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THE EFFECTS OF SPATIAL AND ANGULAR
RESOLUTION IN DISCRETE ORDINATE
CRITICAL-MASS CALCULATIONS

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THE EFFECTS OF SPATIAL AND ANGULAR RESOLUTION IN DISCRETE ORDINATE CRITICAL-MASS CALCULATIONS

Donald C. Coonfield and Douglas C. Hunt

Abstract. The criticality engineer often needs accurate criticality parameters at minimum cost in time and money. To aid in satisfying these requirements, a systematic study is presented of the effects of varying the number of spatial intervals and the number of angular directions in discrete ordinates critical-mass calculations on reflected and moderated systems. The calculations are done by varying the spatial and angular meshes in the Computer Code DTF-II. The results obtained are compared with experimentally measured critical masses. Based on these comparisons and on the asymptotic behavior of computed critical masses as the space-angle mesh is refined, criteria for space-angle mesh specification are obtained. One specific conclusion is that for all the systems studied S_{16} calculations are necessary.

INTRODUCTION

In nuclear material processing plants the need for critical parameters obtained quickly, accurately, and with minimum expense frequently arises. The Computer Code DTF-II(1)¹ has long been used to obtain some of these parameters. The purpose of the report is to present some general space-angle mesh criteria needed for DTF calculations by the criticality engineer to obtain results in a more efficient manner. To this end, the effects of spatial and angular resolution in several types of reflected and moderated systems are investigated. The systems most extensively studied are highly enriched (93.2 percent ^{235}U) uranium metal spherical shells which are reflected and internally moderated by oil. The shell inner radius is varied from zero (solid sphere) to infinity (infinite slab). The 4- and 12-centimeter (cm) inner radius calculational data have been presented in an earlier article(2). The current report gives new results for critical spheres and slabs of reflected uranium

metal along with the computed shell results for comparison purposes. The critical masses of such systems have been measured at the Rocky Flats Plant, Nuclear Safety Laboratory. A complete description of these measurements has been reported by Tuck(3).

Two additional series of DTF calculations are given to investigate the possibility of extending the mesh criteria obtained for the uranium metal systems to uranium solution systems(4,5).

To further test the mesh criteria obtained for the uranium metal systems, the critical mass of (1) a water-reflected plutonium metal sphere, and of (2) water-reflected plutonium nitrate solution spheres at two concentrations is determined using the optimum mesh specification. These results are compared with experiments(6,7).

CALCULATIONAL METHOD

The DTF Code is used for all the critical-mass calculations. It is a later development of Carlson's S_n method(8) which approximates a solution to the Boltzmann transport equation by difference techniques. The DTF Code converges on a quantity λ (lambda) with a specified precision ϵ (epsilon). A problem is terminated when the quantity is within the specified ϵ of unity. Because of the precision specified in the calculations, the critical dimensions are reported to two significant decimal digits only. A more extensive discussion has been reported by the authors earlier(9).

Table I lists the contents and densities of materials used in the calculations. In all cases, the Hansen and Roach 16-group neutron, cross sections are used(10). Uniform fission densities of one neutron per cubic centimeter for each spatial interval are applied as the initial source distribution for the problems.

¹ Numerals in parentheses relate to bibliography at end of text.

TABLE I. Composition and Densities of Materials Used in the Transport Computations.

System	Region	Material	Density grams per (cubic centimeter)
Uranium Metal	Fuel	Uranium (93.12 weight percent uranium 235 and 6.88 weight percent uranium 238)	18.1 grams of uranium
	Moderator and Reflector	Oil $\left(\frac{\text{Hydrogen}}{\text{Carbon}} = 1.82\right)$	0.024
Low Density Uranyl Fluoride (UO_2F_2)	Fuel	Oil $\left(\frac{\text{Hydrogen}}{\text{Carbon}} = 1.82\right)$	0.88
	Reflector	Water	1.0
High Density UO_2F_2	Fuel	UO_2F_2 $\left(\frac{\text{Hydrogen}}{\text{Uranium 235}} = 524\right)$	0.494 grams of uranium 235
	Reflector	Water	1.0
Plutonium Metal	Fuel	UO_2F_2 $\left(\frac{\text{Hydrogen}}{\text{Uranium 235}} = 49.9\right)$	0.483 grams of uranium 235
	Reflector	Water	1.0
Low Density Plutonium Nitrate	Fuel	Plutonium (94.8 weight percent plutonium 239 and 5.2 weight percent plutonium 240)	19.74 grams of plutonium
	Reflector	Water	1.0
High Density Plutonium Nitrate	Fuel	Plutonium (95.4 weight percent plutonium 239 and 4.6 weight percent plutonium 240) $\left(\frac{\text{Hydrogen}}{\text{Plutonium 239}} = 780\right)$	0.033 grams of plutonium
	Reflector	Water	1.0

RESULTS

Figures 1, 2, 3, and 4 give the computed critical masses of respectively, the oil reflected or moderated uranium metal sphere, 4-cm shell, 12-cm shell, and infinite slab as they depend on the space-angle mesh. The plots are parametric in n (of S_n) and have the spatial mesh as the independent variable. In Figures 1 through 4, the approach to asymptotic

behavior is essentially the same for all angular specifications implying the spatial mesh may be specified independent of the angular mesh. From these figures, a mesh of 25 spatial intervals in each of the moderator, fuel, and reflector regions (corresponding to approximately one mesh point every three mean-free paths for thermal neutrons) usually saturates the effect of adding more mesh points. A 40-point mesh always saturates the effect. The plots in the

FIGURE 1. The calculated critical masses of oil reflected spheres of uranium metal as a function of spatial and angular variation.

FIGURE 2. The calculated critical masses of four-centimeter inner radius uranium-metal shells as a function of spatial and angular variation.

FIGURE 3. The calculated critical masses of twelve-centimeter inner radius uranium-metal shells as a function of spatial and angular variation.

FIGURE 4. The calculated critical thickness of uranium-metal slabs as a function of spatial and angular variation.

figures assume unsaturated (10 point) meshes in regions other than the one in which the space mesh is being varied. The asymptotic values will usually be different as the mesh is refined, if saturated meshes are used in the other regions. However earlier work(2) shows that this does not change the mesh refinement needed to saturate the effect of adding more mesh points.

The above treatment was also applied to uranium solution systems (see Table I for a description) to determine if similar mesh specification criteria apply. These results appear in Figures 5, 6, 7, and 8. Figures 5 and 6 give the space mesh variation effect (for S_{16} calculations) on the low and high concentration solutions, respectively. In the calculations, the number of mesh points in the fuel and reflector regions are varied simultaneously. A 35-point mesh in each region nearly saturates the effect of adding more mesh points. This corresponds in the fuel region to approximately one mesh point every thermal neutron mean-free path. Figures 7 and 8 show the variation in critical radius with the order of angular quadrature for the low and high concentration uranium solution systems. The 35-point space mesh is assumed in the fuel and reflector regions. Asymptotic behavior is approached for

S_n ($n=16$) calculations, but even a higher quadrature order appears needed to completely saturate the angular mesh dependence.

The computed and experimental results for the reflected plutonium metal sphere and the reflected plutonium solution spheres (specified in Table I) are given in Table II. The use of an optimum mesh specification (S_{16} and space mesh points every two thermal neutron mean-free paths) in these cases is described in the conclusions.

FIGURE 5. The calculated critical radius of the 49.4-gram uranium 235 per liter uranyl fluoride system as a function of the number of spatial intervals in both material regions.

FIGURE 6. The calculated critical radius of the 483-gram uranium 235 per liter uranyl fluoride system as a function of the number of spatial intervals in both material regions.

FIGURE 7. The calculated critical radius of the 49.4-gram uranium 235 per liter uranyl fluoride sphere as a function of the angular variation.

FIGURE 8. The calculated critical radius of the 483-gram uranium 235 per liter uranyl fluoride sphere as a function of the angular variation.

TABLE II. A Comparison of the Calculated Results, Using the Proposed Criteria, with Experimental Results.

System	Fuel Region Critical Radius	
	Calculated Results	Experimental Results
	(centimeters)	
Low Density Uranyl Fluoride (UO_2F_2)	$r = 15.88$	$r = 16.002$
High Density UO_2F_2	$r = 11.44$	$r = 11.418$
Plutonium Metal	$r = 4.13$	$r = 4.12$
Low Density Plutonium Nitrate	$r = 16.88$	$r = 17.78$
High Density Plutonium Nitrate	$r = 12.83$	$r = 14.61$

CONCLUSIONS

The study indicates that to eliminate effects in discrete ordinates calculations due to mesh specification, one should (1) use 17 angular directions at least (S_{16} calculations) and (2) use a spatial mesh in each region with at least one mesh point every 2 or 3 thermal neutron mean-free paths.

The comparisons in Table II show that applying these mesh criteria, and using Hansen-Roach cross sections, give good calculation-experiment agreement for plutonium metal and uranium solution systems. In earlier work(2), the authors show that these criteria, with a modified Hansen-Roach cross section set, give good agreement with experiment on the uranium metal systems discussed earlier. The plutonium-solution systems calculations are conservative but not in good agreement with the experimental results. Possibly a modified 16-group cross section set is needed for plutonium solutions. A similar experiment-theory discrepancy, where Monte Carlo calculations with Hansen-Roach cross sections are used, has been reported by Dickinson(11).

BIBLIOGRAPHY

1. B. G. Carlson, W. J. Worlton, W. Guber, and M. Shapiro. "DTF Users Manual." *UNC Physics—Mathematics 3321*. United Nuclear Corporation. White Plains, New York. Volume I, November 1963. Volume II, May 1964.
2. D. C. Hunt and D. C. Coonfield. "Enriched Uranium Metal Criticality Calculations." *Nuclear Technology*, 12:260. 1971.
3. G. Tuck. *Enriched Uranium—Metal Measurements, No. 1*. RFP-907. Rocky Flats Division, The Dow Chemical Company. Golden, Colorado. July 26, 1967.
4. J. L. Thomas. "Critical Parameters of U^{235} — Enriched Solutions in Spherical Geometry." ORNL-1926. *Physics Division, Semiannual Progress Report for Period Ending March 10, 1955*. Oak Ridge National Laboratory, Oak Ridge, Tennessee. September 7, 1955.
5. J. K. Fox, L. W. Gilley, and D. Callihan. *Critical Mass Studies, Part IX Aqueous U^{235} Solutions*. ORNL-2367. Oak Ridge National Laboratory, Oak Ridge, Tennessee. March 4, 1958.
6. D. R. Smith and W. U. Geer. "Critical Mass of a Water-Reflected Plutonium Sphere." *Nuclear Applications and Technology*, 7:405. November 1969.
7. C. R. Richey. "Theoretical Analysis of Homogeneous Plutonium Critical Experiments." *Nuclear Science and Engineering*, 31:32. 1968.
8. *Methods in Computational Physics. Statistical Physics Volume 1*. Editors, Berni Alder et al. Academic Press Company, New York. 1963.
9. D. C. Coonfield and D. C. Hunt. *The Effects of Spatial Resolution on Critical Mass Calculations*. RFP-1133. Rocky Flats Division, The Dow Chemical Company, Golden, Colorado. May 31, 1968.
10. G. E. Hansen and W. H. Roach. *Six and Sixteen Group Cross Section for Fast and Intermediate Critical Assemblies*. LAMS-2543. University of California, Los Alamos Scientific Laboratory, Los Alamos, New Mexico. December 1960.
11. Deanne Dickinson. *Calculational Study of Arrays of Cylinders of Fissile Solution*. RFP-1821. Rocky Flats Division, Dow Chemical U.S.A., Golden, Colorado, March 24, 1972.