



**Effect of Particle Histories Termination Parameters  
on Monte Carlo Estimates in Fusion Reactor  
Blanket Scoping Studies**

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**February 1977**

**UWFDM-192**

***FUSION TECHNOLOGY INSTITUTE  
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UWFDM-192

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Effect of Particle Histories Termination Parameters on  
Monte Carlo Estimates in Fusion Reactor Blanket  
Scoping Studies

By

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May 1977

UWFDM-192

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## Abstract

For survey and scoping studies of reactor blankets by Monte Carlo, where small numbers of processed particles are considered, the effect of the particle histories termination parameters by Russian Roulette, on tritium production estimates, is studied. For such a small number of histories, slight trends in the results occur depending on the choice of the particle survival probabilities and the Russian Roulette triggering weights, and justify the use of the 95% confidence interval, rather than the 68% confidence interval for more reliable results, if no prior analysis is carried out. If such an analysis for the choice of these parameters is done, then the 68% confidence interval can still be used. Results from Monte Carlo for a sample size of 1000 particles are compared in this study to the results from an  $S_4 - P_3$  discrete ordinates calculation with satisfactory agreement, within two standard deviations.

It is recommended that one use the highest possible (e.g. 90%) survival probability and the lowest possible (e.g.  $10^{-8}$ ) Russian Roulette triggering weights, so as not to greatly affect the resulting computation time and at the same time control any bias in the results.

The collision estimator has been used in the investigation.

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## 1. Introduction

The current and expected future interest in both conventional and advanced power reactor systems safety necessitates dependable three-dimensional studies of fission, fusion and hybrid systems. This is where the Monte Carlo method finds its natural field of application and is superior to discrete methods. It also incorporates the possibility of time-dependent studies, and detailed cross sections representation when needed. Monte Carlo techniques may be designed to reproduce a physical system in as much detail as is necessary, and so provide a powerful tool for solving problems with very few compromises with the physics. Discrete ordinates is quite powerful for solving time independent two-dimensional problems; much work has been done in recent years to increase the speed of calculations and reduce ray effects. Three-dimensional or two-dimensional-time-dependent discrete calculations are not yet practical. Monte Carlo calculations on the other hand can include three-dimensional geometries of arbitrary complexity and also time dependence. Parallel computers are now being designed for future applications of Monte Carlo, where many particles can be followed in a simulation instead of the present sequential approach.

The shielding community tends to depend more heavily on discrete ordinates methods except in cases where the geometry is complex. At ORNL, discrete ordinates calculations have been coupled to Monte Carlo calculations, where the former treats the problem in a two-dimensional way, and the latter treats parts which are three-dimensional in their nature.<sup>(12)</sup> At Bettis Laboratory, Monte Carlo is used mostly for methods testing.<sup>(12)</sup> However,

at Los Alamos, Cashwell<sup>(12)</sup> reports that: "The reverse is happening; in that Monte Carlo is being used much more than ever before. A lot of problems have very difficult geometries, and in addition some people are not willing to compromise on the treatment of the cross sections." At Livermore also, some codes use as many as 2000 group cross sections. Whitesides<sup>(12)</sup> reports that: "Monte Carlo is used to check the accuracy of the discrete ordinates calculations. In criticality calculations, for the same geometry and the same cross sections, Monte Carlo does as well as any other method."

In fusion reactor blanket studies, Ragheb and Maynard<sup>(3,4)</sup> used Monte Carlo for three-dimensional cell calculations. They also used it for three-dimensional parametric scoping studies. In the USSR,<sup>(13)</sup> Monte Carlo is also used for scoping studies. Steiner<sup>(7)</sup> used Monte Carlo as a standard for assessing the effect of using different quadrature orders in discrete ordinates calculations on tritium breeding estimates, for a standard blanket model. Chapin<sup>(5)</sup> uses Monte Carlo to treat a hexagonal toroid blanket model. Abdou, Milton, Jung and Gelbard<sup>(11)</sup> used Monte Carlo in a cylindrical model to study the effects of vacuum pumping and beam penetrations in an experimental tokamak power reactor design.

In magnetic confinement systems, Monte Carlo is expected to find wider application in the future in the treatment of three-dimensional cell calculations, and of penetrations for radio frequency heating, neutral beams, fuel injection, vacuum pumping, divertor slots, and for maintenance and access. This is necessary to protect the magnets and auxiliary systems from



streaming and scattered components of radiation, which may cause excessive heating, induced activation, and radiation damage. Also in inertial confinement systems, Monte Carlo will be needed to study the three-dimensional nature of laser or electron beams penetrations, and for protection of the optical transport, and of the cryogenic pellet fabrication and injection systems.

With complete reliance in the past on one-dimensional discrete ordinates methods, for the treatment of fusion reactor blankets, and with Monte Carlo entering the picture for more sophisticated calculations, discrepancies between results obtained by Monte Carlo and by discrete ordinates appeared in the reported results of several authors. Ragheb and Maynard<sup>(3)</sup> attributed the difference in results in their work to the different natures of their discussed one-dimensional and three-dimensional models as regards compositions and configurations, and excluded the possibility of an error in their modified version of the Monte Carlo code<sup>(1,2,3)</sup> employed by a comparative one-dimensional benchmark calculation using both discrete ordinates and Monte Carlo.

Chapin<sup>(5)</sup> considered the one-dimensional case of an infinite cylinder consisting of a one region blanket composed of homogenized niobium structure and lithium with volume fractions of 6% and 94% respectively, and solved it by Monte Carlo and discrete ordinates. The results of his calculations for tritium breeding from  $L_1-6$  and  $L_1-7$  are shown in Table 1. The Monte Carlo code used in the investigation was the MORSE<sup>(1,2)</sup> code with combinatorial geometry. The ANISN<sup>(5)</sup> discrete ordinates transport code was also used. A seven group neutron cross section set was formed by collapsing a 52 group

Table 1 Comparison of Monte Carlo and Discrete Ordinates Results for Tritium Production Per Source Neutron. Infinite Cylinder case<sup>†</sup> of a One Region Blanket Composed of Homogenized Structure and Lithium.

Zone Number	Zone Radii (cm)	T6, reactions per source neutron from L <sub>i</sub> <sup>6</sup>		T7, reactions per source neutron from L <sub>i</sub> <sup>7</sup>	
		D. O.	Monte Carlo	D. O.	Monte Carlo
1	230 - 240	0.106030	0.104880 ± 0.001490	0.059081	0.059909 ± 0.001434
2	240 - 250	0.087218	0.083785 ± 0.001198	0.036885	0.038207 ± 0.002029
3	250 - 260	0.069766	0.068753 ± 0.000941	0.022941	0.023350 ± 0.000699
4	260 - 270	0.054142	0.053345 ± 0.000977	0.014200	0.014918 ± 0.000561
5	270 - 280	0.040322	0.039758 ± 0.000624	0.008731	0.009839 ± 0.000646
6	280 - 290	0.027952	0.027520 ± 0.000682	0.005296	0.006220 ± 0.000410
Total, Zones 1-6		0.385430	0.378040 ± 0.002520	0.147130	0.152940 ± 0.002750
Total, Whole Blanket		0.818900	0.824430 ± 0.011250	0.654070	0.625680 ± 0.004760

Total (T6 + T7): D. O. 1.472970  
Monte Carlo 1.450110 ± 0.012216

<sup>†</sup> From: D. L. Chapin, "Comparative analysis of a fusion reactor blanket in cylindrical and toroidal geometry using Monte Carlo", MATT-1234, Princeton University, Plasma Physics Laboratory, March, 1976.

set over the benchmark blanket<sup>(7)</sup> spectrum. The anisotropic scattering was represented by a  $P_3$  Legendre expansion, and  $S_8$  quadrature for the discrete ordinate calculations. Chapin reports that: "the T7 values agree well for the inner zones, but are within about two standard deviations for the outer zones. The total rates in the six zones and in the entire blanket are in closest agreement for T6, and differ by less than 5% for T7. These differences might arise from several factors, such as the small number of cross section groups, the Legendre expansion order of the anisotropic scattering, the angular quadrature order, or the number of mesh intervals used in the vacuum zone for the ANISN calculation." Even though there is a good agreement between the Monte Carlo and discrete ordinate results, one notices that the total (T6 + T7) D.O. (discrete ordinates) result does not lie within one s.d. (standard deviation) of the M.C. (Monte Carlo) result, the total T7 from D.O. within 3 s.d., the T7 in zones 1-6 within 2 s.d., and the T6 in zones 1-6 within 2 s.d. The M.C. result for T7 is larger than the D.O. result in the first 6 zones, but lower over the whole blanket, and for T6 it is lower in the first 6 zones, but larger over the whole blanket.

Monte Carlo being free from the effect of the angular quadrature used in discrete ordinates calculations, Steiner<sup>(7)</sup> used a Monte Carlo calculation with a large number of histories for the standard blanket model as a basis to assess different  $S_N$  results. Results of his calculations are displayed in Table 2. He concludes: "For the assumed blanket geometry, the  $S_4$  approximation gives a system tritium breeding value which is within  $\pm 0.5\%$  of the

Table 2 Comparison of Monte Carlo and Discrete Ordinates Results For Tritium Production Per Source Neutron. The Standard Blanket Case<sup>†</sup>.

Region	P <sub>3-S</sub> <sub>4</sub>	P <sub>3-S</sub> <sub>8</sub>	P <sub>3-S</sub> <sub>12</sub>	P <sub>3-S</sub> <sub>16</sub>	Monte Carlo
	T7				
4	0.0806	0.0780	0.0762	0.0763	0.0752 ± 0.0009
6	0.2812	0.2818	0.2857	0.2858	0.2847 ± 0.0023
7	0.1098	0.1149	0.1168	0.1165	0.1153 ± 0.0017
8	0.0458	0.0467	0.0472	0.0471	0.0472 ± 0.0011
10	0.0009	0.0008	0.0008	0.0008	0.0009 ± 0.0001
T7 Totals	0.5183	0.5222	0.5267	0.5265	0.5233 ± 0.0032
T6					
4	0.0480	0.0476	0.0471	0.0472	0.0467 ± 0.0004
6	0.2912	0.2895	0.2883	0.2884	0.2880 ± 0.0013
7	0.2364	0.2371	0.2370	0.2369	0.2369 ± 0.0010
8	0.2944	0.2957	0.2960	0.2959	0.2946 ± 0.0020
10	0.0634	0.0639	0.0640	0.0640	0.0655 ± 0.0012
T6 Totals	0.9334	0.9338	0.9324	0.9324	0.9317 ± 0.0028
T6 + T7 Totals	1.45170	1.44558	1.4591	1.4589	1.4550 ± 0.004252

<sup>†</sup> From: D. Steiner, "Analysis of a benchmark calculation of tritium breeding in a fusion reactor blanket: The United States calculation", ORNL-TM-4177, April, 1973.

Monte Carlo system value. Thus, the  $S_4$  approximation is adequate for survey calculations on system tritium breeding. An  $S_{12}$  approximation is recommended in those cases where accurate spatial information is desired." The ENDF/B-III cross sections data were used for both calculations. Discrepancies in the D.O. results were attributed to differences in the angular quadrature sets used, the negative-flux correction algorithms (for coarse mesh spacing), the mesh size taken in the vacuum region, the niobium resonance capture cross sections and the elastic scattering matrices (due to differences in the flux weighting functions). The M.C. and D.O. results compare favorably. Careful scrutinization, however, reveals some discrepancies. The total (T6 + T7) D.O. for  $P_3 - S_8$  does not lie within 1 s.d. of the M.C. result, the total T7 D.O. result for  $P_3 - S_{12}$  and  $P_3 - S_{16}$  within 1 s.d. of the M.C. result, and the total T7 for  $P_3 - S_4$  within 2 s.d. One also notices that  $P_3 - S_{12}$  and  $P_3 - S_{16}$  results are higher than the M.C. results, and that the  $P_3 - S_4$  and  $P_3 - S_8$  are lower for the total T7 and (T6 + T7).

Our concern is the causes and magnitudes of discrepancies obtainable in M.C. calculations; a subject which has not yet been reported in the open literature.

In this work, we follow an approach similar to, but in reverse to, the one adopted by Steiner; in the sense that we choose a D.O. calculation to assess the effect of using different parameters in a M.C. calculation. Our primary interest here is the effect of choosing different Russian Roulette parameters on tritium breeding estimates. Russian Roulette is here considered as a (necessary) means for terminating particle histories and not

as an importance sampling device. We are also concerned with small numbers of generated particles histories as would generally be used in scoping and optimization studies. We follow an empirical approach, and discover, in fact, that some minimal trends do occur for different choices of particle histories termination parameters, when small numbers of histories are used to obtain estimates. Suggestions for handling the situations encountered are proposed.

In the next sections, the Russian Roulette technique in Monte Carlo calculations is briefly discussed, the physical model for our investigation, via the standard blanket model, and the estimator employed is exposed, the cross section data are summarized, and the results of the investigation are shown, followed by a set of conclusions and recommendations.

## 2. The Russian Roulette Technique in Monte Carlo Calculations

"Russian Roulette" and "Splitting" as variance-reducing techniques were developed by von Neumann and Ulam as well as Harris and Herman Kahn around 1948.<sup>(8)</sup> It is a fractional sampling method which can be applied in the following manner: when the number of particles gets too large in a simulation, one of them is picked out and with some probability ( $p$ ) is discarded from the sample; otherwise it is allowed to survive but its weight (originally unity) is multiplied by  $(1 - p)^{-1}$ . This is repeated until the number of particles is reduced to manageable size. To increase the sample size, "splitting" can be used where a particle of weight  $W_0$  may be replaced by  $n$  identical particles of weights  $W_1, W_2, \dots, W_n$ , where  $\sum_{i=1}^n W_i = W_0$ , which then proceed independently in the simulation. By such weighting methods, the total number

of tracks and their relative numbers in various regions of space or ranges of energy can be controlled, thus providing a form of importance sampling. One then should arrange for the number of paths in any class to be proportional to the contribution of that class to the final result, and for avoidance of paths which do not contribute much to the final answer. The formal definition of the Russian Roulette estimator is treated by Spanier and Gelbard.<sup>(9)</sup>

In Monte Carlo simulations, even though Russian Roulette may not be used as an importance sampling method, it is nevertheless always needed for termination of particle histories when we are not interested in them anymore.<sup>(10)</sup> We are considering Russian Roulette in the present work in that context and not as an importance sampling method.

The way it is applied in the Monte Carlo code<sup>(1,2)</sup> we are using is as follows: after a particle has suffered a collision, a test is first performed to determine if the Russian Roulette and splitting option have been specified, then a comparison of the particle's weight is made with the Russian Roulette triggering weight  $W_\ell$  (specified by the user) to determine if the particle will experience Russian Roulette. If the particle is killed, its weight is set equal to zero, and if it survives, it assumes a new weight,  $W_n$ , which is also specified by the user. The killing is performed with probability:

$$p_k = 1 - \frac{W}{W_n}$$

and the survival probability is:

$$p_s = \frac{W}{W_n}, \quad p_s + p_k = 1$$

where:  $W$  is the current particle weight. Thus two parameters:

1) The Russian Roulette triggering parameter  $W_\ell$

and 2) The survival probability  $p_s$

may be used to uniquely specify a Russian Roulette scheme. In the MØRSE sample problem, <sup>(1)</sup> treating a point neutron source in an infinite air medium values of  $W_\ell = 10^{-2}$  and  $W_n = 10^{-1}$  have been used for all groups and regions, corresponding to a survival probability of  $p_s = 0.10$ .

If Russian Roulette is used solely for terminating particle histories, and if a relatively small number of histories is used, as in scoping and optimization studies for blanket studies, the following questions arise: Since Russian Roulette will not lose its basic nature as an importance sampling method, would a bias occur if a small number of histories are used? What is the magnitude of the bias? How can a bias be avoided or reduced to tolerable size?

### 3. Physical Model for the Investigation

To answer the questions raised in the previous section, we choose an empirical approach to test for the existence of the suspected phenomenon and to see if its magnitude justifies further theoretical investigations. We adopted as our physical model for the investigation the "standard blanket model" of Steiner.<sup>(7)</sup> This is shown in Figure 1. The geometry is a one-dimensional cylindrical geometry. The fusion-neutron source was taken as an isotropic source of 14-Mev neutrons uniformly distributed in the plasma region of the blanket model. In the Monte Carlo simulation the infinite cylinder was



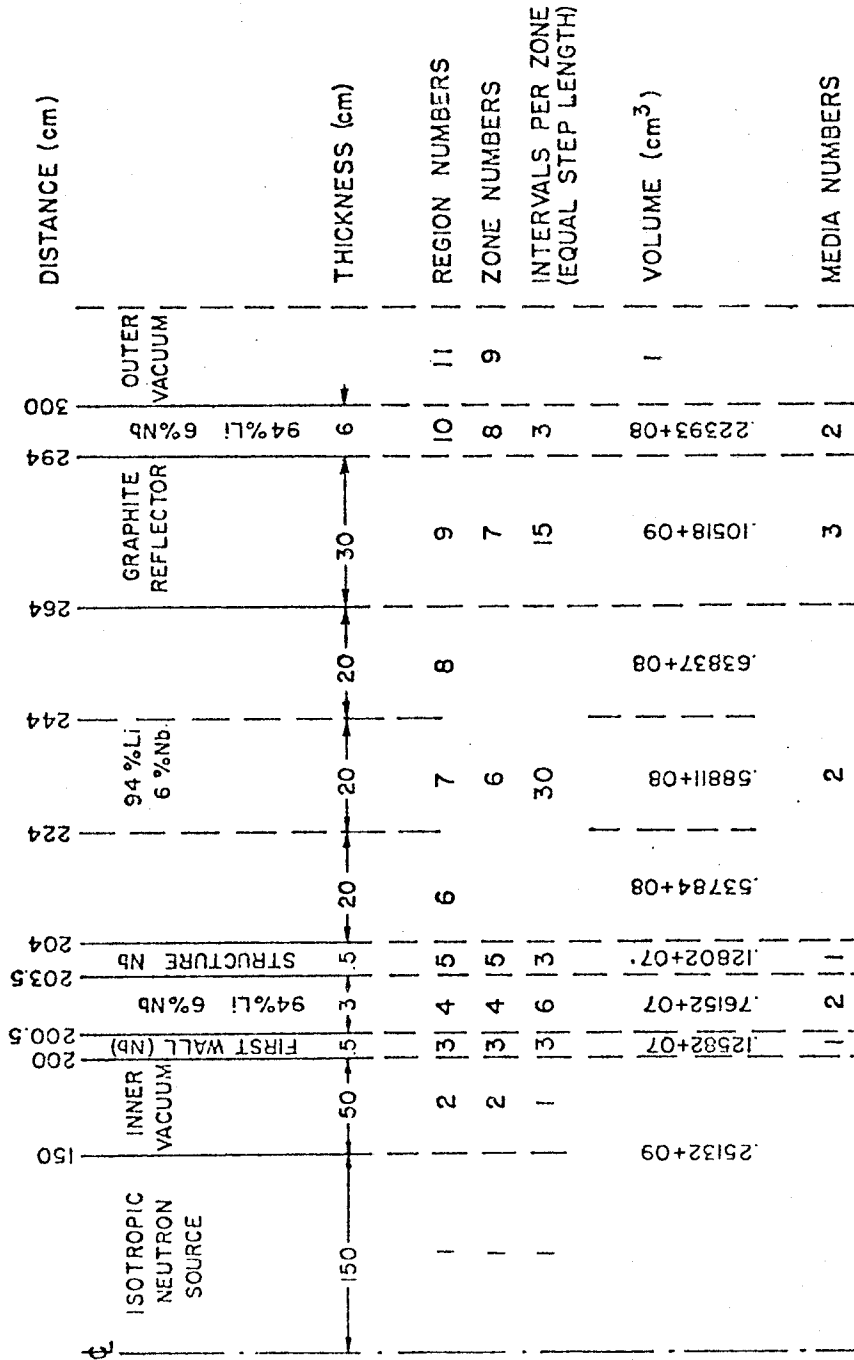


Figure 1: The Standard Blanket Model

represented by a cylinder of 2000 cm length with top and bottom as completely reflecting boundaries. The first wall consists of three regions, the first and third being of niobium structure, and the second one consisting of a mixture of niobium structure and lithium coolant. This is followed by a mixture of Nb and  $L_i$  representing the blanket region, which in turn is subdivided into three subregions. The blanket is followed by a carbon reflector, then by a scrapeoff region of homogenized  $N_b$  structure and  $L_i$  coolant.

The collision density fluence estimator averaged over geometry regions is used as:<sup>(1,2)</sup>

$$\rho_V(E_i) = \frac{\sum_{j=1}^{N_{Vi}} w_j}{n \cdot v_V \cdot \sum_{TV}(E_i)}$$

where  $\rho_V(E_i)$ : fluence in region  $v$  at energy  $E_i$  per source neutron.

$N_{Vi}$  : number of particles of energy  $E_i$  scattering in region  $v$ ,

$w_j$  : weight of the  $j^{\text{th}}$  particle of energy  $E_i$  scattering in region  $v$  per ev,

$n$  : total number of particles,

$v_V$  : volume of region  $v$ ,

$\sum_{TV}(E_i)$  : total macroscopic cross section for groups  $E_i$  in region  $V$ .

The fluence estimate  $\rho_V(E_i)$  has units of particles/(ev.  $\text{cm}^2$  source particles).

Integral parameters, namely reactions rates over volumes are computed as:

$$F_V^Z = (\sum_{RV}^Z, \Phi_V) v_V = v_V \cdot \sum_{i=1}^G \rho_V(E_i) \cdot \Delta E_i \cdot \sum_{RV}^Z(E_i) \text{ Reactions/sec} \quad (2)$$

where  $\Delta E_i$  is the  $i$ -th group energy width,

$\sum_{RV}^Z(E_i)$  is the macroscopic reaction cross section for reaction  $z$  in region  $v$

$G$  is the number of groups

$$\Phi_V(E_i) = \rho_V(E_i) \cdot \Delta E_i$$

( , ) denotes an inner product.

Further investigations should consider other estimators such as the track length per unit volume estimator.

#### 4. Cross Section Data

Version 4 of ENDF/B<sup>(14)</sup> (ENDF/B-IV) was used as the reference for cross section data. These were processed into a broad-group energy structure consisting of 46 groups with the top 5 groups in the GAM-II<sup>(15)</sup> energy group-structure, and one thermal group. The group structure is shown in Table 3.

The reaction rates of interest are the tritium breeding reactions  $L_i^6(n, \alpha)T$  and  $L_i^7(n, n' \alpha)T$ , both for the "hot" and "cold" cases and the  $Nb(n, 2n)$ ,  $L_i^6(n, 2n)$  and  $L_i^7(n, 2n)$  reactions. These were processed into a 46 group format and the macroscopic cross sections for each are displayed in Tables 3 and 4. The nuclides number densities for the different materials are shown in Table 5.

Table 3: Group Structure and Tritium Production Macroscopic Cross Sections for Lithium

GROUP	UPPER EDGE (eV)	$\Sigma(T6+T7)$ Hot	$\Sigma(T6+T7)$ Cold	$\Sigma T6$ (Hot)	$\Sigma T6$ (Cold)	$\Sigma(T7)$
1	1.4918+07	1.3389-02	1.3389-02	8.2813-05	8.2813-05	1.3306-02
2	1.3499+07	1.4606-02	1.4606-02	9.1765-05	9.1765-05	1.4514-02
3	1.2214+07	1.5765-02	1.5765-02	1.0455-04	1.0455-04	1.5661-02
4	1.1052+07	1.6597-02	1.6597-02	1.1621-04	1.1621-04	1.6481-02
5	1.0000+07	1.6943-02	1.6943-02	1.2987-04	1.2987-04	1.6813-02
6	9.0484+06	1.7143-02	1.7143-02	1.4662-04	1.4662-04	1.6996-02
7	8.1873+06	1.7279-02	1.7279-02	1.6363-04	1.6363-04	1.7115-02
8	7.4082+06	1.7094-02	1.7094-02	1.8304-04	1.8304-04	1.6911-02
9	6.7032+06	1.6323-02	1.6323-02	2.0528-04	2.0528-04	1.6117-02
10	6.0653+06	1.4726-02	1.4726-02	2.2941-04	2.2941-04	1.4496-02
11	5.4881+06	1.0574-02	1.0574-02	2.5814-04	2.5814-04	1.0316-02
12	4.9659+06	5.1557-03	5.1557-03	2.8667-04	2.8667-04	4.8690-03
13	4.4933+06	2.1450-03	2.1450-03	3.2073-04	3.2073-04	1.8242-03
14	4.0657+06	1.0458-03	1.0458-03	3.6091-04	3.6091-04	6.8484-04
15	3.6788+06	7.6162-04	7.6162-04	4.0312-04	4.0312-04	3.5850-04
16	3.3287+06	5.6784-04	5.6784-04	4.4309-04	4.4309-04	1.2475-04
17	3.0119+06	5.3729-04	5.3729-04	4.9820-04	4.9820-04	3.9086-05
18	2.7253+06	5.7420-04	5.7420-04	5.7420-04	5.7420-04	0.0000
19	2.4660+06	6.6077-04	6.6077-04	6.6077-04	6.6077-04	
20	1.8268+06	7.5556-04	7.5556-04	7.5556-04	7.5556-04	
21	1.5534+06	8.2965-04	8.2965-04	8.2965-04	8.2965-04	
22	1.0026+06	8.7912-04	8.7912-04	8.7912-04	8.7912-04	
23	7.4274+05	9.4158-04	9.4158-04	9.4158-04	9.4158-04	
24	5.5023+05	1.2479-03	1.2479-03	1.2479-03	1.2479-03	
25	4.0762+05	2.8216-03	2.8216-03	2.8216-03	2.8216-03	
26	3.0197+05	8.8556-03	8.8556-03	8.8556-03	8.8556-03	
27	2.2371+05	6.2738-03	6.2738-03	6.2738-03	6.2738-03	
28	1.6573+05	2.8476-03	2.8476-03	2.8476-03	2.8476-03	
29	1.2277+05	2.1327-03	2.1327-03	2.1327-03	2.1327-03	
30	6.7379+04	2.4206-03	2.4206-03	2.4206-03	2.4206-03	
31	3.1828+04	3.3348-03	3.3348-03	3.3348-03	3.3348-03	
32	1.5034+04	4.7882-03	4.7882-03	4.7882-03	4.7882-03	
33	7.1017+03	6.9377-03	6.9377-03	6.9377-03	6.9377-03	
34	3.3546+03	1.0092-02	1.0092-02	1.0092-02	1.0092-02	
35	1.5846+03	1.4691-02	1.4691-02	1.4691-02	1.4691-02	
36	7.4852+02	2.1420-02	2.1420-02	2.1420-02	2.1420-02	
37	3.5355+02	3.1147-02	3.1147-02	3.1147-02	3.1147-02	
38	1.6702+02	4.5344-02	4.5344-02	4.5344-02	4.5344-02	
39	7.8893+01	6.5996-02	6.5996-02	6.5996-02	6.5996-02	
40	3.7267+01	9.6051-02	9.6051-02	9.6051-02	9.6051-02	
41	1.7603+01	1.3979-01	1.3979-01	1.3979-01	1.3979-01	
42	8.3153+00	2.0343-01	2.0343-01	2.0343-01	2.0343-01	
43	3.9279+00	2.9602-01	2.9602-01	2.9602-01	2.9602-01	
44	1.8554+00	4.3076-01	4.3076-01	4.3076-01	4.3076-01	
45	8.7643-01	6.2679-01	6.2679-01	6.2679-01	6.2679-01	
46	4.1399-01	2.6948+00	1.6415+00	2.6948+00	1.6415+00	

1.0000-04  
(Lower edge)

Table 4 Macroscopic Cross Sections for Major (n,2n) Reactions

GROUP	Nb(n,2n) Blanket	Nb(n,2n) Structure	$L_i^6(n,2n)$	$L_i^7(n,2n)$
1	5.7244-03	0.2066-02	2.2661-04	8.9850-04
2	3.0387-03	5.0639-02	2.0174-04	8.3235-04
3	2.3146-03	3.8572-02	1.6871-04	7.2381-04
4	1.3075-03	2.1788-02	1.2998-04	5.4586-04
5	2.0559-04	3.4262-03	9.0458-05	2.0692-04
6	2.0885-06	3.4804-05	5.1036-05	2.5780-05
7	0.0000	0.0000	2.2547-05	0.0000
8			4.7799-06	
9			4.9713-08	
10			0.0000	
11				
12				

Table 5 Nuclides Number Densities for the Material  
Mixtures of the Benchmark Blanket Model

Medium	Region	Constituents	Number Density
1000	1	Isotropic neutron source	---
1000	2	Inner Vacuum	---
1	3, 5	Niobium	0.055560 atoms/b. cm
2	4,6,7,8,10	Niobium	0.003334 atoms/b. cm
		Lithium-6	0.003234 atoms/b. cm
		Lithium-7	0.040380 atoms/b. cm
3	9	Carbon	0.080040 atoms/b. cm
0	11	Outer Vacuum	---

## 5. Results of Calculations

The MORSE code package<sup>(1,2)</sup> obtainable from the Radiation Shielding Information Center was used in the Monte Carlo part of the investigation, while the ANISN<sup>(6)</sup> code was used in the discrete ordinates part.  $S_4$  quadrature was used for the discrete ordinates calculation. Since we are concerned with survey calculations, 1000 histories per calculation was chosen as a reasonable number. These are distributed over 20 experiments (batches) in each case. We assume, for simplicity, that the discrete ordinates result is the truth and use it as a basis of comparison for the different Monte Carlo results. A more thorough investigation would also consider the effect of quadrature order and mesh interval size and other factors<sup>(7)</sup>, which will certainly give different discrete ordinates results.

The results for the six cases treated are displayed below. In cases A, B, and C we fixed the Russian Roulette triggering weight at  $10^{-5}$  and varied the particle survival probability among three values: 10%, 50%, and 90%. Figure 2 compares the Monte Carlo and discrete ordinates results for case B over the blanket regions for the tritium production per source neutron. The results are remarkably good given that we are using a very small number of histories (1000) compared to what is normally used by other investigators. In reference 11, this ranges from 16,000 to 50,000. (Their study included a shield, however, and not a blanket). The Monte Carlo result is shown with three standard deviations of the mean. The discrete ordinates results all lie within one s.d. except for the result in the first blanket region which lies within 2 s.d.'s. Figure 3 shows the effect of choice of the survival probability

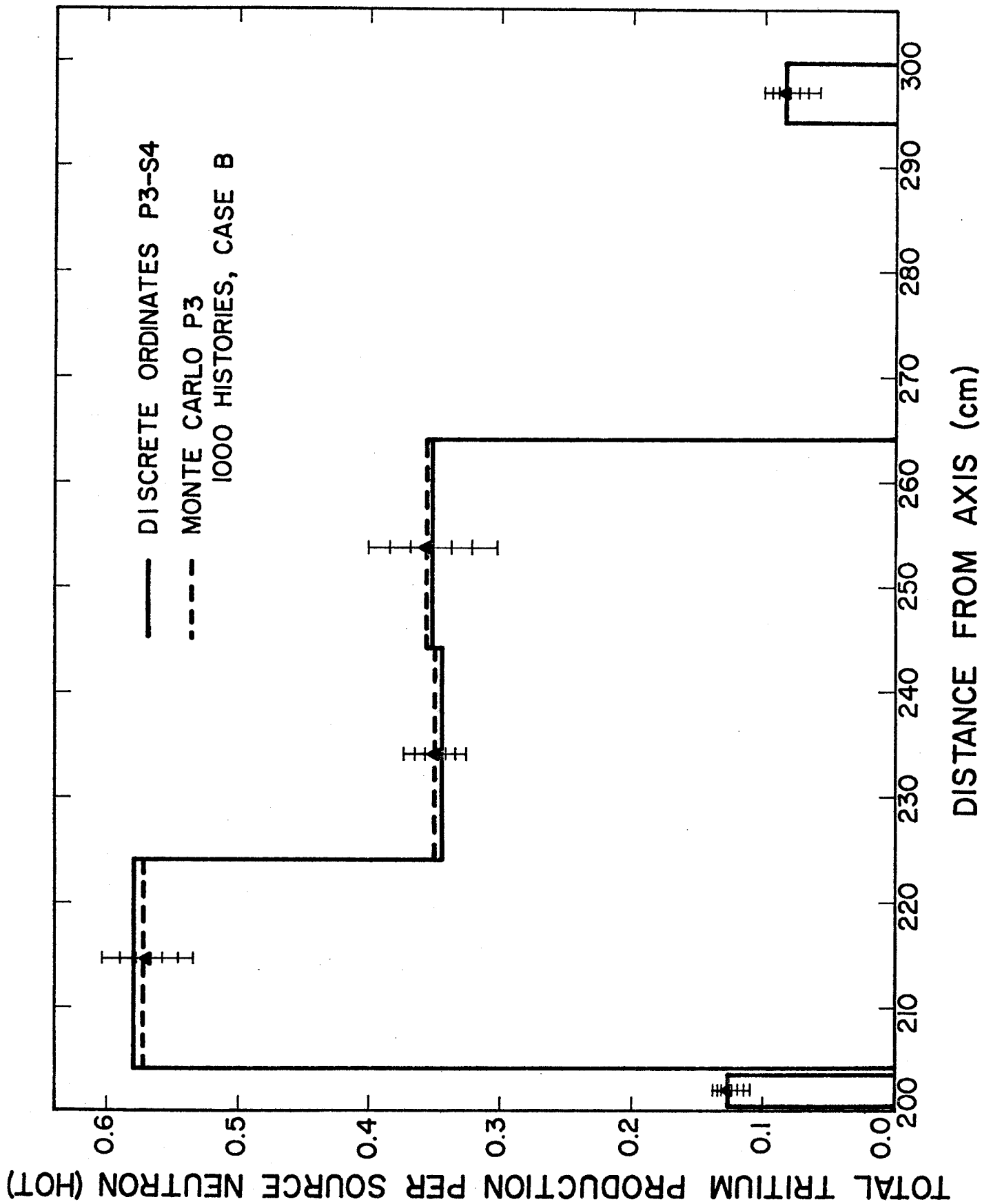


FIGURE 2



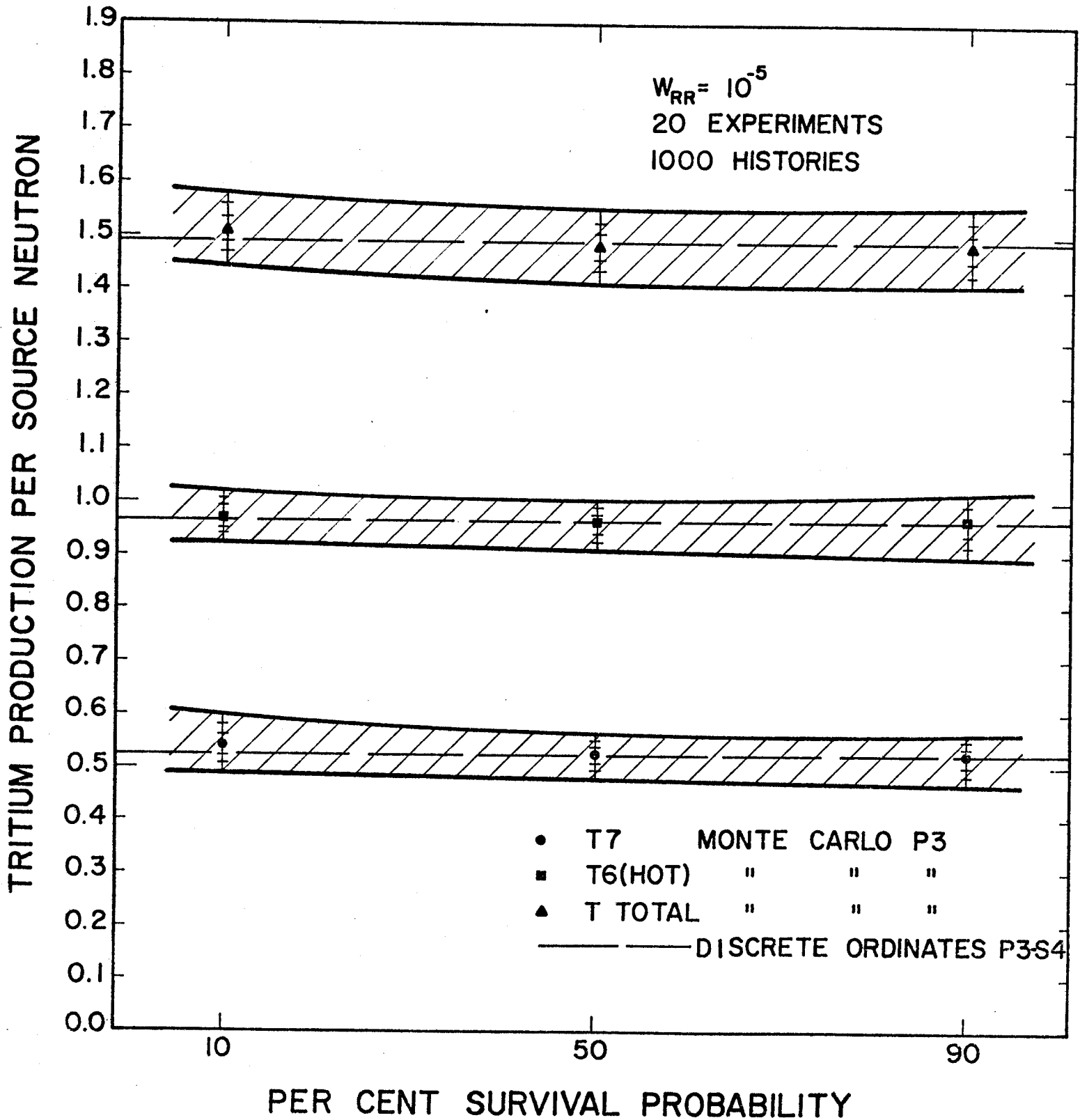


FIGURE 3

on the estimates of tritium production per source neutron, for the hot case. The production from  $L_i^6$ ,  $L_i^7$  and the total are shown. Three standard deviations from the mean are shown. All the results lie within 1 s.d. except for the total (T6 + T7) and the T7 results for  $p_s = 10\%$  which lie within 2 s.d.'s. Figure 3 reveals a slight trend to overestimate the breeding when the survival probability is low. This is understandable since in that case the surviving particles from Russian Roulette are assigned a relatively large weight, and not enough particle histories have been used to smooth out the result. However, the overestimate is not severe and the use of a 95.44% confidence interval (2 s.d.) rather than the customarily used 68.26% confidence interval (1 s.d.) will provide a meaningful and reliable result when Monte Carlo is used for this type of scoping study. When using a larger survival probability, and consequently a lower excess weight for the surviving particles, the overestimation phenomenon becomes much less important. Thus a large survival probability is recommended whenever possible: an ideal (but impractical) simulation is one that follows a particle until its weight reaches zero. Table 14 shows that the computation cost did not change appreciably by using a large survival probability (90% instead of 10%). An interesting result which deserves further investigation is that the minimum variance was obtained when the 50% survival probability was used. Would that mean that there exists an optimal survival probability for a given problem? We leave the question open for the interested investigator. Tables 6, 7, and 8 compare the results for total tritium production, T6, and T7 respectively by region of the blanket model, for the hot and cold cross section sets. Most M.C. results contain the D.O. within one or two s.d.'s. Rarely

Table 6 Comparison of Monte Carlo and Discrete Ordinates Calculations By Region: The Total Tritium Production Per Source Neutron, For Different Russian Roulette Survival Probabilities

Case A: Survival Probability = 90%

Case B: Survival Probability = 50%

Case C: Survival Probability = 10%

Number of histories = 1000

Number of batches = 20

Weight below which Russian Roulette is played =  $10^{-5}$

Region	Case	T6 + T7 (cold)	s.d.	T6 + T7 (hot)	s.d.
4	D.O.	0.1276		0.1276	
	A	0.119690 ± 0.005197	2	0.119690 ± 0.005197	2
	B	0.124020 ± 0.004725	1	0.124020 ± 0.004725	1
	C	0.124590 ± 0.004591	1	0.124590 ± 0.004591	1
6	D.O.	0.5795		0.5795	
	A	0.574780 ± 0.013231	1	0.574780 ± 0.013231	1
	B	0.567520 ± 0.011339	2	0.567520 ± 0.011339	2
	C	0.573630 ± 0.011616	1	0.573630 ± 0.011616	1
7	D.O.	0.3460		0.3460	
	A	0.342410 ± 0.010656	1	0.342410 ± 0.010656	1
	B	0.351180 ± 0.008175	1	0.351180 ± 0.008175	1
	C	0.352500 ± 0.011816	1	0.352500 ± 0.011816	1
8	D.O.	0.3304		0.3522	
	A	0.339100 ± 0.013347	1	0.360240 ± 0.014363	1
	B	0.334040 ± 0.014090	1	0.358210 ± 0.015548	1
	C	0.348700 ± 0.010827	1	0.370000 ± 0.011999	2
10	D.O.	0.0613		0.0831	
	A	0.059450 ± 0.008059	1	0.082035 ± 0.011702	1
	B	0.060222 ± 0.005838	1	0.081329 ± 0.007983	1
	C	0.067729 ± 0.006824	1	0.092949 ± 0.009784	2
Totals	D.O.	1.4448		1.4884	
	A	1.435430 ± 0.024604	1	1.479155 ± 0.025668	1
	B	1.436982 ± 0.021221	1	1.482259 ± 0.022873	1
	C	1.467149 ± 0.021434	2	1.513669 ± 0.023137	2

Table 7 Comparison of Monte Carlo and Discrete Ordinates Calculations By Region. The  ${}^6L_j(n,\alpha t)$  Reaction For Different Russian Roulette Survival Probabilities

Case A: Survival Probability = 90%

Case B: Survival Probability = 50% Weight below which Russian Roulette is

Case C: Survival Probability = 10% played =  $10^{-5}$

Number of histories = 1000

Number of batches = 20

Region	Case	T6 (hot)	s.d.	T7 (cold)	s.d.
4	D.O.	0.0480		0.0480	
	A	0.048466 ± 0.001839	1	0.048466 ± 0.001839	1
	B	0.044180 ± 0.002097	2	0.044180 ± 0.002097	2
	C	0.047601 ± 0.001649	1	0.047601 ± 0.001649	1
6	D.O.	0.2921		0.2921	
	A	0.290440 ± 0.007485	1	0.290440 ± 0.007485	1
	B	0.282350 ± 0.006991	2	0.282350 ± 0.006991	2
	C	0.285480 ± 0.006606	2	0.285480 ± 0.006606	2
7	D.O.	0.2351		0.2351	
	A	0.235240 ± 0.005730	1	0.235240 ± 0.005730	1
	B	0.237190 ± 0.004625	1	0.237190 ± 0.004625	1
	C	0.226440 ± 0.004889	2	0.226440 ± 0.004889	2
8	D.O.	0.3079		0.2861	
	A	0.304540 ± 0.012705	1	0.283400 ± 0.011189	1
	B	0.313920 ± 0.012070	1	0.289740 ± 0.010657	1
	C	0.319200 ± 0.010649	2	0.297900 ± 0.008821	2
10	D.O.	0.0823		0.0605	
	A	0.081626 ± 0.011570	1	0.059041 ± 0.007950	1
	B	0.081068 ± 0.008049	1	0.059960 ± 0.005909	1
	C	0.092726 ± 0.009746	2	0.067506 ± 0.006797	2
Totals	D.O.	0.9654		0.9218	
	A	0.956226 ± 0.019686	1	0.916587 ± 0.016752	1
	B	0.958708 ± 0.016886	1	0.913420 ± 0.014938	1
	C	0.971447 ± 0.016693	1	0.924927 ± 0.013938	1

Table 8

Comparison of Monte Carlo and Discrete Ordinates Calculations by Regions:

The  ${}^7\text{Li}(n,n'\alpha t)$  Reaction for Different Russian Roulette Survival Probabilities

Case A: Survival Probability = 90%

Case B: Survival Probability = 50% Weight below which Russian Roulette is played =  $10^{-5}$

Case C: Survival Probability = 10%

Number of histories = 1000

Number of batches = 20

Region	Case	T7 (Cold)	s.d.
4	D.O.	0.0796	
	A	0.071220 $\pm$ 0.004425	2
	B	0.079836 $\pm$ 0.003854	1
	C	0.076988 $\pm$ 0.004289	1
6	D.O.	0.2874	
	A	0.284330 $\pm$ 0.010551	1
	B	0.285170 $\pm$ 0.010343	1
	C	0.288140 $\pm$ 0.012278	1
7	D.O.	0.1109	
	A	0.107170 $\pm$ 0.007132	1
	B	0.113990 $\pm$ 0.006280	1
	C	0.126060 $\pm$ 0.101737	2
8	D.O.	0.0443	
	A	0.055701 $\pm$ 0.008195	2
	B	0.044295 $\pm$ 0.005637	1
	C	0.050797 $\pm$ 0.005213	2
10	D.O.	0.0008	
	A	0.000408 $\pm$ 0.000351	2
	B	0.000262 $\pm$ 0.000188	3
	C	0.000223 $\pm$ 0.000197	3
Totals	D.O.	0.5230	
	A	0.518829 $\pm$ 0.015781	1
	B	0.523553 $\pm$ 0.013896	1
	C	0.542208 $\pm$ 0.017653	2

Table 9 The (n,2n) Reaction In Different Materials And Regions For Different Russian Roulette Survival Probabilities

Case A: Survival Probability = 90%  
 Case B: Survival Probability = 50%  
 Case C: Survival Probability = 10%

Russian Roulette triggering weight =  $10^{-5}$

Region	Case	$N_b$	$L_i^6$	Material	$L_i^7$	Total
3	A	0.051205 ± 0.003641	---	---	---	0.051205 ± 0.003641
	B	0.054473 ± 0.003419	---	---	---	0.054473 ± 0.003419
	C	0.055557 ± 0.003589	---	---	---	0.055557 ± 0.003589
	D.0.	0.0557	---	---	---	0.0557
4	A	0.015302 ± 0.001077	0.000966 ± 0.000067	0.003790 ± 0.000266	0.020058 ± 0.001111	
	B	0.016793 ± 0.000979	0.001070 ± 0.000061	0.004183 ± 0.000242	0.022046 ± 0.001010	
	C	0.016518 ± 0.001006	0.001049 ± 0.000062	0.004124 ± 0.000249	0.021691 ± 0.001038	
	D.0.	0.0169	0.0011	0.0042	0.0222	
5	A	0.044493 ± 0.003547	---	---	---	0.044493 ± 0.003547
	B	0.035266 ± 0.002361	---	---	---	0.035266 ± 0.002361
	C	0.033154 ± 0.003783	---	---	---	0.033154 ± 0.003783
	D.0.	0.0396	---	---	---	0.0396
6	A	0.048671 ± 0.001493	0.003225 ± 0.000097	0.012628 ± 0.000390	0.064524 ± 0.001497	
	B	0.050026 ± 0.001134	0.003322 ± 0.000081	0.012992 ± 0.000309	0.066340 ± 0.001178	
	C	0.049142 ± 0.001768	0.003267 ± 0.000117	0.012733 ± 0.000456	0.065142 ± 0.001830	
	D.0.	0.0495	0.0033	0.0129	0.0657	
7	A	0.016014 ± 0.001337	0.001109 ± 0.000087	0.004315 ± 0.000343	0.021438 ± 0.001383	
	B	0.016384 ± 0.001088	0.001135 ± 0.000069	0.004433 ± 0.000275	0.021952 ± 0.001124	
	C	0.017646 ± 0.001393	0.001230 ± 0.000095	0.004818 ± 0.000374	0.023694 ± 0.001445	
	D.0.	0.0151	0.0011	0.0041	0.0203	
8	A	0.007300 ± 0.001107	0.000516 ± 0.000077	0.002042 ± 0.000307	0.009858 ± 0.001151	
	B	0.0055700 ± 0.000667	0.000400 ± 0.000047	0.001563 ± 0.000184	0.007533 ± 0.000694	
	C	0.0065341 ± 0.000757	0.000458 ± 0.000051	0.001793 ± 0.000204	0.008785 ± 0.000786	
	D.0.	0.0052	0.0004	0.0014	0.0070	
10	A	0.000000 ± 0.000000	0.000000 ± 0.000000	0.000000 ± 0.000000	0.000000 ± 0.000000	
	B	0.000000 ± 0.000000	0.000000 ± 0.000000	0.000000 ± 0.000000	0.000000 ± 0.000000	
	C	0.000000 ± 0.000000	0.000000 ± 0.000000	0.000000 ± 0.000000	0.000000 ± 0.000000	
	D.0.	0.0001	0.0000	0.0000	0.0001	
Totals	A	0.182985 ± 0.005678	0.005816 ± 0.000166	0.022775 ± 0.000659	0.211576 ± 0.005719	
	B	0.178512 ± 0.004597	0.005927 ± 0.000131	0.023171 ± 0.000513	0.207610 ± 0.004627	
	C	0.178551 ± 0.005818	0.006003 ± 0.000171	0.023468 ± 0.000672	0.208022 ± 0.005859	
	D.0.	0.1820	0.0058	0.0227	0.2105	

does it include it within 3 s.d.'s such as the T7 production in the scrapeoff region. Table 9 displays a comparison of the (n,2n) reaction estimates by M.C. and D.O. by region. Results also agree satisfactorily, even when such a small number of used histories.

In cases D, E, and F we kept the survival probability at 50% and varied Russian Roulette triggering weight between  $10^{-4}$ ,  $10^{-5}$  and  $10^{-8}$ . Following a particle to a small enough weight means following neutrons which reach the low energy groups and contribute to more higher order components of the corresponding Neumann series of the solution. That explains the slight trend of Figure 4 of more tritium production estimates when a lower Russian Roulette triggering weight is used. One would be tempted to superficially relate the trend to more production of T6 in the thermal region, but that will not explain the increase of the T7 estimate too. The trend, however, is not very serious, since using a 95.44% confidence interval would assure us of reliable results even with a small number of histories. Tables 11, 12, and 13 show the results per region for the total (T6 + T7), T6, and T7 for the hot and cold cases. The only instance, as in cases A, B, and C, where the result lies within 3 s.d.'s is for the T7 production in the scrapeoff region, whose result lies within 3 s.d.'s. We experimented with a larger number of histories, and the result improved. Since the contribution of that region to the total breeding is very small (~0.05%), this does not affect the overall conclusions. Table 13 displays a comparison of the (n,2n) result for different cases. From Table 14, an obvious increase in the computation cost by going to lower Russian Roulette triggering weights is noticed.

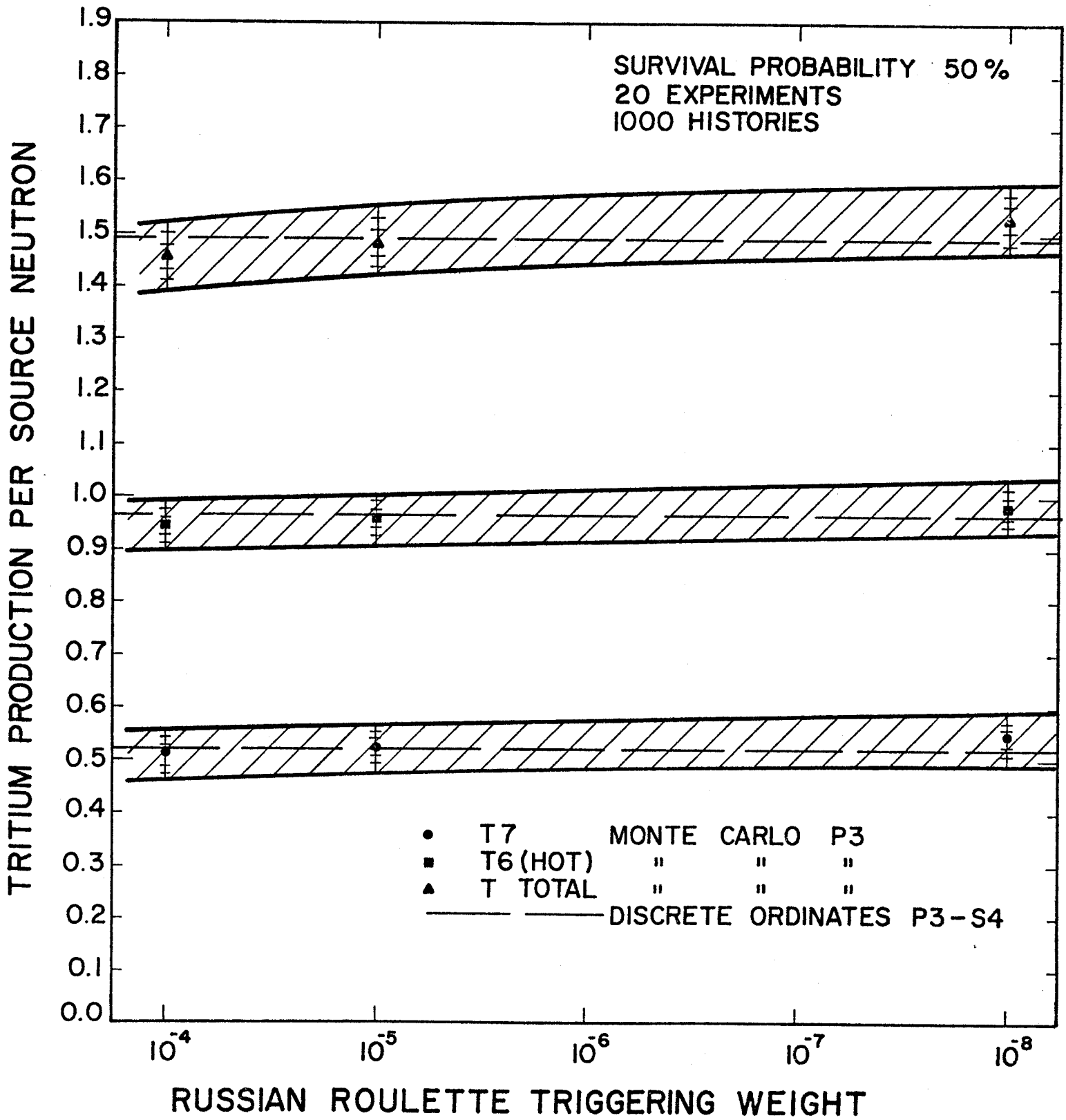


FIGURE 4



Table 10 Comparison of Monte Carlo and Discrete Ordinates Calculations By Region. The Total Tritium Production Per Source Neutron, For Different Russian Roulette Triggering Weights.

Case D: Weight below which Russian Roulette is played =  $10^{-8}$   
 Case E: Weight below which Russian Roulette is played =  $10^{-5}$   
 Case F: Weight below which Russian Roulette is played =  $10^{-4}$

Survival  
Probability = 50%

Region	Case	T6 + T7 (cold)	s.d.	T6 + T7 (hot)	s.d.
4	D.O.	0.1276		0.1276	
	D	0.121490 ± 0.004726	2	0.121490 ± 0.004726	2
	E	0.124020 ± 0.004725	1	0.124020 ± 0.004725	1
	F	0.122070 ± 0.004747	2	0.122070 ± 0.004747	2
6	D.O.	0.5795		0.5795	
	D	0.582120 ± 0.011328	1	0.582120 ± 0.011328	1
	E	0.567520 ± 0.011339	2	0.567520 ± 0.011339	2
	F	0.567090 ± 0.012816	1	0.567090 ± 0.012816	1
7	D.O.	0.3460		0.3460	
	D	0.363690 ± 0.009190	2	0.363690 ± 0.009190	2
	E	0.351180 ± 0.008175	1	0.351180 ± 0.008175	1
	F	0.352390 ± 0.009328	1	0.352390 ± 0.009328	1
8	D.O.	0.3304		0.3522	
	D	0.351100 ± 0.011895	2	0.377430 ± 0.014346	2
	E	0.334040 ± 0.014090	1	0.358210 ± 0.015548	1
	F	0.310310 ± 0.010271	2	0.325930 ± 0.011280	3
10	D.O.	0.0613		0.0831	
	D	0.062749 ± 0.004635	1	0.083346 ± 0.007036	1
	E	0.060222 ± 0.005838	1	0.081329 ± 0.007983	1
	F	0.063825 ± 0.005454	1	0.085359 ± 0.007791	1
Totals	D.O.	1.4448		1.4884	
	D	1.481149 ± 0.019952	2	1.528076 ± 0.022146	2
	E	1.436982 ± 0.021221	1	1.482259 ± 0.022873	1
	F	1.415685 ± 0.020225	2	1.452839 ± 0.021488	2

Table 11 Comparison of Monte Carlo and Discrete Ordinates Calculations By Region. The  ${}^6L_j(n, \alpha t)$  Reaction For Different Russian Roulette Triggering Weights.

Case D: Weight below which Russian Roulette is played =  $10^{-8}$   
 Case E: Weight below which Russian Roulette is played =  $10^{-5}$   
 Case F: Weight below which Russian Roulette is played =  $10^{-4}$       Survival Probability = 50%

Number of histories = 1000  
 Number of batches = 20

Region	Case	T6 (hot)	s.d.	T7 (cold)	s.d.
4	D.O.	0.0480		0.0480	
	D	0.047470 ± 0.001775	1	0.047470 ± 0.001775	1
	E	0.044180 ± 0.002097	2	0.044180 ± 0.002097	2
	F	0.045998 ± 0.002071	1	0.045998 ± 0.002071	1
6	D.O.	0.2921		0.2921	
	D	0.292970 ± 0.006349	1	0.292970 ± 0.006349	1
	E	0.282350 ± 0.006991	2	0.282350 ± 0.006991	2
	F	0.292460 ± 0.005770	1	0.292460 ± 0.005770	1
7	D.O.	0.2351		0.2351	
	D	0.235550 ± 0.004614	1	0.235550 ± 0.004614	1
	E	0.237190 ± 0.004625	1	0.237190 ± 0.004625	1
	F	0.237640 ± 0.005601	1	0.237640 ± 0.005601	1
8	D.O.	0.3079		0.2861	
	D	0.324260 ± 0.013895	2	0.297930 ± 0.010472	2
	E	0.313920 ± 0.012070	1	0.289740 ± 0.010657	1
	F	0.282270 ± 0.009233	3	0.2666500 ± 0.008311	3
10	D.O.	0.0823		0.0605	
	D	0.082653 ± 0.007134	1	0.062056 ± 0.004706	1
	E	0.081068 ± 0.008049	1	0.059960 ± 0.005909	1
	F	0.084926 ± 0.007778	1	0.063392 ± 0.005452	1
Totals	D.O.	0.9654		0.9218	
	D	0.982903 ± 0.017570	1	0.935976 ± 0.014020	2
	E	0.958708 ± 0.016886	1	0.913420 ± 0.014938	1
	F	0.943294 ± 0.014653	2	0.906140 ± 0.012952	2

Table 12 Comparison of Monte Carlo and Discrete Ordinates Calculations by Region  
 The  $T_7$  ( $n, n'$ ) Reaction for Different Russian Roulette Triggering  
 Weights

Case D: Weight below which Russian Roulette is played =  $10^{-8}$   
 Case E: Weight below which Russian Roulette is played =  $10^{-5}$   
 Case F: Weight below which Russian Roulette is played =  $10^{-4}$

Survival  
 Probability = 50%

Number of histories = 1000  
 Number of batches = 20

Region	Case	$T_7$ (CoId)	s.d.
4	D.O.	0.0796	
	D	0.074024+0.004482	2
	E	0.079836+0.003854	1
	F	0.076071+0.004727	1
6	D.O.	0.2874	
	D	0.289150+0.009733	1
	E	0.285170+0.010343	1
	F	0.274630+0.012765	2
7	D.O.	0.1109	
	D	0.128140+0.008779	2
	E	0.113990+0.006280	1
	F	0.114760+0.005476	2
8	D.O.	0.0443	
	D	0.053164+0.006372	2
	E	0.044295+0.005637	1
	F	0.043655+0.006148	1
10	D.O.	0.0008	
	D	0.000693+0.000401	1
	E	0.000262+0.000188	3
	F	0.000433+0.000278	2
Totals	D.O.	0.5230	
	D	0.545171+0.015253	2
	E	0.523553+0.013896	1
	F	0.509549+0.015911	1

Table 13 The (n,2n) Reaction in Different Materials and Regions for Different Russian Roulette Triggering Weights

Case D: Russian Roulette triggering weight =  $10^{-8}$   
 Case E: Russian Roulette triggering weight =  $10^{-5}$   
 Case F: Russian Roulette triggering weight =  $10^{-4}$  Survival Probability = 50%

Region	Case	Material			Total
		$N_b$	$L_i-6$	$L_i-7$	
3	D	0.053721+0.002937	-	-	0.053721+0.002937
	E	0.054473+0.003419	-	-	0.054473+0.003419
	F	0.049448+0.003192	-	-	0.049448+0.003192
	D.O.	0.0557	-	-	0.0557
4	D	0.015819+0.000985	0.000999+0.000064	0.003957+0.000255	0.020775+0.001019
	E	0.016793+0.000979	0.001070+0.000061	0.004183+0.000242	0.022046+0.001010
	F	0.015698+0.000937	0.001006+0.000058	0.003943+0.000235	0.020775+0.000968
	D.O.	0.0169	0.0011	0.0042	0.0222
5	D	0.044228+0.003528	-	-	0.044228+0.003528
	E	0.035266+0.002361	-	-	0.035266+0.002361
	F	0.043061+0.005123	-	-	0.043061+0.005123
	D.O.	0.0396	-	-	0.0396
6	D	0.050195+0.001528	0.003326+0.000101	0.013067+0.000402	0.066588+0.001583
	E	0.050026+0.001134	0.003322+0.000081	0.012992+0.000309	0.066340+0.001178
	F	0.047968+0.001752	0.003167+0.000122	0.012429+0.000484	0.063564+0.001822
	D.O.	0.0495	0.0033	0.0129	0.0657
7	D	0.018247+0.001319	0.001265+0.000087	0.004938+0.000346	0.024450+0.001366
	E	0.016384+0.001088	0.001135+0.000069	0.004433+0.000275	0.021952+0.001124
	F	0.015796+0.000987	0.001113+0.000064	0.004296+0.000261	0.021205+0.001023
	D.O.	0.0151	0.0011	0.0041	0.0203
8	D	0.005363+0.000511	0.000402+0.000039	0.001501+0.000141	0.007266+0.000532
	E	0.005570+0.000667	0.000400+0.000047	0.001563+0.000184	0.007533+0.000694
	F	0.004708+0.000722	0.000349+0.000050	0.001334+0.000198	0.006391+0.000750
	D.O.	0.0052	0.0004	0.0014	0.0070
10	D	0.000001+0.000001	0.000001+0.000001	0.000001+0.000001	0.000003+0.000002
	E	0.000000+0.000000	0.000000+0.000000	0.000000+0.000000	0.000000+0.000000
	F	0.000003+0.000003	0.000001+0.000001	0.000003+0.000003	0.000007+0.000004
	D.O.	0.0001	0.0000	0.0000	0.0001
Totals	D	0.187574+0.005136	0.005993+0.000153	0.023464+0.000605	0.217031+0.005174
	E	0.178512+0.004597	0.005927+0.000131	0.023171+0.000513	0.207610+0.004627
	F	0.176682+0.006471	0.005636+0.000158	0.022005+0.000630	0.204323+0.006504
	D.O.	0.1820	0.0058	0.0227	0.2105

Table 14 Comparison of Monte Carlo and Discrete Ordinates Calculations:  
The Particle Escape Probability\* for Different Russian Roulette  
Parameters and Calculation Costs

Case A Survival Probability = 90% Weight below which Russian Roulette is played =  $10^{-5}$   
 Case B Survival Probability = 50%  
 Case C Survival Probability = 10%  
 Case D Weight below which Russian Roulette is played =  $10^{-8}$   
 Case E Weight below which Russian Roulette is played =  $10^{-5}$  Survival Probability = 50%  
 Case F Weight below which Russian Roulette is played =  $10^{-4}$

Case	Total CPU Time (minutes)	CPU Cost \$	Memory Cost \$	Sum of Costs \$	Total Particle Escape Probability Per Neutron	Number of Escaping Particles	Number of Splittings	Particles Killed by Russian Roulette Number	Total Wt.
D.O.	-	-	-	-	0.040000	-	-	-	-
A	8.25	7.43	4.30	11.73	0.046456	73	4	931	0.003507
B	7.88	7.10	4.12	11.22	0.050700	83	8	925	0.004793
C	8.05	7.25	4.20	11.45	0.041743	76	7	931	0.004965
D	8.70	7.84	4.35	12.19	0.028422 <sup>‡</sup>	69	7	938	0.000038
E	7.88	7.10	4.12	11.22	0.050700	83	8	925	0.004793
F	7.57	6.82	3.95	10.77	0.053524	85	2	917	0.051447

<sup>‡</sup>Splitting was carried out for those particles whose weight exceeded: 2.0

\*Particle escape probability =  $\frac{\text{Total weight of escaping particles}}{\text{Total weight of source particles}}$

#A larger number of processed particles (2000 histories) changed that result to 0.037062

However, the increase is not very serious; it seems better to try to get most of the contributions to the Neumann series terms by going to smaller weights, whenever the increase in computation cost is not serious.

It should be noticed that in some choices, e.g. case B, taking a 68.26% confidence interval may be satisfactory, but requires a preliminary investigation for the best choice of the Russian Roulette parameters; by comparison to a discrete ordinates calculation with high order quadrature, or a Monte Carlo calculation with a large number of histories.

## 6. Conclusions and Recommendations

Monte Carlo can satisfactorily be used for survey and scoping studies using a small number of histories. Users must be careful, however, in their choice of the particle termination (Russian Roulette) parameters. Our study recommends using the highest possible (e.g. 90%) survival probability and the lowest possible (e.g.  $10^{-8}$ ) Russian Roulette triggering weights. This will practically prevent a bias while keeping the computation time reasonable. For small numbers of processed particles, the 95.44% (2 s.d.'s) rather than the 68.26% (1 s. d.) confidence interval<sup>†</sup> is recommended to display results. The 68.26% may still be used if a large number of processed particles is used, or if a prior investigation has shown that it can be used safely. The latter argument may be interpreted as carrying out a comparison between one-dimensional M.C. calculations and a D.O. (with a high order quadrature) calculation for choosing the particle termination parameters before proceeding to a three-dimensional complex geometry calculation, or between M.C. calculations with a small number of histories and another base M.C. calculation with a large number of histories.

Further investigations are recommended to consider the track length per unit volume estimator, the effect of batch (experiment) size and the number of histories on the M.C. results. The use of small numbers of histories

for M.C. calculations is a challenging subject which can be studied within the framework of the field of Small-Sample Statistical Theory.

### Acknowledgement

This research was supported by a grant from the Electric Power Research Institute.

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+ We draw attention to the fact that the standard deviations are not errors bars. They are 68%, 95%, and 99% confidence intervals for normally distributed samples. Also, the numbers 68.28%, 95.44%, and 99.74% refer to the probability (frequency) that the given interval contains the true answer, not to the probability (frequency) that the answer is contained in that interval. This is to emphasize the fact that it is the position and size of the interval that varies, and not the true answer. (16)

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