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Abstract

The effect of different choices of the number of experiments (batches) and their size in Monte Carlo simulations of fusion reactor blankets is studied. The error estimation method is exposed, the standard blanket model is used and results are compared to a Discrete Ordinates calculation. Since most of the Monte Carlo results contain the Discrete Ordinates results within two standard deviations, use of the 95% confidence interval is recommended over the currently used 68% interval for such applications. As the experiment sizes or their number increase, the error range decreases with fluctuations, and convergence occurs. For a large number of histories, the size of the error becomes sensitive only to the total number of histories used. A minimum size for the number of experiments is recommended as twenty, with the size of each experiment chosen to sample the source adequately. For the problem treated, a choice of ten for the ratio of the number of histories per experiment to the number of experiments was adequate. It is recommended that existing Monte Carlo codes be modified so as to show fluctuations and convergence of the results as larger numbers of histories are used, to implement tests of normality for an experiment size of twenty, and to derive normality tests for larger numbers of experiments.

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ACKNOWLEDGEMENT

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1. Introduction and Background

The effect of choices of the number of experiments and their sizes in Monte Carlo simulations of fusion reactor blankets is studied. Reliable and safe designs of fission, fusion, and hybrid nuclear reactor systems necessitate dependable tri-dimensional simulations. Monte Carlo is the only available practical possibility for that type of calculation. It can also include time dependence and detailed cross section representation when needed. Under the title "Design Error Blamed for Mutsu Debacle", the Journal "Nuclear News"(1) reports: "Radiation leakage on the NS Mutsu reached 10 million times its design value, because the designers overlooked fast-neutron leakage over the primary shield, concludes a final report by the committee that investigated the ship's radiation shielding. The Committee report said neutron leakage at the upper part of the containment vessel was through a gap between the pressure gap and the upper primary shield ... gamma-rays detected on the upper deck above the reactor were primarily capture gamma rays produced when neutrons from the leakage point were absorbed in the lead secondary shield. The main primary shielding, however, operated satisfactorily." The reactor has been dismantled. Tri-dimensional design methods could have easily predicted the leakage and suggested corrective actions, but unfortunately were not used.

Analog and albedo Monte Carlo are the major methods available for the treatment of voids and penetrations in reactor systems.(2) The albedo data themselves are mostly generated by Monte Carlo.(3) Bi-dimensional Discrete Ordinates coupled to tri-dimensional Monte Carlo has been used at the Oak Ridge National Laboratory.(4) At Bettis Laboratory, Monte Carlo is used mostly for methods testing.(4)

At the Los Alamos and Livermore Laboratories, Monte Carlo is used for problems with difficult geometries and those that need detailed cross sections representation. Whitesides[4] 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." Rief and Kschwendt[14] report in their work on criticality that ". . . the Monte Carlo results generally agree with experimental values better than the S_N results."

In fusion reactor studies, Monte Carlo is finding a wide field of application. In the USSR, Gur'ev et al.[9], report using Monte Carlo to solve the transport equation for the first neutron generation, then using the P1-approximation for the later generations. Their gamma-ray calculations were also carried out by Monte Carlo.[9] For the Livermore fusion design work, Monte Carlo is being used for both mirror[10] and laser[8] fusion systems calculations. Steiner[11] 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[12] used Monte Carlo to treat a hexagonal toroid blanket model. Abdou, Milton, Jung and Gelbard[13] used Monte Carlo in a cylindrical model to study the effects of vacuum pumping and beam penetrations in an experimental tokamak power reactor design. Ragheb and Maynard[5,6] used Monte Carlo for three-dimensional cell calculations, and for three-dimensional parametric studies for a gas-cooled solid blanket design. Ragheb, Cheng and Conn[7] used Monte Carlo in a laser reactor design with a lithium oxide blanket. Monte Carlo is expected to find wider application in the future in both magnetic and inertial confinement system designs: scoping studies, cell calculations, treatment of penetrations for radio frequency heating, neutral beams, electron beams, laser beams and divertor slots. Also for shielding of optical transport, pellet injection, cryogenic pellet fabrication and injection, magnets and field shaping systems. These studies include estimation of breeding, heat generation, induced activation, radiation damage, and shielding requirements.

Particle transport methods are sensitive to calculational parameter choices and a suitable choice of these parameters is important for reliable and meaningful results. For Discrete Ordinates calculations the final results will depend among other things on the choice of the Legendre expansion order of the anisotropic scattering, the angular quadrature order, the number of mesh intervals, and the number of energy groups. Table 1 shows how Discrete Ordinates calculations are sensitive to the angular quadrature used. This table is taken from a work by Steiner[11] in which he studied that effect and compared his results to a reference Monte Carlo calculation, since Monte Carlo is free from the effect of angular quadrature found in Discrete Ordinates methods. Monte Carlo results share the sensitivity to the Legendre expansion order and the number of energy groups with Discrete Ordinates, but then have their own parameters which affect the final results. Ragheb, Gohar and

Table 1. Comparison of Monte Carlo and Discrete Ordinate Results For Tritium Production Per Source Neutron. The Standard Blanket Case.†

Region	P_3-S_4	P_3-S_8	P_3-S_{12}	P_3-S_{16}	Monte Carlo
	T7: Tritium Production From Li^7				
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: Tritium Production From Li^6				
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

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

Maynard[7] studied the effect of particle histories termination parameters on Monte Carlo estimates in Fusion Reactor Blanket studies. They are concerned with scoping studies where a relatively small number of particle histories are used. They addressed themselves to Russian Roulette as a means of terminating particle histories and not as an importance sampling method. They recommended, for moderate numbers of histories, the use of the highest possible survival probability and lowest Russian Roulette triggering weight to avoid possible biases in the results. In their study, they fixed the experiment size at 1000 histories and the total number of experiments at 20, and pointed out that different choices of these two parameters may have an effect on the calculational results. The purpose of that work is to study the effect of the choices of these two parameters on the tritium breeding estimates using Steiner's[11] standard blanket model. The purpose of the investigation is also to study the behavior of the solution as the number of treated particles increases, and to recommend procedures for making suitable choices of these parameters.

In the following, we deduce a generalized formula for the estimation of the variance of Monte Carlo simulation estimates. The formulae used in some Monte Carlo codes: MCN,[15] MORSE,[16,17] and TARTNP,[18] are discussed and some errors in the documentation of the latter two codes regarding these formulae, according to our derivation, are pointed out, for the prospective user. Our physical model for the investigation: the standard fusion blanket model of Steiner[11] is described, as well as the Monte

Carlo estimator employed. Results of empirical calculations for estimates of tritium breeding as a function of the number of experiments (also called by some authors: batches, statistical aggregates, or samples) and as function of the number of histories in each experiment are discussed. A set of empirical recommendations for similar calculations, and for further work and modification to the presently used Monte Carlo codes, are proposed.

2. Formulae for Estimating the Variance of Monte Carlo Estimates

In a Monte Carlo neutron or gamma ray calculation, one generates a number of random walks for n particles. Each particle is assigned a weight w which changes along the history depending upon the Markov chain random walk model, and the problem collision and transport kernels. Sampling from a normalized source distribution, the original weight is chosen as $w_0 \equiv 1$, and that value decreases if the random walk subjects the particle to scattering or absorption reactions, and increases for particle generation reactions such as (n, 2n) and fission reactions. Particle histories are terminated when the weight decreases below a value assigned by the user, by a Russian Roulette procedure. Estimates of quantities of interest may be obtained by summing the weights in specified regions of interest or at certain points, and using different estimators as weighting functions for these summations.

Assume over a region of interest, a certain estimator yields contribution y_i for the i-th random walk. The Monte Carlo code MCN[15] uses the following method. The sample mean is defined as:

$$\bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i \qquad (1)$$

and the sample variance of y is taken as:

$$\hat{\sigma}^2(y) = \frac{1}{n-1}\left[\sum_{i=1}^{n}(y_i-\bar{y})^2\right] = \frac{n}{n-1}\left[\frac{\sum_{i=1}^{n} y_i^{\,2}}{n} - \bar{y}^2\right]$$

$$= \frac{n}{n-1}\left[\overline{y^2} - \bar{y}^2\right] \qquad (2)$$

To estimate the error of the sample mean, use is made of:

$$\sigma_{\bar{y}}^2 = \frac{\hat{\sigma}^2(y)}{n} = \frac{1}{n-1}\left[\overline{y^2} - \bar{y}^2\right]$$

Because n is usually large, the code MCN[15] uses the following formula for the standard deviation of the sample mean:

$$\sigma_{\bar{y}} = \left[\frac{\overline{y^2} - \bar{y}^2}{n}\right]^{1/2} \qquad (3)$$

which is then interpreted to mean that there is a 68.3% chance that the error is no larger than the value listed, by use of the Central Limit Theorem.

According to Burrows and MacMillan,[19] this method suffers from the disadvantage that: lacking knowledge of the probability distribution of the y_i's, one has no basis for setting confidence limits on μ; the true answer, from $\sigma_{\bar{y}}$. If, however, one divides the whole sample of n particles into N experiments, (also called by some authors: batches, statistical aggregates, groups, or simply samples) such that:

$$n = \sum_{i=1}^{n} n_i \qquad (4)$$

where: n_i is the number of histories treated in the i-th experiment; (these need not be equal)

by the Central Limit Theorem, the distribution of the estimates over the N experiments is asympotically normal for large N, and one can compute confidence limits for μ.

Let us define: x_{ij} as the score by a given estimator over the i-th experiment at its j-th history.

and: $$X_{ij} = \frac{x_{ij}}{\text{Total weight of source particles}} \qquad (5)$$

If we are sampling a normalized source, each source particle will be assigned a unit weight, and the total weight of source particles will just be equal to the total number of treated histories; thus, in that case:

$$X_{ij} = \frac{x_{ij}}{n} \qquad (5)'$$

The mean can be computed over the N experiments as:

$$\bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i \qquad (6)$$

where: $$x_i = \frac{1}{n_i} \sum_{j=1}^{n_i} X_{ij} \qquad (7)$$

Similarly to equation (2) but noting that we are considering the variance over the N experiments, rather than over the total number of histories n,

$$\sigma^2 (x) = \frac{1}{N} \sum_{i=1}^{N} (x_i - \bar{x})^2 = \frac{1}{N} \left[\sum_{i=1}^{N} x_i^2 - \frac{1}{N} \left(\sum_{i=1}^{N} x_i \right)^2 \right]$$

and assuming N is sufficiently large to yield a normal (gaussian) distribution, an estimate of the sample variance can be obtained as:

$$\hat{\sigma}^2 (x) = \frac{N}{N-1} \sigma^2(x) = \frac{1}{N-1} \left[\sum_{i=1}^{N} x_i^2 - \frac{1}{N} \left(\sum_{i=1}^{N} x_i \right)^2 \right] \qquad (8)$$

From the laws of large numbers, the variance of the mean is:

$$\sigma_{\bar{x}}^2 = \frac{\hat{\sigma}^2(x)}{N} \text{ , thus:}$$

$$\sigma_{\bar{x}} = \left[\frac{1}{N(N-1)} \left\{ \sum_{i=1}^{N} x_i^2 - \frac{1}{N} \left(\sum_{i=1}^{N} x_i \right)^2 \right\} \right]^{1/2} \qquad (9)$$

$$x_i = \frac{1}{n_i} \sum_{j=1}^{n_i} X_{ij}$$

where:

$$X_{ij} = \frac{x_{ij}}{n}, \text{ for unit weight source particles}$$

n is the total number of treated histories $n = \sum_{i=1}^{N} n_i$

n_i is the number of histories in the i-th experiment;

N is the number of experiments

x_{ij} is the score at the ith experiment at its j-th history.

Our derived equation 9 should be used when a simulation is divided into a number of experiments or batches for error estimation purposes. Since many Monte Carlo codes have different working formulae for that type of calculation, let us try to derive them using our equation 9 to check their validity and establish their limitations. For the special case in which all the experiments sizes are equal: n_i = constant, we have from equation 4:

$$n = \sum_{i=1}^{N} n_i = N.n_i \qquad (10)$$

One can then rewrite equation 9 as (using equation 10):

$$\sigma_{\bar{x}}^2 = \frac{1}{N-1} \left[\frac{1}{N} \frac{n_i}{n_i} \sum_{i=1}^{N} x_i^2 - \frac{1}{N^2} \frac{n_i^2}{n_i^2} \left(\sum_{i=1}^{N} x_i \right)^2 \right]$$

$$= \frac{1}{N-1} \left[\frac{1}{n} \sum_{i=1}^{N} n_i x_i^2 - \frac{1}{n^2} \left(\sum_{i=1}^{N} n_i x_i \right)^2 \right] \qquad (11)$$

which is the working formula for the MORSE [17,18] Monte Carlo code (page 201 of Reference 17). Since this formula derives from our formula 9 for the special case n_i = constant, the statement in the MORSE code documentation: " ...... calculates variances and fractional standard deviations (f.s.d.) for batch statistics allowing for <u>unequally weighted</u> batches" is in error. In our numerical calculations we used n_i = constant, in which case the formula used in the MORSE code is still valid. Our formula 9 is the one valid for unequally <u>sized</u> experiments, but equally weighted (by $\frac{1}{N}$) for the estimation of the mean $\bar{x}$.

Suppose we defined: $X'_{ij} \equiv x_{ij} = nX_{ij}$

so that we have:
$$x'_i = \frac{1}{n_i} \sum_{j=1}^{n_i} X'_{ij} = \frac{1}{n_i} \sum_{j=1}^{n_i} x_{ij} = nx_i \tag{12}$$

which means that our scores are not divided by the total weight of source particles. We may want to postpone dividing by that total weight to the end of the calculation to save some computer operations, or if we intend to decide the total number of histories n sequentially as the calculation proceeds, and not at its starting point. In that case using equation 12, the estimate of the mean becomes:

$$\bar{x} = \frac{1}{Nn} \sum_{i=1}^{N} x'_i \tag{6'}$$

and the variance of the mean becomes, by using equation (9):

$$\sigma^2_{\bar{x}} = \frac{1}{N(N-1)} \left[\sum_{i=1}^{N} \left(\frac{x'_i}{n} \right)^2 - \frac{1}{N} \left(\sum_{i=1}^{N} \frac{x'_i}{n} \right)^2 \right]$$

Thus:
$$\sigma_{\bar{x}} = \frac{1}{n} \left\{ \frac{1}{N(N-1)} \left[\sum_{i=1}^{N} \left(x'_i \right)^2 - \frac{1}{N} \left(\sum_{i=1}^{N} x'_i \right)^2 \right] \right\}^{1/2} \tag{9'}$$

which corrects the working equation of the code TARTNP [18], page 15, reported in its documentation as:

$$\sigma_n = \frac{1}{n} \cdot \frac{1}{N(N-1)} \left[\sum_{i=1}^{N} \left(x'_i \right)^2 - \frac{1}{N} \left(\sum_{i=1}^{N} x'_i \right)^2 \right]^{1/2}$$

Our derivation shows that what is defined as the standard deviation of the mean <u>for a single history</u>, σ_n, is nothing but the standard deviation of the mean $\sigma_{\bar{x}}$ itself. The additional factor $\frac{1}{n}$ just depends on how the scores are gathered, i.e. on how we define our X_{ij}'s.

The use of equation 9 allows the assignment of confidence intervals based on the assumption of normality. Burrows and Macmillan [19] described a test of normality to be applied to the experimental averages of x_i or x'_i, introduced by Shapiro and Wilks[19] which applied only for the case of N=20 experiments.

We use the multiple experiments approach in our investigation and study the effect of different numbers of experiments N, and the experiments size n_i on Monte Carlo estimates of tritium breeding in fusion reactor blanket studies.

3. Physical Model for the Investigation.

Our aim is to study the effects of different choices of N, the number of experiments, and of n_i, the sizes of the experiments on Monte Carlo estimates of means and variances in fusion reactor blanket studies. In the literature, we were unable to find theoretical recommendations on how to choose N and n_i for a total number of histories n in equation 9, for reliable and meaningful results; so we resorted to an empirical approach. The "Standard Blanket model" of Steiner(11) is adopted as the physical model for the investigation. This is shown in Figure 1. We compare our Monte Carlo results to a Discrete Ordinates calculation using a S_4 quadrature.

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 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 Li 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 Nb structure and Li coolant. No magnet shield is included.

The collision density fluence estimator for reaction Z averaged over geometry region v is used as:

$$F_v^z = \sum_{i=1}^{G} \frac{\Sigma_{RV}^{z}(E_i)}{\Sigma_{Tv}(E_i)} \left(\frac{\sum_{j=1}^{N_{v_i}} {}^{i}W_j}{n} \right) \frac{\text{Reactions}}{\text{Source particle}} \tag{13}$$

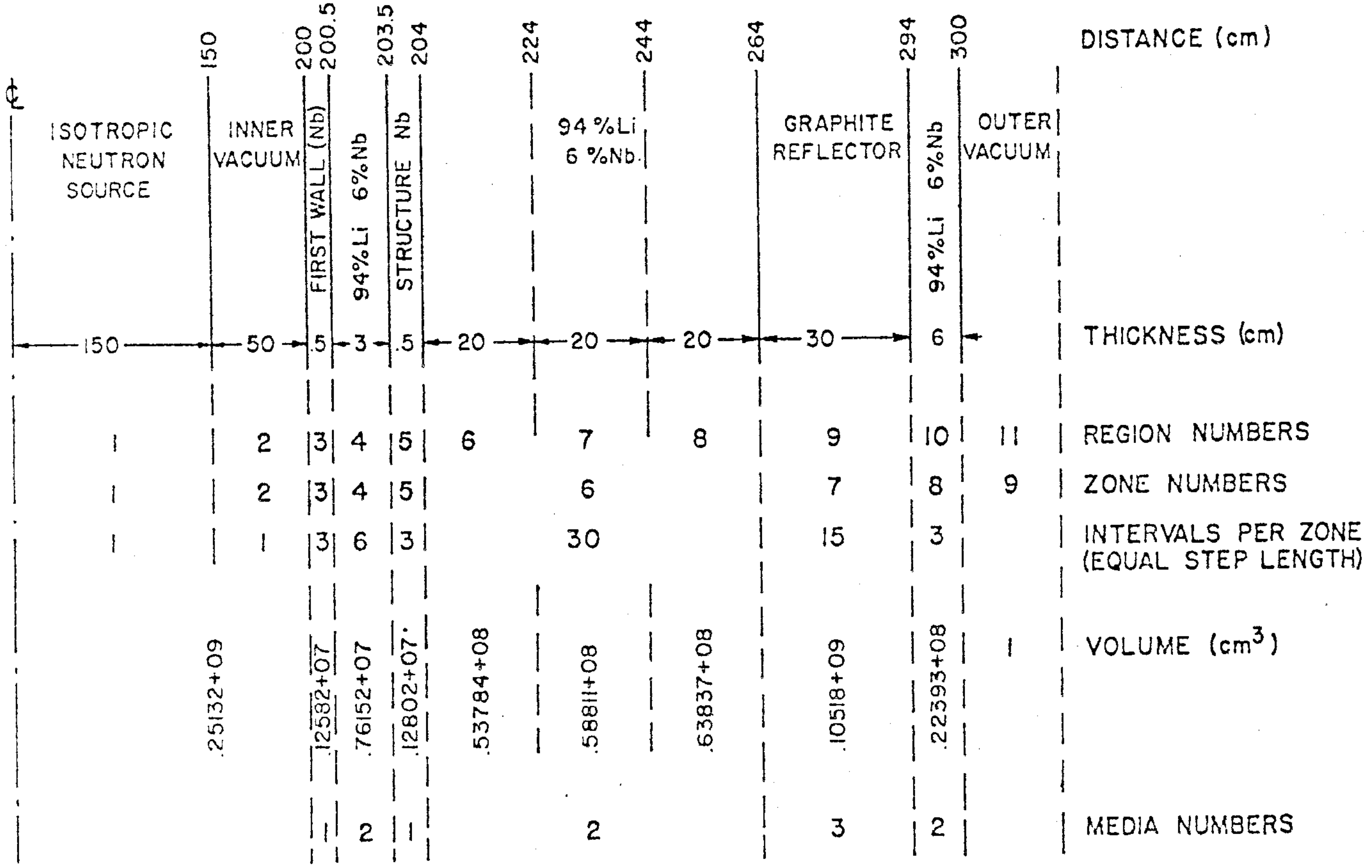


Figure 1: The Standard blanket model configuration

Table 2 Nuclides Number Densities for the Material Mixtures of the Standard 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 Lithium-6 Lithium-7	0.003334 atoms/b. cm 0.003234 atoms/b. cm 0.040380 atoms/b. cm
3	9	Carbon	0.080040 atoms/b. cm
0	11	Outer Vacuum	---

where: W_j : weight of the j-th particle of energy E_i scattering in region v.

N_{v_i} : number of particles of energy E_i scattering in region v.

n : is the total weight of source particle = total number of histories, for unit weight source particles.

G : is the number of treated groups.

$\Sigma_{Tv}(E_i)$: total macroscopic cross section for groups E_i in region v.

$\Sigma^{z}_{R,v}(E_i)$: is the macroscopic reaction cross section for reaction z in region v for groups E_i.

Note that the estimator of equation 13 corresponds to the x_j's in equation 9.

Version IV of ENDF/B[20] was used as the reference for cross sections data. These were processed into a broad-group energy structure consisting of 46 neutron groups and one thermal group.

The 46 group reaction rates of interest are the tritium breeding reactions:

Li-6(n,α) T

Li-7(n,n'α) T

both for the "hot" and "cold" cases, and the (n,2n) reactions:

Nb (n,2n)

Li-6(n,2n)

Li-7(n,2n)

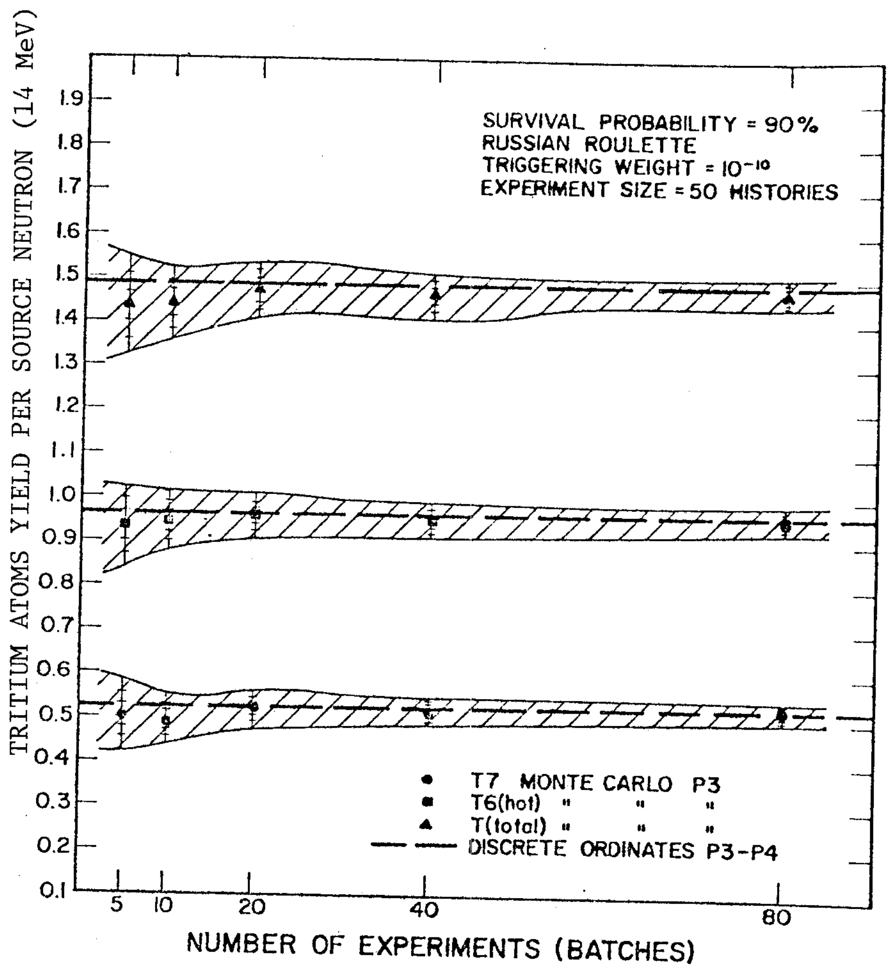
The nuclides number densities for the different materials are shown in Table 2.

4. Results of Calculations

The MORSE code package [16,17,6] obtainable from the Radiation Shielding Information Center was used in the Monte Carlo (M.C.) part of the investigation, while the ANISN [21] code was used for the Discrete Ordinates (D.O.) part with S_4 quadrature. A P_3 Legendre expansion for the angular distributions of the cross sections was used in both types of calculations. Even though different quadratures will give different Discrete Ordinates results (See Table 1), we assume here our obtained D.O. result to be the truth and compare to it the M.C. results.

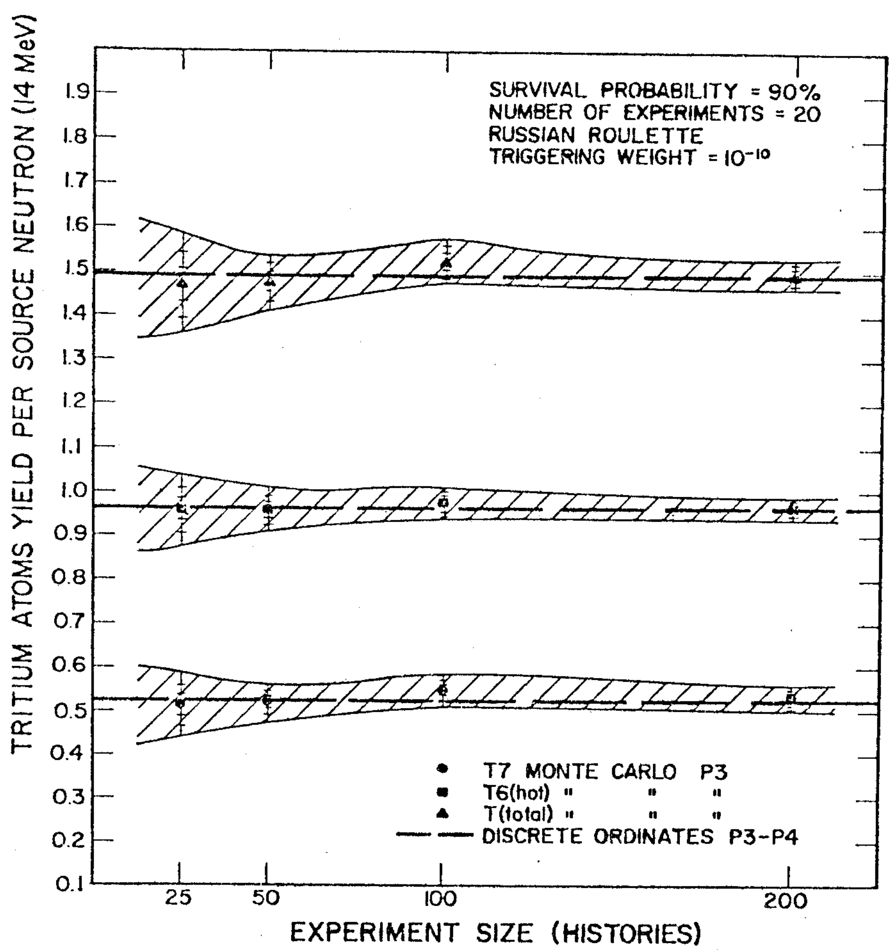
To eliminate the possible bias which can be obtained by the application of Russian Roulette as a particle termination process for moderate number of histories, (pointed out to by Ragheb, Gohar and Maynard [22] in a previous work) we chose as a Russian Roulette triggering weight 10^{-10}, and as a survival probability: 90% in all energy groups and all regions of geometry.

In the first part of the investigation we study the effect of increasing the number of experiments (batches) keeping the size of each experiment constant and equal to 50 histories. Cases A, B, C, D, E correspond to 5, 10, 20, 40, and 80 experiments each. The results per region are displayed in Table 3 for the total tritium from Li^6 (T6) and Li^7 (T7) production per source neutron for the hot and cold cases. Table 4 shows the production from Li^6 alone, and Table 5 from Li^7. Results are compared to the D.O. results in each region. It can be noticed that most D.O. results for the totals lie within two standard deviations of the M.C. results even for a small number of histories, and may even lie within one standard deviation; rarely do they lie within three standard deviations.



TRITIUM ATOMS YIELD PER SOURCE NEUTRON (14 MeV)
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
SURVIVAL PROBABILITY = 90%
RUSSIAN ROULETTE
TRIGGERING WEIGHT = 10^{-10}
EXPERIMENT SIZE = 50 HISTORIES
T7 MONTE CARLO P3
T6(hot) " " "
T(total) " " "
DISCRETE ORDINATES P3-P4
5
10
20
40
80
NUMBER OF EXPERIMENTS (BATCHES)

Figure 2



SURVIVAL PROBABILITY = 90%
NUMBER OF EXPERIMENTS = 20
RUSSIAN ROULETTE
TRIGGERING WEIGHT = 10⁻¹⁰
TRITIUM ATOMS YIELD PER SOURCE NEUTRON (14 MeV)
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
T7 MONTE CARLO P3
T6(hot) " " "
T(total) " " "
DISCRETE ORDINATES P3-P4
25
50
100
200
EXPERIMENT SIZE (HISTORIES)

Figure 3

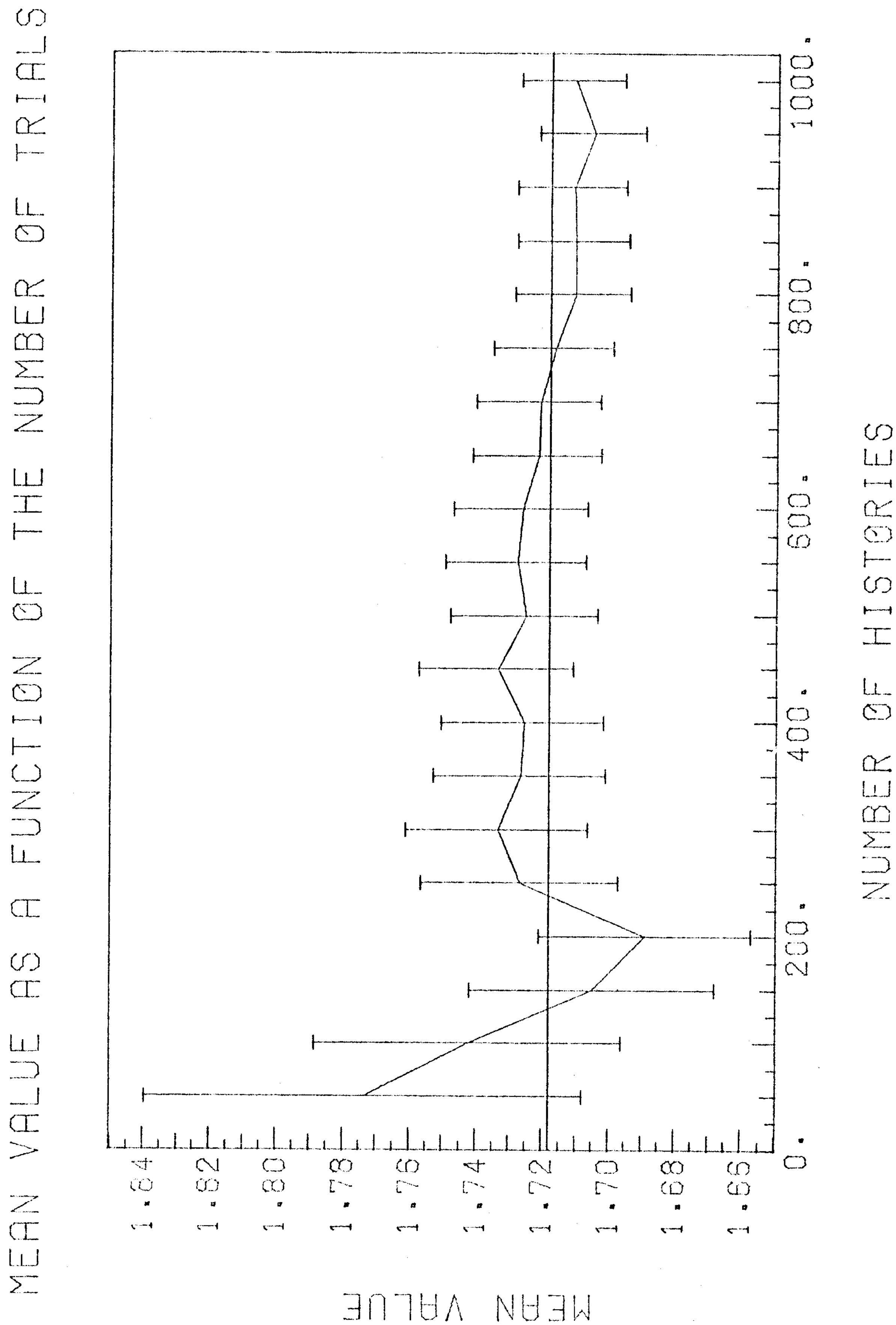

MEAN VALUE AS A FUNCTION ØF THE NUMBER ØF TRIALS
MEAN VALUE
1.84
1.82
1.80
1.78
1.76
1.74
1.72
1.70
1.68
1.66
0.
200.
400.
600.
800.
1000.
NUMBER ØF HISTØRIES

Figure 4

Figure 2 displays the totals over the whole blanket for T6, T7 and (T6 + T7) for different numbers of experiments. Three standard deviations for the estimates are shown. Even though the choice of 50 histories per experiment would not have sampled the source adequately and results in an under-estimate at small number of histories (250 histories), one can notice that the D.0 results have been contained within two standard deviations of the Monte Carlo estimates. With the increase in the number of experiments to 40 and 80, the M.C. result approaches the D.O. result and the error margin narrows significantly.

In the second part of the investigation, we fixed the number of experiments at twenty and treated four cases in which the size of each experiment was set at 25, 50, 100 and 200 for cases F, G, H,and I, respectively. Tables 6, 7 and 8 compare the results obtained per region for the total (T6 + T7), T6, and T7 respectively. As in the last case, most M.C. results contain the D.O. result within 2 standard deviations.

Figure 3 displays the results for the total tritium production summed over all regions for different numbers of experiments sizes. The M.C. results here too contain the D.O. result within two standard deviations, but show a fluctuation around it, then converge when a large number of histories is used. This type of fluctuations and convergence is typical of Monte Carlo calculations. Figure 4 shows the same type of behavior for an analog Monte Carlo calculation of the integral: $\theta = \int_0^1 e^x dx$. The curves of figures 2 and 3 show a similar behavior in that both converge to the D.O. result at large numbers of histories; however, whenever fluctuations are observed in figure 3, a monotonic approach to the D.O. result from below is observed in figure 2. For large numbers of histories (e.g.4000) the final result seems to be dependent on the total number of histories and not much on the experiment size or the number of experiments. For 4000 histories, we obtained a result of 1.496316 $\pm$ 0.010740 when we used 20 experiments with 200 histories each (Case I), and 1.475316 $\pm$ 0.011630 (Case E) when 80 experiments were used with 50 histories each: the standard deviation is of the same order. This is to be compared with the D.O. result of 1.4884 (dependent itself on the angular quadrature). The first M.C. result contains the D.O. result within one standard deviation, while the second contains it within two standard deviations.

Table 9 displays the results for the estimates of the (n,2n) reactions contributions from different reactions in different regions for cases F, G, H and I, and compares the M.C. and D.O. results. The total M.C. estimates contain the D.O. result within one standard deviation. Table 10 shows the Monte Carlo statistics for the different cases with the total particle escape probability defined as the total weight of escaping particles per source neutron. For the same number of histories (e.g. 4000) a large number of experiments results in a slightly higher computer cost.

TABLE 3

COMPARISON OF MONTE CARLO AND DISCRETE ORDINATES CALCULATIONS BY REGION

The Total Tritium Production Per Source Neutron
for Different Numbers of Experiments

Case A: Number of Experiments: 5
Case B: Number of Experiments: 10
Case C: Number of Experiments: 20
Case D: Number of Experiments: 40
Case E: Number of Experiments: 80

Experiment Size = 50
Survival Probability = 90%
Russian Roulette Triggering Weight = 10^{-10}

Region	Case	T6 + T7 (Cold)	T6 + T7 (Hot)
4	A	0.112860 ± 0.007047	0.112860 ± 0.007047
	B	0.117330 ± 0.005996	0.117330 ± 0.005996
	C	0.120880 ± 0.004661	0.120880 ± 0.004661
	D	0.117090 ± 0.003184	0.117090 ± 0.003184
	E	0.120470 ± 0.002709	0.120470 ± 0.002709
	D.O.	0.1276	0.1276
6	A	0.569510 ± 0.015337	0.569510 ± 0.015337
	B	0.557760 ± 0.014597	0.557760 ± 0.014597
	C	0.558540 ± 0.011249	0.558540 ± 0.011249
	D	0.558310 ± 0.008955	0.558310 ± 0.008955
	E	0.559210 ± 0.006067	0.559210 ± 0.006067
	D.O.	0.5795	0.5795
7	A	0.343230 ± 0.022307	0.343230 ± 0.022307
	B	0.340400 ± 0.015689	0.340400 ± 0.015689
	C	0.354310 ± 0.012957	0.354310 ± 0.012957
	D	0.354180 ± 0.007958	0.354180 ± 0.007958
	E	0.351960 ± 0.004906	0.351960 ± 0.004906
	D.O.	0.3460	0.3460
8	A	0.324650 ± 0.014564	0.351500 ± 0.022844
	B	0.320540 ± 0.011575	0.348700 ± 0.015458
	C	0.334580 ± 0.009164	0.362230 ± 0.011323
	D	0.329820 ± 0.007497	0.350980 ± 0.008936
	E	0.338450 ± 0.006011	0.360510 ± 0.006742
	D.O.	0.3304	0.370
10	A	0.045036 ± 0.010954	0.059111 ± 0.012994
	B	0.053050 ± 0.010916	0.072949 ± 0.011009
	C	0.058457 ± 0.006374	0.080075 ± 0.007962
	D	0.060249 ± 0.004691	0.083204 ± 0.006594
	E	0.060159 ± 0.003362	0.083166 ± 0.004647
	D.O.	0.0613	0.0831
TOTALS	A	1.395286 ± 0.033385 (2 s.d.)	1.436211 ± 0.038382 (2 s.d.)
	B	1.389080 ± 0.025156 (3 s.d.)	1.437139 ± 0.029246 (2 s.d.)
	C	1.426768 ± 0.020994 (1 s.d.)	1.476035 ± 0.022533 (1 s.d.)
	D	1.419649 ± 0.015227 (2 s.d.)	1.463764 ± 0.016643 (2 s.d.)
	E	1.430249 ± 0.010754 (2 s.d.)	1.475316 ± 0.011630 (2 s.d.)
	D.O.	1.4448	1.4884

TABLE 4

COMPARISON OF MONTE CARLO AND DISCRETE ORDINATES CALCULATIONS BY REGION

The $^{6}Li(n,\alpha t)$ Reaction for Different Number of Experiments

Case A: Number of Experiments: 5
Case B: Number of Experiments: 10
Case C: Number of Experiments: 20
Case D: Number of Experiments: 40
Case E: Number of Experiments: 80

Experiment Size = 50
Survival Probability = 90%
Russian Roulette Triggering Weight = 10^{-10}

Region	Case	T6(Hot)	T6(Cold)
4	A	0.050518 ± 0.004889	0.050518 ± 0.004889
	B	0.053389 ± 0.003116	0.053389 ± 0.003116
	C	0.049744 ± 0.002288	0.049744 ± 0.002288
	D	0.047268 ± 0.001613	0.047268 ± 0.001613
	E	0.047743 ± 0.001205	0.047743 ± 0.001205
	D.O.	0.0480	0.0480
6	A	0.297170 ± 0.012844	0.297179 ± 0.012844
	B	0.288240 ± 0.010469	0.288240 ± 0.010469
	C	0.285470 ± 0.007162	0.285470 ± 0.007162
	D	0.286700 ± 0.004880	0.286700 ± 0.004880
	E	0.286370 ± 0.003645	0.286370 ± 0.003645
	D.O.	0.2921	0.2921
7	A	0.238550 ± 0.003273	0.238550 ± 0.003273
	B	0.229700 ± 0.004920	0.229700 ± 0.004920
	C	0.233650 ± 0.006049	0.233650 ± 0.006049
	D	0.233790 ± 0.004568	0.233790 ± 0.004568
	E	0.230550 ± 0.003009	0.230550 ± 0.003009
	D.O.	0.2351	0.2351
8	A	0.288780 ± 0.023873	0.261940 ± 0.017498
	B	0.301810 ± 0.015613	0.273650 ± 0.011729
	C	0.310050 ± 0.010849	0.282390 ± 0.008734
	D	0.299810 ± 0.008116	0.278650 ± 0.006520
	E	0.308120 ± 0.005676	0.286070 ± 0.004806
	D.O.	0.3079	0.2861
10	A	0.057261 ± 0.013767	0.043185 ± 0.011615
	B	0.071739 ± 0.011130	0.051839 ± 0.008030
	C	0.079330 ± 0.009040	0.057712 ± 0.006418
	D	0.082426 ± 0.006630	0.059471 ± 0.004727
	E	0.082431 ± 0.004624	0.059424 ± 0.003335
	D.O.	0.0823	0.0605
TOTALS	A	0.932279 ± 0.030968 (2 s.d.)	0.891363 ± 0.025311 (2 s.d.)
	B	0.944878 ± 0.022609 (1 s.d.)	0.896818 ± 0.018589 (2 s.d.)
	C	0.958244 ± 0.017104 (1 s.d.)	0.908966 ± 0.014512 (1 s.d.)
	D	0.949994 ± 0.012534 (2 s.d.)	0.905879 ± 0.010590 (2 s.d.)
	E	0.955214 ± 0.008797 (2 s.d.)	0.910157 ± 0.007617 (2 s.d.)
	D.O.	0.9654	0.9218

TABLE 5

COMPARISON OF MONTE CARLO AND DISCRETE ORDINATES CALCULATIONS BY REGION

The Li^7 (n,n′αt) Reaction for Different Number of Experiments

Case A: Number of Experiments: 5
Case B: Number of Experiments: 10
Case C: Number of Experiments: 20
Case D: Number of Experiments: 40
Case E: Number of Experiments: 80

Experiment Size = 50
Survival Probability = 90%
Russian Roulette Triggering Weight = 10^{-10}

Region	Case	T7(Cold)
4	A	0.062340 ± 0.008633
	B	0.063940 ± 0.005694
	C	0.071136 ± 0.004332
	D	0.069823 ± 0.002935
	E	0.072727 ± 0.002436
	D.O.	0.0796
6	A	0.272330 ± 0.012770
	B	0.269520 ± 0.009466
	C	0.273070 ± 0.007507
	D	0.271610 ± 0.006217
	E	0.272840 ± 0.004641
	D.O.	0.2874
7	A	0.104680 ± 0.021768
	B	0.110700 ± 0.014669
	C	0.120650 ± 0.009914
	D	0.120330 ± 0.006202
	E	0.121400 ± 0.003942
	D.O.	0.1109
8	A	0.062715 ± 0.003986
	B	0.046890 ± 0.005934
	C	0.052184 ± 0.004324
	D	0.051169 ± 0.003826
	E	0.052384 ± 0.002959
	D.O.	0.0443
10	A	0.001850 ± 0.000950
	B	0.001210 ± 0.000562
	C	0.000745 ± 0.000324
	D	0.000778 ± 0.000310
	E	0.000735 ± 0.000207
	D.O.	0.0008
Totals	A	0.503915 ± 0.026986 (1 s.d.)
	B	0.492260 ± 0.019306 (2 s.d.)
	C	0.517785 ± 0.013864 (1 s.d.)
	D	0.513770 ± 0.010023 (1 s.d.)
	E	0.520086 ± 0.007195 (1 s.d.)
	D.O.	0.5230

TABLE 6

COMPARISON OF MONTE CARLO AND DISCRETE ORDINATES CALCULATIONS BY REGION

The Total Tritium Production Per Source Neutron
for Different Numbers of Experiment sizes

Case F: Experiment Size = 25
Case G: Experiment Size = 50
Case H: Experiment Size = 100
Case I: Experiment Size = 200

Number of Experiments: 20
Survival Probability: 20%
Russian Roulette Triggering Weight = 10^{-10}

Region	Case	T6 + T7 (Cold)	T6 + T7 (Hot)
4	F	0.105960 ± 0.007630	0.105960 ± 0.007630
	G	0.120880 ± 0.004661	0.120880 ± 0.004661
	H	0.120280 ± 0.004555	0.120280 ± 0.004555
	I	0.125000 ± 0.002648	0.125000 ± 0.002648
	D.O.	0.1276	0.1276
6	F	0.572210 ± 0.012621	0.572210 ± 0.019621
	G	0.558540 ± 0.011249	0.558540 ± 0.011249
	H	0.581030 ± 0.009279	0.581030 ± 0.009279
	I	0.585230 ± 0.005864	0.585230 ± 0.005864
	D.O.	0.5795	0.5795
7	F	0.372400 ± 0.018884	0.372400 ± 0.018884
	G	0.354310 ± 0.012957	0.354310 ± 0.012957
	H	0.360890 ± 0.005536	0.360890 ± 0.005536
	I	0.348360 ± 0.004156	0.348360 ± 0.004156
	D.O.	0.3460	0.3460
8	F	0.324370 ± 0.018551	0.347090 ± 0.021249
	G	0.334580 ± 0.009164	0.362230 ± 0.011323
	H	0.345680 ± 0.008262	0.369070 ± 0.008710
	I	0.333840 ± 0.005435	0.353370 ± 0.005742
	D.O.	0.3304	0.3304
10	F	0.053720 ± 0.008462	0.073257 ± 0.012016
	G	0.058457 ± 0.006374	0.080075 ± 0.007962
	H	0.068933 ± 0.004849	0.095771 ± 0.007097
	I	0.061759 ± 0.003254	0.084356 ± 0.004868
	D.O.	0.0613	0.0831
TOTALS	F	1.428660 ± 0.034865 (1 s.d.)	1.470917 ± 0.034359 (1 s.d.)
	G	1.426768 ± 0.020994 (1 s.d.)	1.476035 ± 0.022533 (1 s.d.)
	H	1.476813 ± 0.016142 (2 s.d.)	1.527041 ± 0.016240 (3 s.d.)
	I	1.454189 ± 0.009940 (1 s.d.)	1.496316 ± 0.010740 (1 s.d.)
	D.O.	1.4448	1.4884

TABLE 7

COMPARISON OF MONTE CARLO AND DISCRETE ORDINATES CALCULATIONS BY REGION

The $^{6}Li(n,\alpha t)$ Reaction for Different Experiment Sizes

Case F: Experiment Size = 25
Case G: Experiment Size = 50
Case H: Experiment Size = 100
Case I: Experiment Size = 200

Number of Experiments: 20
Survival Probability: 90%
Russian Roulette Triggering Weight = 10^{-10}

Region	Case	T6 (Hot)	T6 (Cold)
4	F	0.047129 ± 0.003199	0.047129 ± 0.003199
	G	0.049744 ± 0.002288	0.049744 ± 0.002288
	H	0.046730 ± 0.001483	0.046730 ± 0.001483
	I	0.048081 ± 0.000931	0.048081 ± 0.000931
	D.O.	0.0480	0.0480
6	F	0.293040 ± 0.010025	0.293040 ± 0.010025
	G	0.285470 ± 0.007162	0.285470 ± 0.007162
	H	0.285810 ± 0.004236	0.285810 ± 0.004236
	I	0.293920 ± 0.002648	0.293920 ± 0.002648
	D.O.	0.2921	0.2921
7	F	0.244530 ± 0.008365	0.244530 ± 0.008365
	G	0.233650 ± 0.006049	0.233650 ± 0.006049
	H	0.233270 ± 0.003457	0.233270 ± 0.003457
	I	0.231760 ± 0.002274	0.231760 ± 0.002274
	D.O.	0.2351	0.2351
8	F	0.303380 ± 0.012859	0.280660 ± 0.016823
	G	0.310050 ± 0.010849	0.282390 ± 0.008734
	H	0.317530 ± 0.007198	0.294130 ± 0.006594
	I	0.304300 ± 0.004090	0.284770 ± 0.003611
	D.O.	0.3079	0.3079
10	F	0.071602 ± 0.011738	0.052065 ± 0.008167
	G	0.079330 ± 0.009040	0.057712 ± 0.006418
	H	0.094975 ± 0.007179	0.068137 ± 0.004939
	I	0.083691 ± 0.004968	0.061094 ± 0.003350
	D.O.	0.0823	0.0605
TOTALS	F	0.959681 ± 0.026700 (1 s.d.)	0.917424 ± 0.023031 (1 s.d.)
	G	0.958244 ± 0.017104 (1 s.d.)	0.908966 ± 0.014512 (1 s.d.)
	H	0.978315 ± 0.011638 (2 s.d.)	0.928077 ± 0.009998 (1 s.d.)
	I	0.961752 ± 0.007380 (1 s.d.)	0.919625 ± 0.006100 (1 s.d.)
	D.O.	0.9654	0.9218

TABLE 8

COMPARISON OF MONTE CARLO AND DISCRETE ORDINATES CALCULATIONS BY REGION

The 7Li (n,n ´αt) Reaction for Different Experiment Sizes

Case F: Experiment Size = 25
Case G: Experiment Size = 50
Case H: Experiment Size = 100
Case I: Experiment Size = 200

Number of Experiments: 20
Survival Probability: 90%
Russian Roulette Triggering Weight = 10^{-10}

Region	Case	T7 (Cold)	
4	F	0.058826 ± 0.006267	
	G	0.071136 ± 0.004332	
	H	0.075610 ± 0.003808	
	I	0.076916 ± 0.002377	
	D.O.	0.0796	
6	F	0.279170 ± 0.016918	
	G	0.273070 ± 0.007507	
	H	0.295220 ± 0.007921	
	I	0.291300 ± 0.004932	
	D.O.	0.2874	
7	F	0.127870 ± 0.015199	
	G	0.120650 ± 0.009914	
	H	0.127620 ± 0.005001	
	I	0.116520 ± 0.003310	
	D.O.	0.1109	
8	F	0.043706 ± 0.007173	
	G	0.052184 ± 0.004324	
	H	0.051546 ± 0.003717	
	I	0.049070 ± 0.002713	
	D.O.	0.0443	
10	F	0.001655 ± 0.001165	
	G	0.000745 ± 0.000324	
	H	0.000796 ± 0.000344	
	I	0.000665 ± 0.000231	
	D.O.	0.0008	
TOTALS	F	0.511227 ± 0.024684 (1 s.d.)	
	G	0.517785 ± 0.013864 (1 s.d.)	
	H	0.550792 ± 0.010779 (3 s.d.)	
	I	0.534541 ± 0.006953 (2 s.d.)	
	D.O.	0.5230	

TABLE 9

The (n,2n) Reaction in Different Materials and Regions

Case F: Batch Size = 25
Case G: Batch Size = 50
Case H: Batch Size = 100
Case I: Batch Size = 200

Number of Batches: 20
Survival Probability: 90%
Russian Roulette Triggering Weight = 10^{-10}

Region	Case	Material			Total
		Nb	Li-6	Li-7	
3	F	0.051435 ± 0.005595			0.051435 ± 0.005595
	G	0.058241 ± 0.004029			0.058241 ± 0.004029
	H	0.055388 ± 0.003148			0.055388 ± 0.003148
	I	0.053991 ± 0.002082			0.053991 ± 0.002082
	D.O.	0.0557			0.0557
4	F	0.013465 ± 0.001415	0.000847 ± 0.000089	0.003331 ± 0.000354	0.017643 ± 0.001461
	G	0.015670 ± 0.000953	0.000988 ± 0.000060	0.003890 ± 0.000239	0.020548 ± 0.000984
	H	0.015520 ± 0.000701	0.000993 ± 0.000045	0.003892 ± 0.000175	0.020405 ± 0.000724
	I	0.015956 ± 0.000469	0.001017 ± 0.000030	0.003993 ± 0.000119	0.020966 ± 0.000485
	D.O.	0.0169	0.0011	0.0042	0.0222
5	F	0.043645 ± 0.005364			0.043645 ± 0.005364
	G	0.038203 ± 0.003494			0.038203 ± 0.003494
	H	0.037884 ± 0.002412			0.037884 ± 0.002412
	I	0.038827 ± 0.002276			0.038827 ± 0.002276
	D.O.	0.0396			0.0396
6	F	0.048653 ± 0.002569	0.003219 ± 0.000173	0.012590 ± 0.000671	0.064462 ± 0.002661
	G	0.048813 ± 0.001193	0.003217 ± 0.000075	0.012576 ± 0.000301	0.064606 ± 0.001233
	H	0.050845 ± 0.001391	0.003376 ± 0.000088	0.013212 ± 0.000358	0.067433 ± 0.001439
	I	0.049779 ± 0.000686	0.003302 ± 0.000048	0.012902 ± 0.000192	0.065983 ± 0.000714
	D.O.	0.0495	0.0033	0.0129	0.0657
7	F	0.017827 ± 0.001992	0.001251 ± 0.000138	0.004876 ± 0.000544	0.023954 ± 0.002070
	G	0.016543 ± 0.001475	0.001161 ± 0.000103	0.004506 ± 0.000401	0.022210 ± 0.001532
	H	0.017631 ± 0.000909	0.001242 ± 0.000058	0.004850 ± 0.000233	0.023723 ± 0.000940
	I	0.016506 ± 0.000546	0.001141 ± 0.000036	0.004461 ± 0.000144	0.022108 ± 0.000566
	D.O.	0.0151	0.0011	0.0041	0.0203

TABLE 9 (Cont.)

The (n,2n) Reaction in Different Materials and Regions

Case F: Batch Size = 25
Case G: Batch Size = 50
Case H: Batch Size = 100
Case I: Batch Size = 200

Number of Batches: 20
Survival Probability: 90%
Russian Roulette Triggering Weight = 10^{-10}

Region	Case	Material			Total
		Nb	Li-6	Li-7	
8	F	0.004883 ± 0.001010	0.000358 ± 0.000070	0.001413 ± 0.000281	0.006654 ± 0.001051
	G	0.005548 ± 0.000444	0.000408 ± 0.000029	0.001551 ± 0.000122	0.007507 ± 0.000461
	H	0.005709 ± 0.000615	0.000416 ± 0.000041	0.001613 ± 0.000165	0.007738 ± 0.000638
	I	0.005715 ± 0.000280	0.000416 ± 0.000018	0.001597 ± 0.000072	0.007728 ± 0.000290
	D.O.	0.0052	0.0004	0.0014	0.0070
10	F	0.000063 ± 0.000063	0.000007 ± 0.000005	0.000018 ± 0.000017	0.000088 ± 0.000065
	G	0.000078 ± 0.000054	0.000006 ± 0.000004	0.000022 ± 0.000015	0.000106 ± 0.000056
	H	0.000039 ± 0.000037	0.000003 ± 0.000002	0.000012 ± 0.000010	0.000054 ± 0.000038
	I	0.000070 ± 0.000025	0.000006 ± 0.000002	0.000021 ± 0.000008	0.000097 ± 0.000026
	D.O.	0.0001	0.0000	0.0000	0.0001
TOTALS	F	0.179971 ± 0.008583	0.005682 ± 0.000249	0.022228 ± 0.000975	0.207881 ± 0.008642 (1 s.d.)
	G	0.183096 ± 0.005757	0.005780 ± 0.000144	0.022545 ± 0.000569	0.211421 ± 0.005787 (1 s.d.)
	H	0.183016 ± 0.004400	0.006030 ± 0.000122	0.023579 ± 0.000490	0.212625 ± 0.004429 (1 s.d.)
	I	0.180844 ± 0.003253	0.005882 ± 0.000069	0.022974 ± 0.000278	0.209700 ± 0.003266 (1 s.d.)
	D.O.	0.1820	0.0058	0.0227	0.2105

TABLE 10

Computation Statistics for the Different Treated Cases

Case	Total Particle Escape Probability per Source Neutron	Number of Escaping Particles	Number of Splittings	Particles Killed by Russian Roulette: Number	Particles Killed by Russian Roulette: Total Wt.	Number of Experiments	Particles per Experiment	Total cpu Time (Minutes)	cpu Cost $	Memory Cost $	Sum of Costs + $
A	0.064144	25	0	225	0.62241-08	5	50	2.40	2.17	1.31	3.48
B	0.068698	49	1	452	0.12409-07	10	50	4.53	4.09	2.41	6.50
C	0.054847	82	5	923	0.25614-07	20	50	9.08	8.19	4.72	12.91
D	0.053370	167	5	1842	0.51477-07	40	50	17.73	15.96	9.14	25.10
E	0.051388	330	21	3693	0.10202-06	80	50	35.38	31.85	18.15	51.00
F	0.040108	29	3	474	0.13406-07	20	25	4.57	4.12	2.42	6.54
G	0.054847	82	5	923	0.25614-07	20	50	9.08	8.19	4.72	12.91
H	0.041144	150	9	1859	0.51205-07	20	100	17.73	15.97	9.15	25.12
I	0.043618	302	20	3718	0.10327-06	20	200	35.08	31.58	18.00	49.58

+ Based on weekend runs charges for the UW UNIVAC-1110.

5. Conclusions and Recommendations

In the majority of cases the M.C. results contain the D.O. results within two standard deviations, even for small numbers of histories. Our empirical results show that convergence to the mean occurs, and the variance decreases; as the number of experiments is increased, keeping their size constant, and as the size of the experiments is increased, keeping their number constant. For large numbers of histories, the Monte Carlo estimates in the treated category of problems depends mostly upon the total number of histories used, and in that case the size of the estimated standard deviations becomes insensitive to the number of experiments and their sizes. Comparing the Monte Carlo results to an S_4 Discrete Ordinates calculation for the same quantities, it is recommended that one use the 95% confidence interval rather than the 68% interval currently used, even though many of the M.C. results contain the D.O. results within one standard deviation. This is particularly recommended, when small numbers of particles are used, such as in scoping studies.

It is felt that a minimum of 20 experiments is necessary for experiment (batch) statistics, to provide a reasonable assurance of the normality of the means. Let n be the total number of histories the user is planning or able to use, N the number of experiments, and n_i is the experiment size, kept constant, such that $n = N.n_i$. We recommend the following procedure: N is set at 20 and n_i determined according to the choice of n, for preliminary calculations. The user must then check that his n_i choice allows sampling of his source adequately, and if he has available computer time, increase it until e.g. $\frac{ni}{N} \simeq 10$; since such a ratio has given us adequate results (Case I). If more available computer time is available, the user can then keep the proportion $\frac{ni}{N} \simeq 10$ constant by increasing both n_i and N.

Related to the observed fluctuation around the mean and the convergence, it is recommended that existing Monte Carlo codes be modified so that output is obtained at regular intervals during the calculation. Then convergence to the mean as N increases can be shown for the Monte Carlo results. There is also a need for implementing the available test of normality for N = 20 in existing codes (e.g. MØRSE), and develop tests which apply for N>20. For distributions which are approximately normal, it may be advantageous to reconstruct the distribution from its moments, and using the result, construct the appropriate confidence interval.

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