0927E-13	0.00005	2.2177E-10	0.19275
10	2.6832E-14	0.00011	4.6922E-11	0.06199

4 pi r2 gamma dose rate (cm**2 rad/source)**

detector	total response	fsd total
1	5.8971E-10	0.07463
2	8.0956E-10	0.05328
3	9.9445E-10	0.04316
4	1.1589E-09	0.02569
5	1.1439E-09	0.02597
6	6.4773E-10	0.02692
7	4.9373E-10	0.03021
8	2.7453E-10	0.03264
9	1.1823E-10	0.06700
10	4.9335E-11	0.08268

neutron deaths	No.	weight
killed by Russian roulette	5472	0.49019E+01
escaped	0	0
reached energy cutoff	12534	0.52371E+04
reached time cutoff	0	0

number of scatterings	No.
medium 1	896906

4 pi r2 neutron dose rate (cm**2 rad/source)**
IBM RISC 6000 CGA results

detector	uncoll. response	total response	fsd total
1	3.6315E-09	5.9163E-09	0.02028
2	2.9621E-09	6.0081E-09	0.02402
3	2.4162E-09	6.2945E-09	0.02065
4	1.6076E-09	6.2306E-09	0.02886
5	4.7353E-10	4.5683E-09	0.03747
6	4.1084E-11	2.0395E-09	0.04118
7	1.8188E-11	1.4733E-09	0.04572
8	3.5645E-12	7.3367E-10	0.06506
9	3.0927E-13	2.2097E-10	0.07137
10	2.6832E-14	5.3047E-11	0.10338

4 pi r2 gamma dose rate (cm**2 rad/source)**

detector	total response	fsd total
1	6.2053E-10	0.05940
2	7.9292E-10	0.04630
3	8.9389E-09	0.04430
4	1.1208E-09	0.03807
5	1.1601E-09	0.01990
6	6.2287E-10	0.02411
7	5.2094E-10	0.05266
8	2.8975E-10	0.04473
9	1.1284E-10	0.05760
10	4.8233E-11	0.06660

neutron deaths	No.	weight
killed by Russian roulette	5544	0.49674E+01
escaped	0	0
reached energy cutoff	12385	0.51508E+04
reached time cutoff	0	0

number of scatterings	No.
medium 1	897968

Table 3. Comparison of measured and calculated neutron dose rates for iron slabs

Thickness (cm)	Dose equivalent rate (μSv/h) Experiment	SAS1 SCALE CARBON STEEL	C/E	SAS1 actual steel composition	C/E	SAS4 calculation	C/E
0	165.3	123.5	0.75	123.5	0.75	186.4(1%)	1.13
5	118.2	123.4	1.04	124.0	1.05	131.2(2%)	1.11
15	62.5	79.6	1.27	83.2	1.33	65.9(5%)	1.05
20	46.3	61.6	1.33	66.4	1.43	-	
25	34.6	47.6	1.38	53.1	1.53	33.2(5%)	0.96
35	19.0	28.9	1.52	34.8	1.83	15.8(6%)	0.83

Table 4. Summary of SAS4 3-D dose-rate results

		Neutron (mrem/h)			Gamma (mrem/h)		
		Calc.	Meas.	Ratio (c/m)[c]	Calc.	Meas.	Ratio (c/m)[c]
Side	MC-10 (91.5)[a]	17.5	19.6	0.89	47.9	21.4	2.24
	Castor (91.5)	8.9	11.4	0.78	79.8	30.2	2.64
	TN-24 (91.5)	1.5	2.8	0.54	35.4	12.3	2.88
	TN-24 con. (91.5)	1.9	4.0	0.48	14.8	5.8	2.55
	VSC (91.5)	1.96	1	1.96	49.0	20	2.45
Lid	MC-10 (80×80)[b]	46.7	56.7	0.82	49.4	14.6	3.38
	Castor (40.0)	44.6	51.5	0.87	46.3	38.4	1.21
	TN-24 (58.2)	30.3	28.5	1.06	68.4	37.9	1.80
	TN-24 con. (58.2)	26.4	31.7	0.83	17.0	12.7	1.34
	VSC (58.2)	6.7	10	0.67	6.2	10	0.62
Bottom	MC-10 (80×80)	4.9	4.6	1.07	93.2	62.0	1.50
	Castor (40.0)	45.6	51.3	0.88	47.6	24.5	1.94
	TN-24 (58.2)	66.2	57.9	1.14	189.7	117.0	1.62
	TN-24 con. (58.2)	62.7	75.8	0.83	2.6	3	0.87

[a]Radii or heights of surface detectors in cm.
[b]MC-10 axial surface detectors are 80 cm by 80 cm.
[c]Calculated/measured.

For the neutron and photon results in Table 4, a number of trends are noted. The latest results are generally consistent with previously reported results[3,7] except for the top and bottom gamma results. The predictions of the gamma-ray dose rates for the top and bottom locations increased approximately a factor of 2 from the previously published results due to corrections made in the case inputs. These cases were improperly normalized for contributions due to the endfitting and plenum regions. The latest neutron dose rates are about 10-20% lower than previously calculated results for the top and bottom locations. This decrease is due to a slightly revised burnup shape assumed in the present study (the default burnup shape in SAS4 was used).

The general conclusions reported in Ref. 3 and 7 remain valid here for neutrons and side gamma-rays. With the exception of the three cask side measurements below 4 mrem/hr, the neutron doses agree with the measurements to within 35%. It appears that these measurements have significant uncertainties. For the gamma-ray doses on the cask side, an over prediction of the measured results by over a factor of 2 is seen. The fact that all of these casks have similar calculated-to-experimental ratios indicates a common or similar source of the over prediction. Due to the large amount of attenuation (about 5 orders of magnitude), a slight increase in the iron or concrete cross sections or densities could account for this over prediction. For the gamma-ray dose for the cask lid and bottom, the agreement with the experiment is a factor of about 3 or better, however, all calculations with appreciable contributions from the endfittings and plenum locations are conservative with respect to the experimental values. The procedure used to generate the endfitting and plenum source terms was designed to give conservative results. These results confirm the conservative nature of these sources, however, there appears to be large variations in the initial cobalt loadings as expected.

CONCLUSION

All of the V&V problems were originally run using the SCALE 27N-18G library; however, the problem set can be analyzed with other cross section libraries (sources should be recast into the new group structure). Although the V&V problems were initially run using SCALE 4.2, the SCALE V&V package distributed by RSICC will contain results from the current version of SCALE. The V&V package consists of the input and output files, the results of the calculations, and the utility codes used to process the output. The utility codes collect the relevant results into tabular form so that users can readily compare their results with those from ORNL.

The set of V&V problems described here provide users with methods for assuring the proper installation and functioning of SCALE as well as guidance in the validation of SCALE for their applications. After SCALE 4.4 is released, the V&V package will be finalized. The variety of problems included in this V&V represents a quite thorough testing of the shielding analysis codes in SCALE. This package of problems should prove to be invaluable to users of the SCALE system.

REFERENCES

1. *QA Plan for the SCALE Computational System*, SCALE QAP-005, R0, April 1996.

2. B. L. Broadhead, *Verification and Validation Plan for the SCALE Code System*, SCALE CCV-001, Rev. 1, April 1996.

3. B. L. Broadhead, M. B. Emmett, and J. S. Tang, *Guide to Verification and Validation of the SCALE-4 Radiation Shielding Software*, NUREG/CR-6484 (ORNL/TM-13277), December 1996.

4. *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200, Rev. 5 (ORNL/NUREG/CSD-2/R5), Vols. I-III (March 1997). Available from Radiation Safety Information Computational Center, Oak Ridge National Laboratory, as CCC-545.

5. B. L. Broadhead, M. C. Brady, and C. V. Parks, *Benchmark Shielding Calculations for the NEACRP Working Group on Transportation Packages*, ORNL/CSD/TM-272, Martin Marietta Energy Systems, Inc., Oak Ridge National Laboratory, November 1990.

6. C. V. Parks, et al., *Assessment of Shielding Analysis Methods, Codes, and Data for Spent Fuel Transport/Storage Applications*, ORNL/CSD/TM-246, Martin Marietta Energy Systems, Inc., Oak Ridge National Laboratory, July 1988.

7. B. L. Broadhead, et al., *Evaluation of Shielding Analysis Methods in Spent Fuel Shipping Cask Environments*, EPRI-TR 104329, May 1995.

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