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USE OF PARTISN 2.99 ON THE Y-12 NATIONAL SECURITY COMPLEX SGI HIGH-PERFORMANCE COMPUTER (MANHATTAN)

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ABSTRACT

The ultimate goal of this work is to provide the capability to perform confirmatory calculations for shielding applications and Criticality Accident Alarm Systems (CAAS) placement designs for storage of highly enriched uranium in vault-type storage buildings at the Y-12 National Security Complex. The scope includes the procurement, installation, verification and validation of the Los Alamos National Laboratory multi-processor discrete ordinates transport code PARTISN 2.99 on the Y-12 National Security Complex Engineering Division's SGI high performance computer (Manhattan). The scope also includes the development of a source term, the procurement of an appropriate cross section library based on the material isotopes of the model and the desired particles to be tracked, and the development of an appropriate response function set. The validation is accomplished by modeling standardized two-dimensional and three-dimensional benchmark shielding reference calculations from ANSI/ANS-6.6.1, and the validation of Kansas State University (KSU) Skyshine Experiments in two dimensions. Future work includes the development of a three-dimensional model of a vault-type storage building design in order to serve as primary or confirmatory calculations for CAAS placement. The model design is developed in accordance with various national standards and federal codes.

Key Words: CAAS, multi-processor, discrete ordinates, PARTISN, KSU Skyshine Experiments

1. INTRODUCTION

The purpose of this work is to ultimately provide a new capability for the Y-12 National Security Complex (NSC) during its current modernization effort. The Los Alamos National Laboratory (LANL) multi-processor discrete ordinates transport code PARTISN 2.99 has been installed on the Y-12 SGI high-performance computer (Manhattan) in order to perform primary or confirmatory calculations for shielding applications on a multi-processor platform [1]. Never before has Y-12 been able to perform its own Criticality Accident Alarm Systems (CAAS) placement design analysis or possess configuration control of its CAAS placement in-house. The scope of the work being presented includes procurement, installation, verification, and preliminary validation. Associated data necessary for use of the transport code, such as appropriate cross section libraries, source terms, and response function sets, were developed or procured.

2. DESCRIPTION

The PARTISN code package is a modular computer program package designed to solve the time-independent, multigroup discrete ordinates form of the Boltzmann transport equation [2]. PARTISN 2.99 is a beta test multi-processor successor to the DANTSYS 3.1 discrete ordinates transport code package. The Manhattan currently has up to 64 processors available for use with PARTISN 2.99 when run in its multi-processor form. The multi-processor form expands the mesh size capability for complex models, and in turn, greatly reduces run time required for completion of discrete ordinate transport codes.

2.1 Installation and Verification

PARTISN 2.64 was first installed by electronic transfer from the code developer to the Manhattan computer custodian, which was not successful due to the corruption of several files during the transfer. For verification of PARTISN 2.64, the run of 74 verification problems from compact disc installation was successful. For verification of PARTISN 2.99, the run of 80 verification problems from compact disc installation was successful.

2.2 Cross Section Libraries

The choice of cross section library is conservative in that it considers only the primary photon contribution from a fission source. The LANL-developed MENDF5 is a 30-group neutron cross section library with 99 nuclides which include the material isotopes of the models. MENDF5G is a 30-group neutron and 12-group gamma cross section library with the same 99 nuclides, designed for use in modeling fast systems, based on ENDF/B-V nuclear evaluated data. MENDFG is a subset of the MENDF5G library containing only the 12-group photon library, and is used for the tracking of photons in the validation of the reference calculations and in preliminary confirmatory calculations. Future shielding validation cases will employ the MENDF5G coupled cross section library to include the secondary contribution of photons from (n,γ) reactions from fission of ^{235}U if demonstrated that primary photons alone are not sufficient to activate CAAS sensors**.**

2.3 Response Function Development

For the validation of the ANSI/ANS-6.6.1 reference calculations, the 25 energy point values of ICRU-57 Conversion coefficients for air kerma per unit fluence (K_a / Φ) of monoenergetic photons were integrated over the 12 energy group ranges required for MENDFG [3]. For the validation of the Kansas State University (KSU) Skyshine Experiments, the ANSI/ANS-6.1.1-1977 Gamma Flux to Dose Factors for (rem/hr)/(photons/$cm^2 \cdot s$) were integrated over the 12 energy group ranges required for MENDFG [4].

2.4 Preliminary Validation

2.4.1 ANSI/ANS 6.6.1 reference calculation problem I.1

There are currently no OECD shielding benchmarks using either a Monte Carlo stochastic code package or a discrete ordinates code package. However, ANSI/ANS 6.6.1 reference calculations match several important characteristics of the necessary vault-type storage analysis with PARTISN 2.99: materials including air, ground, and a physical structure made of concrete, a point source term, and particle detectors [5]. See Figure 1 for the Reference Calculation I.1 model.

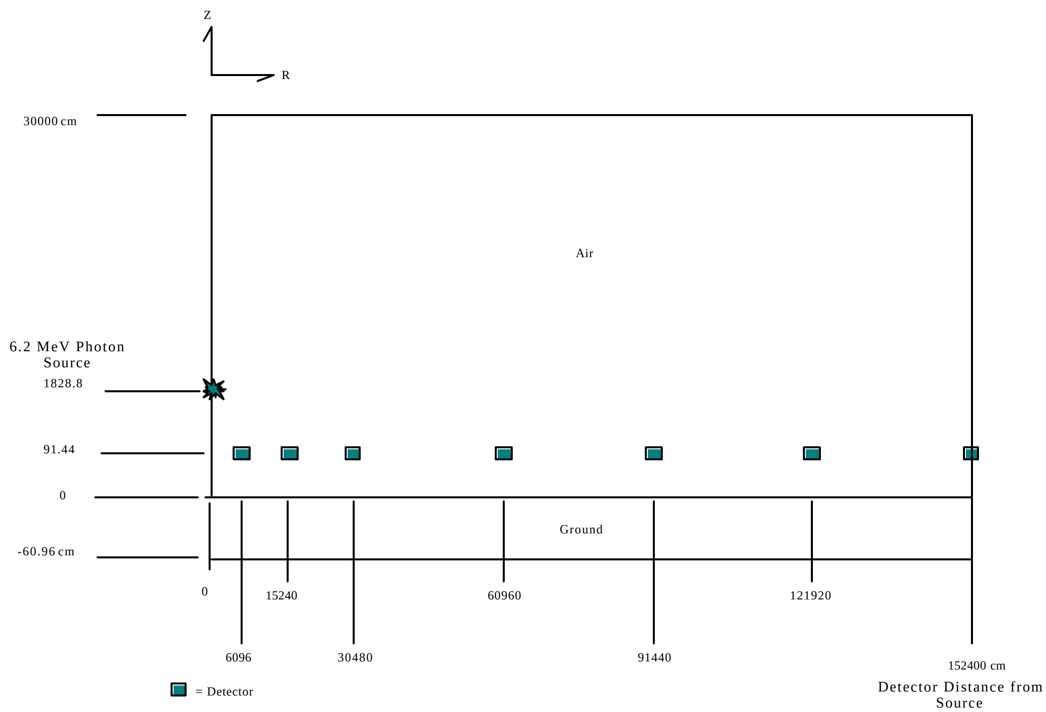

Figure 1. Two-Dimensional Cylindrical Configuration for Reference Calculation Problem I.1 of ANSI/ANS 6.6.1.

2.4.2 Results for ANSI/ANS 6.6.1 Reference Calculation Problem I.1

Results for preliminary validation of PARTISN 2.99 in modeling Reference Problem I.1 are presented in Table I. It is important to understand that a deterministic code which discretely solves the transport equation has a much smaller "target" to hit than that of a stochastic code theoretically based on normal distributions that produce results with associated uncertainties, such as MCNP. This is best illustrated by performing a hand-calculated uncollided flux using a point kernal method. The difficulty of matching an experimental value with the solution of a single equation is due to all the other particle events occurring at the time, e.g., scattering or absorption in air, skyshine, etc., that may not be accounted for in the equation. The difficulty increases as distance from the source increases, as shown in Table 1, with differences of 2-55%.

With this understanding, comparison of Reference Calculation I.1 results to the PARTISN 2.99 results in Table I show relative agreement (37 % difference or less with the outside values of the given Reference Calculation Compilation range, relative to the maximum 55%) as long as the first collision source treatment is applied. Reference Calculation I.1 results show an improving agreement without the first collision source treatment as distance from the source increases, but overall consistency and a smaller % difference from the standard is achieved with the first collision source treatment employed.

Because of ray effects, a ray-tracing first collision source treatment is applied [6]. The computer generated uncollided flux file is used to create a first collision source, which is then fed to the code discrete ordinate solver as a distributed fixed source. The resulting flux distribution from the first collision source calculation is added to the uncollided flux distribution to get the total flux rate in each calculational cell. The detector response is calculated from this total flux distribution. TECPLOT 9.0 is used to graphically illustrate the effective mitigation of ray effects by the use of the ray-tracing first collision source treatment for the Problem I.1 reference calculation.

R-Z geometry is used for the model because X-Y geometry results in a line source and line detector at a single point in space, underestimating the total dose contribution from the isotropic source. R-Z geometry produces a ring source and detector, which considers the total dose contribution from the isotropic source, but that results in the same dose at all points.

Numerical results for input file 12ans6611 (708 by 602 mesh) are the same for versions 2.64 and 2.99 [7], and computer run times were both about 8 minutes using 64 processors. Results for input file 15ans6611 using version 2.99 converged, whereas the results for version 2.64 did not [7]. Run time for version 2.64 using 1 processor was about 150 hours. Run time for version 2.99 using 32 processors was 14 minutes.

Table I. Results Comparison Between ANSI/ANS 6.6.1 Reference Calculation I.1 and Calculational Model Using PARTISN 2.99

Benchmark Problem I.1 Radius	Reference Calculation Problem I.1 Compilation of 7 Code Results (Absorbed Dose)	Hand Calculated Uncollided Flux (Point Kernel)		PARTISN Calculated Absorbed Dose W/out First Collision Source Treatment 12ANS6611.299.rz.o		PARTISN Calculated Absorbed Dose W/ First Collision Source Treatment 15ANS6611.rz.ray2.o	
(ft) (cm)	(rads/yr)	(rads/yr)	(% difference)	(rads/yr)	(% difference)	(rads/yr)	(% difference)
200 (6096)	9.0E-11 to 1.0E-10	8.82E-11	2	8.25E-12	91	7.43E-11	17
500 (15240)	1.5E-11	1.15E-11	23	2.47E-12	84	9.77E-12	35
1000 (30480)	2.5E-12	1.82E-12	27	5.95E-13	76	1.63E-12	35
2000 (60960)	2.5E-13 to 3.5E-13	1.81E-13	28	9.96E-14	60	1.59E-13	37
3000 (91440)	5.0E-14 to 7.5E-14	3.19E-14	36	2.28E-14	54	3.53E-14	29
4000(121920)	1.5E-14 to 2.0E-14	7.10E-15	53	6.49E-15	57	1.01E-14	33
5000(152400)	4.0E-15 to 6.0E-14	1.80E-15	55	1.71E-15	57	2.53E-15	37

2.4.3 ANSI/ANS 6.6.1 Reference Calculation Problem I.2

The configuration for Problem I.2 is identical to Problem I.1 except for the presence of a 4 foot thick concrete rectangular building around the point source. The height of all four concrete walls is 62 feet, and the inside dimensions of the building are 100 feet by 150 feet. There is no roof. X-Y-Z geometry is used for the Problem I.2 model. Detectors are positioned as for Problem I.1. See Figure 2 for a graphical representation.

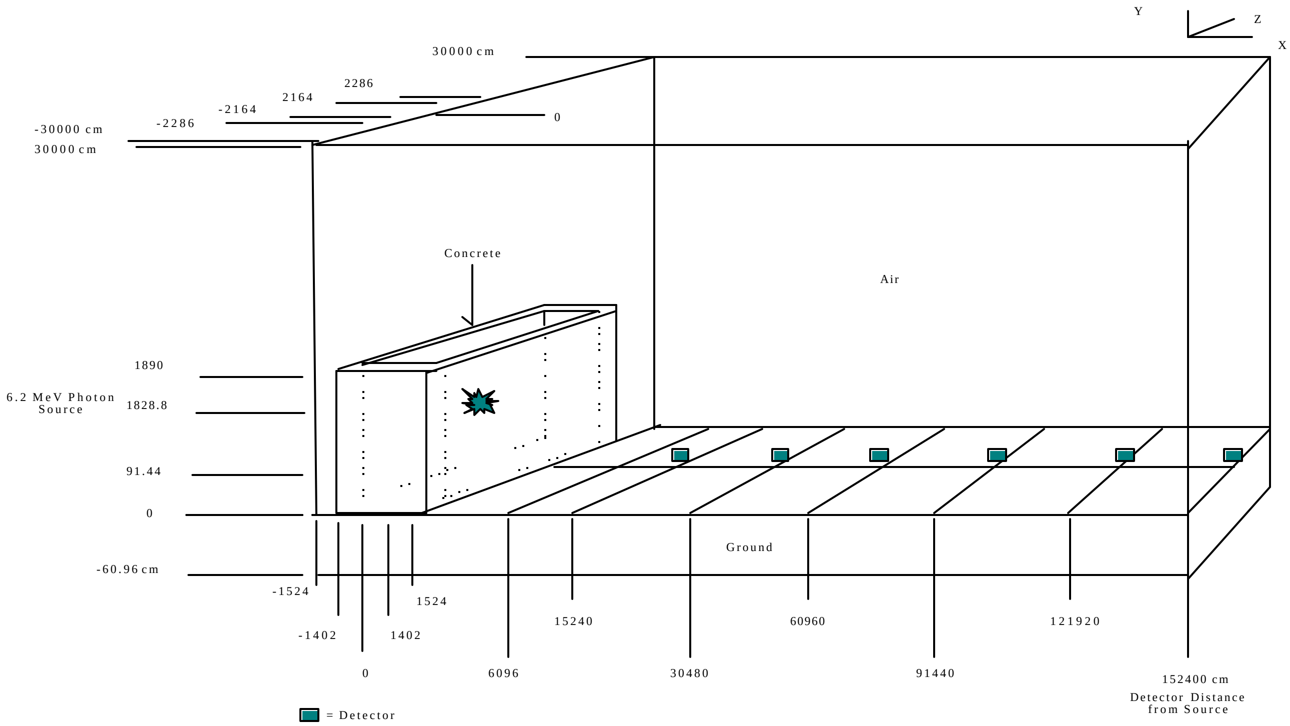

Figure 2. Three-Dimensional Configuration for Reference Calculation I.2 of ANSI/ANS 6.6.1

2.4.4 Results for ANSI/ANS 6.6.1 Reference Calculation Problem I.2

Results for preliminary validation of PARTISN 2.99 in modeling Reference Problem I.2 are presented in Table 2. Because of ray effects, a ray-tracing first collision source treatment is applied [6]. TECPLOT 9.0 is used to graphically illustrate the effective mitigation of ray effects by the use of the ray-tracing first collision source treatment for the Problem I.2 reference calculation.

Comparison of the Reference Calculation I.2 results to the PARTISN 2.99 results in Table II show relative agreement (less than 30 % difference with the outside values of the Reference Calculation Compilation range) except for the first detector closest to the source, with the first collision source treatment applied. As with problem I.1, problem I.2 results show an improving agreement without the first collision source treatment as distance from the source increases, but overall consistency and a smaller % difference from the standard is achieved with the first collision source treatment.

Numerical results for input file 7ans6612 are identical for versions 2.64 and 2.99 [7]. Run time for version 2.64 using 32 processors was 36 hours, but for version 2.99 using 64 processors was only 44 minutes. In an interesting twist, numerical results for input file 10ans6612 using version 2.99 and 16 or 32 processors are almost identical with input file 10ans6612 using version 2.64 and only 1 processor (input file 8ans6612)[7]. Run time for 10ans6612 using version 2.99 and 32 processors was 115 minutes, while run time for 10ans6612 using version 2.99 and 16 processors was 243 minutes. Numerical results for 10ans6612 are exactly the same whether using 16 processors or 32 processors.

Table II. Results Comparison Between ANSI/ANS 6.6.1 Reference Calculation I.2 and Calculational Model Using PARTISN 2.99

Benchmark Problem I.1 Radius	Reference Calculation Problem I.1 Compilation of 7 Code Results (Absorbed Dose)	PARTISN Calculated Absorbed Dose W/out First Collision Source Treatment 7ANS6612.299		PARTISN Calculated Absorbed Dose W/ First Collision Source Treatment 10ANS6612.ray2 (16 processors)		PARTISN Calculated Absorbed Dose W/ First Collision Source Treatment 10ANS6612.ray2 (32 processors)	
(ft) (cm)	**(rads/yr)**	**(rads/yr)**	**(% difference)**	**(rads/yr)**	**(% difference)**	**(rads/yr)**	**(% difference)**
200 (6096)	8.5E-13 to 2.0E-12	7.63E-12	282	5.56E-12	178	5.56E-12	178
500 (15240)	5.0E-13 to 8.0E-13	1.04E-12	30	9.93E-13	24	9.93E-13	24
1000 (30480)	1.8E-13 to 3.0E-13	3.78E-13	26	3.87E-13	22	3.87E-13	22
2000 (60960)	2.2E-14 to 6.0E-14	6.77E-14	13	6.99E-14	17	6.99E-14	17
3000 (91440)	8.0E-15 to 1.64E-14	2.11E-14	32	1.68E-14	5	1.68E-14	5
4000(121920)	1.2E-15 to 5.0E-15	6.85E-15	37	5.07E-15	1.4	5.07E-15	1.4
5000(152400)	7.0E-16 to 2.0E-15	2.15E-15	8	1.26E-15	Within range	1.26E-15	Within range

2.4.5 KSU Skyshine experiments

The Kansas State University Skyshine Experiment models use air, ground, a steel source cask and cart, a concrete structure, three different source strengths, and particle detectors [8]. See Figure 3 for the model.

2.4.6 Results for KSU Skyshine experiments

Results for preliminary validation of PARTISN 2.99 in modeling the Kansas State University (KSU) Skyshine Experiments are presented in Table III. Because of ray effects, a ray-tracing first collision source treatment is applied [6] in using the PARTISN transport code. The computer generated uncollided flux file is used to create a first collision source, which is then fed to the code discrete ordinate solver as a distributed fixed source. The resulting flux distribution from the first collision source calculation is added to the uncollided flux distribution to get the total flux rate in each calculational cell. The detector response is calculated from this total flux distribution.

Comparison of the KSU Skyshine Experiments results to the PARTISN 2.99 results in Table 3 show agreement (34 % difference with experimental results) whether or not the first collision source treatment is employed. However, there is no correlation between agreement with the results and increased distance from the source as was shown with the ANSI/ANS 6.6.1 Reference Calculations. This may be due to the impact of scattering from the steel cask, steel cart, and concrete walls in the KSU configuration. The ray-tracing first collision source treatment redistributes the uncollided flux as a distributed source. The ray-tracing technique appears to have mitigated the ray effects, but subsequently overestimated the dose to different degrees at various detectors.

TECPLOT 9.0 is used to graphically illustrate the effective mitigation of ray effects by the use of the ray-tracing first collision source treatment for all KSU experiments.

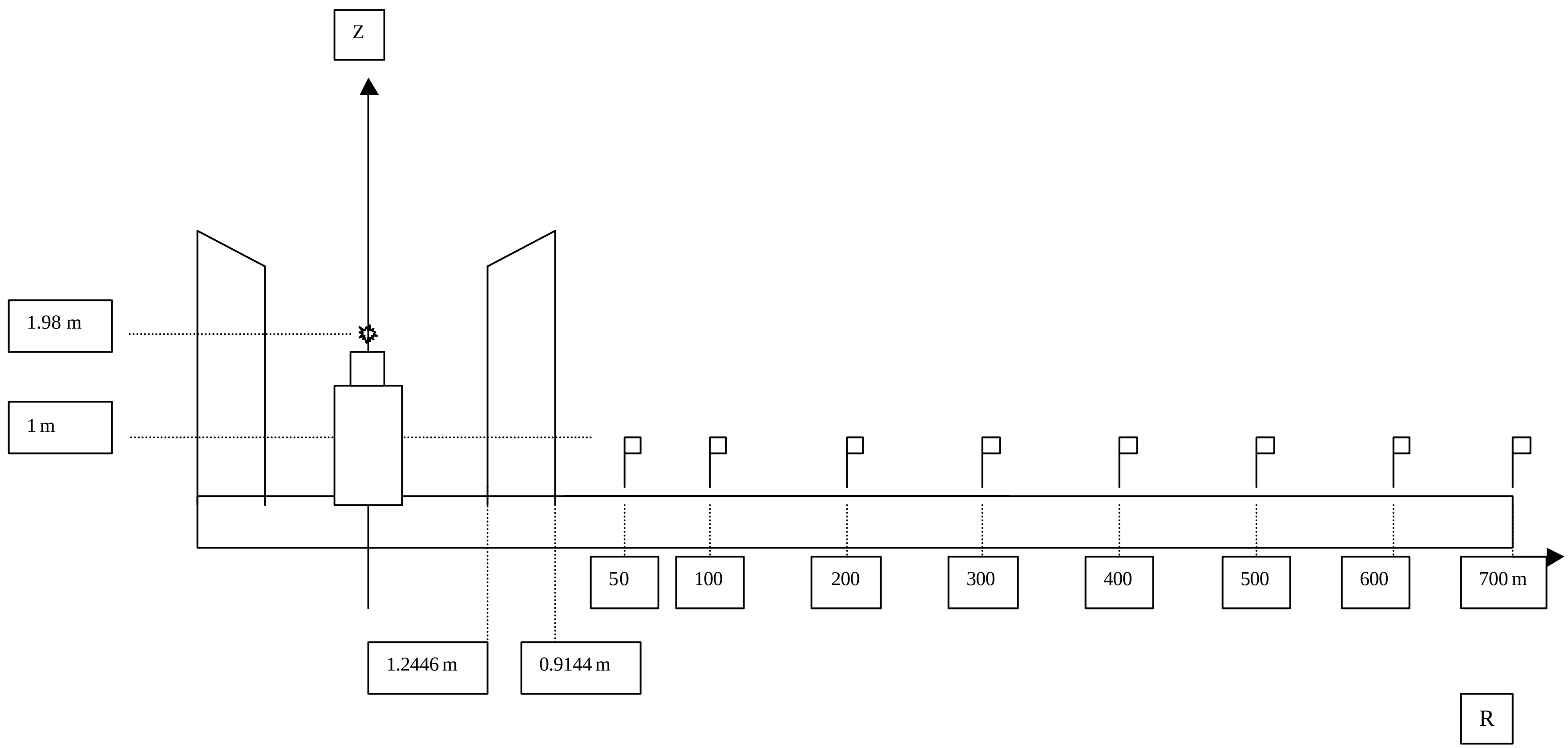

Figure 3. Cylindrical Configuration for Kansas State University Skyshine Experiments.

Table III. Results Comparison Between KSU Skyshine Experiment with Various ^{60}Co Sources and Calculational Model Using PARTISN 2.99

Experiment Distance from Silo Wall to Detector	^{60}Co Source Strength	Experimental Results	MCNP Calculated Result		PARTISN Calculated Result Without First Collision Source Treatment (64 processors)		PARTISN Calculated Result With First Collision Source Treatment (32 processors)	
(cm)	**(Ci)**	**(mR/hr/Ci)**	**(mR/hr/Ci)**	**(± %)**	**(mR/hr/Ci)**	**(% difference)**	**(mR/hr/Ci)**	**(% difference)**
5000	10.33	24.24	23.95	0.61	30.03	19	32.46	25
10000	10.33	9.66	9.17	0.84	11.18	13	12.13	20
20000	10.33	2.425	2.415	0.73	2.99	9	3.25	25
30000	229.1	0.76	0.851	0.44	1.03	26	1.10	31
40000	229.1	0.31	0.327	0.37	0.398	22	0.431	28
50000	229.1	0.117	0.135	0.40	0.161	27	0.178	34
60000	3804	0.0542	0.0541	1.18	0.0587	8	0.0667	19
70000	3804	0.0244	0.0235	1.15	0.0171	30	0.0196	20

3. CONCLUSIONS

The installation of PARTISN 2.99 is verified because of excellent agreement between the results of the problems provided by the code developer (LANL) and the results attained by the user's (Y-12) execution of the same problems. Because of acceptable agreement of 30-50% for shielding applications for discrete ordinate transport codes, the preliminary validation of PARTISN 2.99 is successful. The use of TECPLOT 9.0 to graphically illustrate the results of validation reference calculations and benchmarks with the use of the first collision source treatment is extremely useful in helping the analyst determine where a CAAS detector could be placed and still detect a certain minimum dose or activity. The contour feature of TECPLOT is an excellent tool to graphically generate specific locations of isodose levels and curves from PARTISN 2.99 output.

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REFERENCES

1. ANSI/ANS 8.3, *Criticality Accident Alarm Systems* (1997), American Nuclear Society, 555 North Kensington Avenue, LaGrange Park, Illinois, 60525, American National Standards Institute, Inc. 5/28/97.
2 DANTSYS 3.1, *One-, Two- and Three-Dimensional Multigroup Discrete Ordinates Transport Code System*, CCC-547, contributed by Los Alamos National Laboratory as LA-12969-M, Los Alamos New Mexico, distributed by the Radiation Safety Information Computational Center (RSICC), Oak Ridge National Laboratory, Oak Ridge, Tennessee, March, 1997.
3. *Conversion Coefficients for use in Radiological Protection Against External Radiation*, ICRU-57, International Commission on Radiation Units and Measurements, Bethesda, Maryland, August 1, 1998.
4. ANSI/ANS 6.1.1, *Neutron and Gamma-Ray Fluence-to-Dose Factors* (1991), American Nuclear Society, 555 North Kensington Avenue, LaGrange Park, Illinois, 60525, American National Standards Institute, Inc., 8/26/91.

5. ANSI/ANS 6.6.1, *Calculation and Measurement of Direct and Scattered Gamma Radiation from LWR Nuclear Power Plants* (1987), American Nuclear Society, 555 North Kensington Avenue, LaGrange Park, Illinois, 60525, American National Standards Institute, Inc. 6/24/87.
6. R. S. Baker, *A Stochastic First Collision Source for TWODANT*, LA-UR-94-176, Los Alamos National Laboratory, Los Alamos, New Mexico, 87545, submitted to Eighth International Conference on Radiation Shielding, April 24-27, 1994, Arlington, Texas.
7. S. B. Turner, *Installation, Testing, and Demonstration of Discrete Ordinates Particle Transport Software (PARTISN 2.64/DANTSYS3.1) on the Y-12 National Security Complex Supercomputer (Manhattan*), Y/DD-1001, Revision 0, Y-12 National Security Complex, May 2002. (Unclassified)
8. R.H. Olsher, Hsiao-Hun Hsu, W.F. Harvey, Benchmarking the MCNP Monte Carlo Code with a Photon Skyshine Experiment, *Nuclear Science and Engineering*, **Volume 114**, pg 219-227, 1993.