CLM-P345

CLM-P345

UKAEA RESEARCH GROUP

Preprint

NEUTRONICS CALCULATIONS ON A FUSION REACTOR BENCHMARK MODEL

D STEINER
S BLOW

CULHAM LABORATORY
Abingdon Berkshire

1973

CLM-P 345

NEUTRONICS CALCULATIONS ON A FUSION REACTOR BENCHMARK MODEL

by

D Steiner†

and

S Blow*

(Submitted for publication in Nuclear Fusion)

ABSTRACT

The paper describes the benchmark model of a fusion reactor blanket which was defined at the Neutronics Session of the International Working Sessions on Fusion Reactor Technology, held at Oak Ridge, U.S.A., in June 1971.

The returns made by participants are analysed in detail. The recommended system tritium breeding value for this model, 100 cm in thickness, is 1.439.

The most important deduction made is that inadequacies in nuclear data files and in data processing codes have a far greater influence on tritium breeding values than do refinements of calculationalmethod.

An eight point summary of the results is made at the end of the paper, together with a series of recommended activities for the future.

† Oak Ridge National Laboratory, Tennessee, U.S.A.

* Central Electricity Generating Board, Courtenay House, London.

U.K.A.E.A. Research Group
Culham Laboratory
Abingdon
Berks

July 1973

1. INTRODUCTION

It is most probable that the first generation of fusion reactors will operate on the deuterium-tritium fuel cycle, since this reaction has a cross section at low energies which is much higher than any other possible fusion reaction[1]. The basic reaction is:-

$$D + T = n(14.06\ MeV) + \alpha(3.52\ MeV) \quad ...(1)$$

Although deuterium exists in copious amounts in the world's oceans (at about 0.0153 at % of the hydrogen in sea water), it will be necessary to breed tritium, which is radioactive having a half-life of 12.26 years, in a blanket surrounding the fusion reactor. Tritium production in the blanket will be accomplished via interactions between the fusion neutrons and the two isotopes of natural lithium; that is, via $^{6}Li\ (n, \alpha)\ t$ and $^{7}Li(n, n' \alpha)t$ reactions. It is one of the important functions of neutronics studies to calculate tritium breeding ratios as accurately as possible.

At the Neutronics Session of the International Working Sessions of Fusion Reactor Technology, held at Oak Ridge in June 1971, it was noted[2] that there were serious discrepancies in system breeding ratios quoted by different groups. Typically, values varied from 1.23 up to 1.40, a difference of some 15%. It was, therefore, agreed to undertake a benchmark calculation of tritium breeding using the latest available nuclear data files, and by comparing the results from different codes, see whether calculational methods were at fault.

It is the main purpose of this paper to describe the benchmark model, to discuss the results achieved, and to make recommendations for the future to those engaged in fusion reactor neutronics.

2. BENCHMARK MODEL AND RECOMMENDED BREEDING RATES

The configuration of the blanket model specified in the benchmark problem is shown in Figure 1. The blanket geometry was taken as one dimensional

Distances in cm	0	150	200	200.5	203.5	204				264	294	300
Origin →	Plasma	Vacuum	Nb	94% Li 6% Nb	Nb	20 cm	94% Li 6% Nb	20 cm		C	94% Li 6% Nb	
Zone Number	1	2	3	4	5		6			7	8	
Region Number	1	2	3	4	5	6	7	8		9	10	
Material	A	B	C	D	C		D			E	D	
Number of Intervals Per Zone	1	1	3	6	3		30			15	3	
Thickness (cm)	150	50	0.5	3	0.5		60			30	6	

Note: The intervals in each zone are of equal step length. There are 62 intervals all together.

Fig.1 Configuration of the Benchmark Blanket Model

cylindrical geometry. The fusion-neutron source was idealised as an isotropic source of 14 MeV neutrons distributed uniformly in space throughout the "plasma" region of the blanket model. The specified nuclide number densities for each material of the blanket are given in Table 1.

Nuclear data files are required for the four nuclides Nb, ^{6}Li, ^{7}Li, and C. It was recommended that the American ENDFB-3[3] data files be used, or the exact equivalent of these files held in European nuclear data libraries. It was further specified that the nuclear data be processed into 100 groups with the top 99 groups following the GAM-II structure[4], and one thermal group. In preparing these cross sections the effect of resonance self-shielding would be neglected.

It was agreed to perform Monte Carlo calculations to a statistical accuracy of less than 1% variance, and then to check discrete ordinates transport codes against these values. A $P_3 - S_4$ approximation was recommended in the first instance, with the further intention to investigate the result of variations in the order of angular quadrature (S_n) or of the order of Legendre polynomial expansion (P_ℓ).

The recommended values of tritium breeding rates for the benchmark model are given in Table 2. The value for ^{7}Li was derived by assigning equal weights to the results from the Monte Carlo and the high order ($P_3\ S_{12}$ or $P_3\ S_{16}$) discrete ordinates calculations (see Section 4.1). In deriving the recommended value for ^{6}Li only the ORNL and AERE

Table 1:

Nuclide Number Densities for the Materials of the Benchmark Blanket Model.

Material Code Letter	Constituent	Number Density
A	Isotropic flux source of neutrons	
B	Vacuum	
C	Niobium	0.05556 x 10^{24}/cc
D	Niobium	0.003334 x 10^{24}/cc
	Lithium-6	0.003234 x 10^{24}/cc
	Lithium-7	0.04038 x 10^{24}/cc
E	Carbon	0.0804 x 10^{24}/cc

Table 2:

Recommended Values of Tritium Breeding Rates in the Benchmark Model. Results are for One Source Neutron.

REGION	^{7}Li (n, n'α) t	^{6}Li (n, α) t
3	-	-
4	0.077	0.047
5	-	-
6	0.287	0.285
7	0.117	0.237
8	0.046	0.288
9	-	-
10	0.001	0.054
TOTALS	0.528	0.911

Monte Carlo results were used since there is a question mark against niobium data processing in the LASL ETOG code, which probably distorts the LASL ^{6}Li breeding values (see Section 6.3). From Table 2 the values are:-

^{7}Li (n, n' α) t = 0.528

^{6}Li (n, α) t = 0.911

Total = 1.439

3. HISTORY OF FIRST AND SECOND ROUND ACTIVITIES

Following the Oak Ridge meeting of June 1971, an ad hoc committee was formed to define the benchmark model, and to participate in the calculations. Participants in the first round of activity were invited to calculate reaction rates for the high energy threshold reactions ^{7}Li (n, n' α) t and Nb (n, 2n), and to work out flux values in the various zones of the blanket. Some nine laboratories (see Table 3) contributed, and the results were analysed in a summary sent out by D. Steiner of ORNL in December 1971.

Table 3:

List of Participants in the Benchmark Calculations

ROUND 1

Brookhaven National Laboratory (BNL)
Los Alamos Scientific Laboratory (LASL)
Lawrence Livermore Laboratory (LLL)
U.S. National Aeronautics and Space Administration (NASA)
Oak Ridge National Laboratory (ORNL)
Battelle Pacific North West Laboratories (PNL)
University of Wisconsin (WISCONSIN)
Atomic Energy Research Establishment, Harwell (AERE)
Kernforschungsanlage, Jülich (KFA)

ROUND 2

PARTICIPANT	AFFILIATION
A.L. Aronson	BNL
S. Blow	AERE
D.J. Dudziak[a]	LASL
D.W. Muir[b]	
D. Steiner	ORNL

a Performed the Transport calculations.

b Performed the data processing calculations.

The results of the first round activity showed considerable discrepancies in reaction rates. Values for ^{7}Li (n, n' α) t varied from 0.44 up to 0.57, and for Nb (n, 2n) values varied from 0.065 up to 0.074. It transpired that:-

1) Contributors were using different and discrepant nuclear data files on blanket materials.

2) The data processing codes used were sometimes outdated versions. For example, versions of ETOG[5] and SUPERTOG[6] did not correctly process data for secondary neutron spectra from reactions of the type (n, n' α).

3) The variations in data files used and the faults in processing were undoubtedly masking any variations arising from neutronics code approximations.

It was not possible to include any of the first round contributions in the second round effort, for the basic reason that the recommended ENDFB-3 file on Nb was substantially different from earlier files (see section 5.1).

Table 4:

Summary of Benchmark Calculations

LABORATORY	METHOD OF CALCULATION	CODE USED	BREEDING IN ^7Li [a]	BREEDING IN ^6Li [a]	TOTAL BREEDING[a]
BNL	Discrete Ordinates P_3-S_4	ANISN[7]	0.512	0.883	1.395
LASL	Discrete Ordinates P_3-S_4	DTF-IV[8]	0.507	0.888	1.395
LASL	Discrete Ordinates P_3-S_8	DTF-IV	0.522	0.891	1.413
LASL	Discrete Ordinates P_3-S_{12}	DTF-IV	0.529	0.892	1.421
ORNL	Discrete Ordinates P_3-S_4	ANISN	0.518	0.933	1.451
ORNL	Discrete Ordinates P_3-S_8	ANISN	0.522	0.934	1.456
ORNL	Discrete Ordinates P_3-S_{12}	ANISN	0.527	0.932	1.459
ORNL	Discrete Ordinates P_3-S_{16}	ANISN	0.526	0.932	1.458
ORNL	Monte Carlo[b]	MORSE[9]	0.523 $\pm$0.003	0.932 $\pm$0.003	1.455 $\pm$0.004
AERE	Monte Carlo	SPECIFIC[10]	0.529 $\pm$0.006	0.891 $\pm$0.006	1.420 $\pm$0.008

a) Calculated on the basis of one source neutron.
b) The ORNL Monte Carlo calculations employed the same multigroup cross section sets as were used in the Discrete Ordinates Calculations.

As a result of the first round experience, it was required of second round participants that they use version ENDFB-3 data files, and satisfy themselves that their processing codes were in good order. Participants were invited to calculate ^7Li (n, n′ α) t and ^6Li (n, α) t reaction rates, and to work out the neutron balance in the model i.e. to ensure that neutron production and absorption balanced out.

The responses to the second round were not received as rapidly as the first round responses, and it was not possible to start this summary paper until March 1973, some 15 months after the second round was initiated. The four groups whose contributions were included are given in Table 3. Returns were also received from PNL and KFA. Unfortunately, a discrepancy in neutron balance was observed in the PNL return, whilst the KFA group had not been able to acquire an ENDFB-3 tape in time to use in their calculation. In both cases either other work loads or time schedules prevented a correction being made.

4. RESULTS OF THE CALCULATIONS

Table 4 gives a summary of the system breeding in ^6Li and ^7Li (normalised to one source neutron) calculated by the second round participants. At BNL and ORNL the transport code ANISN[7] was used; at LASL the code DTF-IV[8] was employed. Monte Carlo calculations were performed at ORNL and AERE using the codes MORSE[9] and SPECIFIC[10] respectively. In all cases the calculations were performed with a vacuum boundary condition, that is there was no reflected current of neutrons returned to the blanket. Note that higher-order angular quadrature discrete ordinates calculations were performed in addition to the S_4 calculations.

Table 5 compares the ^7Li breeding rates by region for the high order quadrature calculations, and for the Monte Carlo results. The same is done for the ^6Li reaction in Table 6. Table 7 summarises the AERE multiplication and parasitic absorption rates by region. In Tables 8 and 9 a comparison is made of the series of ORNL discrete ordinates and Monte Carlo calculations for ^7Li and ^6Li breeding. The BNL, LASL and ORNL P_3-S_4 calculations on tritium breeding rates are compared in Table 10. The results presented in Tables 4-10 are summarised in Sections 4.1 to 4.5.

4.1 High Order Discrete Ordinates and Monte Carlo:

The agreement for the ^7Li breeding reaction is very good. The variations in regional values do go up to 5-6% (though Monte Carlo variance values are in some instances up to 3%), but the total values agree to within 1% and to within the Monte Carlo variance uncertainty.

The situation with regard to the ^6Li reaction is not so satisfactory. The ORNL P_3 S_{16} and Monte Carlo calculations match very closely. The total value for the LASL and AERE calculations also agree closely, but they are some 5% lower than the ORNL value. However, the variation by region for LASL and AERE as compared with ORNL differs in detail. The LASL values are consistently lower than ORNL, the reason probably being that the processed Nb absorption cross sections are too high for LASL (Section 6.3). The AERE results compare moderately well with ORNL for all but the outside region, region 10. Here the AERE value is only two-thirds that recorded for ORNL. It would appear at first sight that differences in carbon cross sections

Table 5:

Comparison of Values for ^{7}Li (n, n'α) t Reaction by Region

LAB.	LASL (P_3 S_{12})	ORNL (P_3 S_{16})	ORNL (MC)	AERE (MC)
REGION				
3	-	-	-	-
4	0.0755	0.0763	0.0752 ±0.0009	0.079 ±0.002
5	-	-	-	-
6	0.2870	0.2858	0.2847 ±0.0023	0.288 ±0.005
7	0.1180	0.1165	0.1153 ±0.0017	0.117 ±0.003
8	0.0476	0.0471	0.0472 ±0.0011	0.044 ±0.001
9	-	-	-	-
10	0.0008	0.0008	0.0009 ±0.0001	0.001 ±0.001
TOTAL	0.5289	0.5265	0.5233 ±0.0032	0.529 ±0.006

Table 6:

Comparison of Values for ^{6}Li (n,α) t Reaction by Region

LAB.	LASL (P_3 S_{12})	ORNL (P_3 S_{16})	ORNL (MC)	AERE (MC)
REGION				
3	-	-	-	-
4	0.0454	0.0472	0.0467 ±0.0004	0.047 ±0.001
5	-	-	-	-
6	0.2770	0.2884	0.2880 ±0.0013	0.281 ±0.004
7	0.2260	0.2369	0.2369 ±0.0010	0.237 ±0.003
8	0.2810	0.2959	0.2946 ±0.0020	0.282 ±0.003
9	-	-	-	-
10	0.0624	0.0640	0.0655 ±0.0012	0.044 ±0.002
TOTAL	0.8918	0.9324	0.9317 ±0.0028	0.891 ±0.006

Table 7:

Summary of AERE Neutron Multiplication and Parasitic Absorption Values by Region

REGION	MULTIPLICATION	PARASITIC ABSORPTION
3	0.052 ±0.0014	0.029 ±0.0010
4	0.026 ±0.0007	0.012 ±0.0004
5	0.037 ±0.0010	0.028 ±0.0008
6	0.078 ±0.0010	0.070 ±0.0010
7	0.026 ±0.0005	0.059 ±0.0008
8	0.009 ±0.0003	0.053 ±0.0006
9	-	0.010 ±0.0005
10	0.0001	0.001 ±0.0001
TOTAL	0.228 ±0.002	0.263 ±0.002

Table 8: Comparison of ORNL Discrete Ordinates and Monte Carlo Calculations by Region: The ^{7}Li (n, n' α)t Reaction.

^{7}Li (n, n' α)t					
CALCULATION	P_3-S_4	P_3-S_8	P_3-S_{12}	P_3-S_{16}	MONTE CARLO
REGION					
3	-	-	-	-	-
4	0.0806	0.0780	0.0762	0.0763	0.0752 $\pm$0.0009
5	-	-	-	-	-
6	0.2812	0.2818	0.2857	0.2858	0.2847 $\pm$0.0023
7	0.1098	0.1149	0.1168	0.1165	0.1153 $\pm$0.0017
8	0.0458	0.0467	0.0472	0.0471	0.0472 $\pm$0.0011
9	-	-	-	-	-
10	0.0009	0.0008	0.0008	0.0008	0.0009 $\pm$0.0001
TOTALS	0.5183	0.5222	0.5267	0.5265	0.5233 $\pm$0.0032

Table 9: Comparison of ORNL Discrete Ordinates and Monte Carlo Calculations by Region: The ^{6}Li (n, α)t Reaction.

^{6}Li (n, α)t					
CALCULATION	P_3-S_4	P_3-S_8	P_3-S_{12}	P_3-S_{16}	MONTE CARLO
REGION					
3	-	-	-	-	-
4	0.0480	0.0476	0.0471	0.0472	0.0467 $\pm$0.0004
5	-	-	-	-	-
6	0.2912	0.2895	0.2883	0.2884	0.2880 $\pm$0.0013
7	0.02364	0.02371	0.2370	0.2369	0.2369 $\pm$0.0010
8	0.2944	0.2957	0.2960	0.2959	0.2946 $\pm$0.0020
9	-	-	-	-	-
10	0.0634	0.0639	0.0640	0.0640	0.0655 $\pm$0.0012
TOTALS	0.9334	0.9338	0.9324	0.9324	0.9317 $\pm$0.0028

Table 10: Comparison of P_3-S_4 Discrete Ordinates Calculations by Region

	^{7}Li (n, n' α)t			^{6}Li (n, α)t		
LABORATORY	BNL	LASL	ORNL	BNL	LASL	ORNL
REGION						
3	-	-	-	-	-	-
4	0.0815	0.0823	0.0806	0.0471	0.0466	0.0480
5	-	-	-	-	-	-
6	0.2796	0.2680	0.2812	0.2845	0.2790	0.2912
7	0.1064	0.1070	0.1098	0.2244	0.2230	0.2364
8	0.0434	0.0488	0.0458	0.2691	0.2770	0.2944
9	-	-	-	-	-	-
10	0.0008	0.0011	0.0009	0.0578	0.0627	0.0634
TOTALS	0.5117	0.5072	0.5183	0.8829	0.8883	0.9334

between ENDFB-3 and UKNDL must be to blame (further discussed in Section 5.4). If the region 10 value for AERE were the same as the ORNL value then the difference in system values would be only 2% - almost within variance limits.

4.2 Neutron Economy:

The total neutron source value in the AERE calculations (equal to input plus multiplication) is equal to 1.228. This should match with total absorption plus surface leakage. The values for ^{6}Li (n, α)t for parasitic absorption, and for leakage are respectively: 0.891, 0.263, and 0.072. These total to 1.226 which agrees with the source value within variance error. The values for system leakage in the American calculations are nearer 0.04, again reflecting this curious difference which is manifest with regard to neutron leakage through region 10.

4.3 The ORNL Discrete Ordinates and Monte Carlo Calculations:

All the ORNL calculations were performed with the same set of multigroup cross sections. Thus the ORNL discrete ordinates and Monte Carlo results can be compared on the basis of identical input cross sections. Each of the discrete ordinates system values for breeding in ^{6}Li is in good agreement with the Monte Carlo system value. The largest discrepancy among the region values for breeding in ^{6}Li occurs in the S_4 region 4 value which is $\sim$ 3% higher than the Monte Carlo region 4 value. The S_4 system value for breeding in ^{7}Li differs from the Monte Carlo value by only $\sim$ 1%. The S_4 region 4 value is, however, some 7% higher than the Monte Carlo region 4 value. The S_8 results for breeding in ^{7}Li are in good agreement with the Monte Carlo results in all regions except region 4, where the S_8 result is $\sim$ 4% higher. The S_{12} results are in good agreement with the Monte Carlo results, and there is no significant improvement on progressing to S_{16}.

4.4 The Discrete Ordinates P_3-S_4 results:

The BNL system value for breeding in ^{7}Li is $\sim$ 1% greater than the LASL value; the ORNL value is $\sim$ 2% greater than LASL. The differences observed among the region values do not exhibit a consistent trend. As noted in 4.1 the agreement between ORNL and LASL values improved considerably on increasing the order of quadrature.

The ORNL system value for breeding in ^{6}Li is $\sim$ 5% higher than both the LASL and BNL values. The ORNL region values are consistently higher than the BNL and LASL region values, and this difference is relatively insensitive to the order of angular quadrature. It is thought to be due to differences in processed Nb absorption cross sections (discussed in Section 6.3).

4.5 Further Calculational Details:

The Monte Carlo calculations are not sensitive to details other than those specified in the benchmark model description (Section 2) unless a splitting option is called for. This is a well-known device for improving statistical accuracy in regions remote from the source by allowing particles crossing boundaries to "split" into two or more new particles with appropriately lower weights. A total of four splitting regions were used in the AERE calculations; no details were given for the MORSE work.

An examination of the details of the discrete ordinates calculations revealed differences in (1) the negative-flux correction algorithm, (2) the number of intervals taken in the plasma region (region 1 in figure 1), (3) the number of intervals taken in the vacuum region (region 2 in figure 1), and (4) the angular quadrature sets.

A comparison of the P_3-S_4 results from BNL and ORNL showed that the discrepancies in the ^{7}Li breeding results were due to differences in both the mesh size taken in the vacuum region and the elastic scattering matrices. With the same mesh spacing and elastic scattering elements, the differences between ORNL and BNL disappeared.

A comparison of the P_3-S_4 results from LASL and ORNL showed that discrepancies in ^{7}Li breeding results were due to differences in the angular quadrature sets and in the negative-flux correction algorithms. Again, with the same details operating, the ORNL results closely approached those of LASL.

As already noted in Section 4.4, the differences in ^{6}Li breeding values were thought to be due to differences in processed Nb cross sections; at any rate the values were insensitive to alterations in calculational details.

It was noted earlier (in Section 4.3) that the LASL and ORNL discrete ordinates calculation improved in agreement as the order of angular quadrature increased (for ^{7}Li results). It is, therefore, reasonable to assume that as the order of angular quadrature increases the results become less sensitive to differences in the angular quadrature sets and the negative-flux correction algorithms.

Two further points are considered in Sections 4.6 and 4.7, dealing with energy group structure and order of Legendre expansion.

4.6 Energy Group Structure:

One of the actions requested in round 2 was that results on the benchmark model should be checked with an energy group structure altered from GAM-II[4] to see if this had any effect. Specifically, contributors were asked to test the influence of using 50 energy groups between 14 MeV and 2.7 MeV, instead of the 17 given by the GAM II structure.

This alteration was effected at AERE but no significant differences occurred. This is not surprising, however, since an alteration in the energy group structure makes no difference to the neutron life histories. The point is that the energy group structure used in nuclear data preparation is independent of the structure used for tracking in the SPECIFIC[10] code.

Experience with ANISN has shown that results may be sensitive to energy group structure[11]. The matter should be further investigated.

4.7 Order of Legendre Expansion, P_ℓ:

The question of the appropriate order for Legendre expansion in considering anisotropy of elastic scattering has not been subjected to the same scrutiny as variations in the order of angular quadrature, S_n. It appeared to become established at an early stage in these benchmark calculations that there was no benefit to be derived in going beyond P_3, and certainly the close agreement between P_3 S12 and Monte Carlo results would appear to confirm this.

Nevertheless, the fact remains that a P_3 expansion cannot possibly give an accurate representation of the severely forward peaked scattering which takes place between many nuclides and 14 MeV neutrons. Even a P_{20} expansion - the largest allowed in the ENDFB format - may not be good enough. Some 50-60% of interactions at 14 MeV will be due to elastic scatter, and the lighter nuclides, which can cause greatest energy loss in the neutrons, should be the most susceptible to these inaccuracies. It would be a worthwhile project to attempt to discover why it is that an accurate representation of anisotropy is not required in these benchmark calculations.

5. NUCLEAR DATA

The three returns from ORNL, BNL and LASL to the second round all used the ENDFB-3 library[3]. The AERE return used the U.K. Nuclear Data Library[12]. It is important to appreciate that though files in the ENDFB and the UKNDL may be based on the same evaluations, they will not be in the same form. For example, the resonance region is dealt with in ENDFB by listing resonance parameters; in UKNDL actual cross sections are worked out at numerous points in the energy range. In ENDFB secondary neutron angular distributions may be specified either as coefficients multiplying a Legendre polynomial expansion or as a group to group scattering matrix; in UKNDL pairs of values of probability and centre of mass scattering cosine are recorded. This means that it is not easy to compare library listings for a particular nuclide directly. However, these differences in library format should not be significant so long as the data is processed appropriately for a neutronics calculation. The evaluations for the nuclides of interest in the benchmark calculations are discussed below, the ENDFB and UKNDL identification numbers being shown in Table 11.

Table 11: The ENDFB-3 and UKNDL Identification Numbers for the Nuclides of Interest

NUCLIDE	ENDFB NUMBER	UKNDL NUMBER
^{93}Nb	1164	79-B
^{6}Li	1115	914
^{7}Li	1116	215-D
^{12}C	1165	68-A

5.1 Niobium 93:

The original evaluation and construction of the ENDFB file was carried out by Allen and Drake in 1967[13]. It has been realised for some time that the original (n, 2n) cross section needed to be increased by a substantial factor[14]. Basically, the old (n, 2n) cross section has been increased by a factor 2.5, and a consequential reduction made in the inelastic cross section to retain the same overall value for the non-elastic cross section. The new evaluation of Nb has been given ENDFB code number MAT 1164. The UKNDL data file number (DFN) of 79-B was also taken directly from Allen and Drake with the appropriate alterations in (n, 2n) and (n,n′).

5.2 Lithium - 6:

An evaluation by Sowerby at AERE has led to the production of DFN 914. This is basically the same as the old file above 2 MeV, but the low energy cross sections have been altered according to the prescription of Diment and Uttley[15]. Battat and Labauve of LASL have produced the ENDFB-3 MAT 1115, this being based on the AERE evaluation.

5.3 Lithium - 7:

The UKNDL file in current use is 215-D. This is based on the Pendlebury AWRE evaluation of 1964[16], which gave DFN 176. Low energy cross sections were altered to produce 215-A and the width of the scattering resonance at 260 keV was reduced to the O K value to give DFN 215-D. Battat and Labauve produced the ENDFB-3 MAT 1116 based on DFN 215-A. The differences between 1116 and 215-D are probably insignificant to these benchmark calculations.

5.4 Carbon - 12:

It is possible that there is some discrepancy between ENDFB-3 and UKNDL data for this nuclide. Data on breeding ratios discussed in earlier sections suggest that the UKNDL file does not "thermalise" the fusion neutrons as efficiently as the ENDFB-3 file, MAT 1165. A number of modifications have been effected to create this file since the original Slaggie and Reynolds evaluation in 1966[17]. It is thought that DFN 51 is equivalent to MAT 1165. The actual file used in the AERE calculations was 68-A which is believed to be very little different from DFN 51. The most recent evaluation by Douglas at AWRE has produced DFN 902-A. There is undoubtedly a need to review the situation on carbon files.

6. PROCESSING CODES

The processing codes used by the four groups contributing to the second round of calculations are shown in Table 12. Also shown are the method of flux weighting used to obtain group cross sections, and the assumed temperature used for dealing with the thermal group.

Table 12:

Information on Processing Codes and Thermal Group Cross Sections

LABORATORY	Processing Code	Flux Weighting Used to Obtain Group-Averaged Cross Sections	Assumption Regarding Thermal Group Cross Sections
BNL	ETOG[5]	$1/E$	MAXWELLIAN AT 300 K
LASL	ETOG[5]	CONSTANT	MAXWELLIAN AT 1170 K
ORNL	SUPERTOG[6]	$1/E$	MAXWELLIAN AT 300 K
AERE	MOWLD[18]	NOT RELEVANT	NO THERMAL SPECTRUM ADJUSTMENT

The AERE contribution used sub-program MOWLD from the Aldermaston DICE V suite[18]. This code operates by reducing UKNDL cross section values to a standard set of 300 energy points. Careful visual inspection in the past has indicated that this reduction is computed correctly. However, it is not possible to compare the AERE processed cross sections with the American data directly, because the former does not reduce to the 100 GAM II group structure.

An examination of the multigroup cross section sets produced by ETOG and SUPERTOG revealed differences in the elastic scattering matrices and the thermal group absorption cross section of all nuclides, and in the resonance capture cross sections of niobium. These three items are discussed below.

6.1 Elastic Scattering Matrices:

Differences of from 1-7% in elastic transfer elements were observed though the total elastic cross sections varied by less than 0.05%. The differences between the LASL and ORNL results were found to be due to the difference in weighting function used (see Table 12). It was considered that the current version of ETOG at BNL appears to contain an error which is observed in all GAM II energy groups from 1 to 59.

6.2 Thermal Absorption:

The BNL and ORNL thermal group absorption cross sections were about a factor 2 greater than the LASL values, the difference arising from the ambient temperature assumption (see Table 12). However, only 7% of the system absorptions occur in the thermal group. In addition, for this model the absorption cross section even for the LASL value is so high as to prevent any thermal group leakage from region to region. Therefore, the differences in thermal group cross sections have a negligible effect on the tritium breeding calculations.

6.3 Niobium Resonance Capture:

About 36% of all parasitic absorption in the benchmark model occurs as a result of resonance capture in niobium in the energy range defined by groups 60 to 70. Table 13 shows that the ORNL niobium resonance capture cross sections are consistently lower than both the BNL and LASL values; in some groups the discrepancy is as much as a factor of three. These discrepancies were identified as arising from differences between the ETOG (BNL and LASL versions) and SUPERTOG (ORNL version) calculations of the resolved resonance contribution to the niobium capture cross section. Further examinations [19, 20] substantiated the SUPERTOG results. In passing, it is noted that a more recent version of ETOG at Westinghouse appears to yield results in close agreement with the SUPERTOG results.

Niobium resonance region cross sections have an important bearing on tritium breeding rates because the Nb (nγ) and ^{6}Li (nα) t reactions are in competition for lower energy neutrons. The higher ^{6}Li (nα) t breeding rate recorded in the ORNL calculations as compared with LASL and BNL (see Table 10) is undoubtedly due to the lower values produced by SUPERTOG for the niobium capture cross sections.

Table 13:

The BNL and ORNL Niobium Resonance Capture Cross Sections Relative to the LASL Values

LABORATORY	LASL	BNL	ORNL
ENERGY GROUP INDEX	(IN BARNS)	(RELATIVE)	(RELATIVE)
60	0.5055	1.0045	0.9775
61	2.7184	0.9905	0.3721
62	1.9879	0.9854	0.3315
63	3.0367	0.9988	0.3604
64	1.3695	1.0149	0.6520
65	2.4594	1.0056	0.7185
66	1.6435	0.9881	0.8194
67	2.4654	0.9734	0.7985
68	3.3268	0.9841	0.8815
69	1.8162	0.9145	0.8875
70	2.3787	0.9241	0.8507

7. SUMMARY

A series of points summarising the actions and the results of the benchmark calculations are made below.

7.1 A benchmark calculation of tritium breeding in a fusion reactor blanket model was performed using ENDFB-3 as the reference for cross section data. The ENDFB-3 data was processed into multigroup sets using the ETOG code (at BNL and LASL) and the SUPERTOG code (at ORNL). The equivalent UKNDL data was processed by MOWLD into a form suitable for Monte Carlo calculations at AERE.

7.2 Neutronics calculations were performed using the discrete ordinates codes ANISN (at BNL and ORNL) and DTF-IV (at LASL) and the Monte Carlo codes MORSE (at ORNL) and SPECIFIC (at AERE).

7.3 The evaluated values for ^{7}Li breeding and ^{6}Li breeding rates were, respectively, 0.528 and 0.911, giving a total of 1.439. Differences among high order discrete ordinates calculations and Monte Carlo calculations of ^{7}Li system breeding were only of the order ∿ 1%. The differences of up to 15% which instigated this benchmark survey must have been caused by the use of out-of-date nuclear data files, and inadequate data processing, and are not due to calculational methods.

Again, the differences of ∿ 5% observed in ^{6}Li system breeding are almost certainly due to the use of non-equivalent data files and incorrect data processing (see 7.4 and 7.5).

7.4 There are probably important differences between the ENDFB-3 and current UKNDL data files on carbon. These manifest themselves by producing a substantially lower value for ^{6}Li breeding in the outside region (region 10) of the blanket for the UKNDL based data.

7.5 It was surmised that the differences (∿ 5%) in ^{6}Li total breeding values observed between ORNL on the one hand, and BNL and LASL on the other, were caused by a shortcoming in the versions of the processing code ETOG used at BNL and LASL .

7.6 Variations in energy group structure, and extension of Legendre expansion beyond P_3 do not appear to have a significant effect on the results.

7.7 For the assumed blanket geometry, the S_4 approximation gives a system tritium breeding value which is within ∿ 0.5% of the Monte Carlo system value. Thus, the S_4 approximation is adequate for survey calculations on system tritium breeding.

7.8 An S_{12} approximation is necessary in those cases where accurate spatial information is required.

8. RECOMMENDATIONS

In anticipating future work on benchmark survey of fusion reactor blankets the following suggestions are made:-

8.1 That a Monte Carlo calculation be performed to an accuracy of ∿ 0.5% to define reaction rates in the model.

8.2 That survey work can be carried out by comparing the results of low order P_ℓ S_n calculations with the Monte Carlo standard, in order to determine the order of expansion required to fulfil a specified level of accuracy.

8.3 That survey work using low order transport codes be compared with survey work using variational techniques [21].

8.4 That further details be given in future on calculational parameters such as splitting meshes for Monte Carlo calculations, and choice of mesh spacing, details of negative flux corrections and angular quadrature sets, for discrete ordinates methods.

8.5 That a proper amount of effort be expended by groups in ensuring that nuclear data libraries are kept up-to-date, and that processing codes are functioning accurately. These two items have been observed to have a much more profound effect on computed reaction rates than do refinements of calculational methods.

8.6 That the influence of extending Legendre expansions beyond P_3 and of varying energy group structure be scrutinised.

8.7 That a benchmark model which includes a magnet shield as well as a breeding blanket should be studied.

8.8 That tritium breeding rates (and other pertinent reaction rates) be measured in a benchmark experiment which simulates as closely as possible the model already investigated.

ACKNOWLEDGEMENTS: The authors would like to express their heartfelt gratitude to the many contributors who took part in both first and second round activities in this benchmark study. In particular they would like to remark on the enthusiastic atmosphere of the Neutronics Session of the International Working Week on Fusion Reactor Technology held at Oak Ridge in the Summer of 1971. It was there that the idea for the benchmark work was proposed and the impetus necessary for its completion generated.

REFERENCES

1. CROCKER, V.S., BLOW, S. and WATSON, C.J.H. "Nuclear Cross-Section Requirements for Fusion Reactors", United Kingdom Atomic Energy Authority Report CLM-P240 (1970).

2. BLOW, S. "The Role of Neutronics Calculations in Fusion Reactor Technology", Proceedings of the International Working Sessions of Fusion Reactor Technology, June 28 - July 2, 1971, Oak Ridge National Laboratory. pp 74-76.

3. HONECK, H.C. "ENDFB. Specifications for an Evaluated Nuclear Data File for Reactor Applications", Brookhaven National Laboratory, BNL - 50066 (1966).

4. JOANOU, G.D. and DUDEK, J.S. "GAM II: A B_3 Code for the Calculation of Fast Neutron Spectra and Associated Multigroup Constants", General Atomic, GA - 4265 (1963).

5. KUNSER, D.E. and DANNELS, R.A. "ETOG-1. A Fortran IV Program to Process Data from the ENDFB File to MUFT, GAM and ANISN Format". Westinghouse Electric Corporation, WCAP-3845-1 (1969).

6. WRIGHT, R.Q. et al. "SUPERTOG: A Program to Generate Fine Group Constants and P_n Scattering Matrices from ENDFB", Oak Ridge National Laboratory, ORNL-TM-2679 (1969).

7. ENGLE, W.W. Jr. "ANISN - A User's Manual", Oak Ridge Gaseous Diffusion Plant, K-1693 (1967).

8. LATHROP, K.D. "DTF-IV. A Fortran Program for Solving the Multigroup Transport Equation with Anisotopic Scattering", Los Alamos Scientific Laboratory, LA-3373 (1965).

9. STRAKER, E.A. et al. "The MORSE Code - a Multigroup Neutron and Gamma-Ray Monte Carlo Transport Code", Oak Ridge National Laboratory, ORNL-4585 (1970).

10. HOLBROUGH, D.W. and LIPSCOMBE, B.A. "SPECIFIC II. A Monte Carlo Programme for High Energy Neutron Spectrum Estimation". United Kingdom Atomic Energy Authority, AERE - R6622 (1971).

11. EGERTON, J.A. Atomic Energy Research Establishment, Personal Communication (1972).

12. PARKER, K. "The Aldermaston Nuclear Data Library as at May 1963". UKAEA Report AWRE O-70/63.

13. ALLEN, M.S. and DRAKE, M.K. "Neutron Cross Sections for Niobium" General Dynamics, GA-8133 (1967).

14. BLOW, S. "The (n, 2n) reaction in Niobium, and its Relevance to Fusion Reactor Technology". Journal of Nuclear Energy 26, 9 (1972).

15. DIMENT, K.M. and UTTLEY, C.A. "The Cross Sections of Lithium - 6", UKAEA Progress Report AERE - PR/NP 15 and AERE - PR/NP 16 (1969).

16. PENDLEBURY, E.W. "Neutron Cross Sections of Lithium - 7 in the energy range 0.001 eV - 15 MeV" UKAEA Report AWRE O-61/64 (1964).

17. SLAGGIE, E.L. and REYNOLDS, J.T. "Carbon - 12 Evaluated Cross Sections" KAPL - 3099 (1966).

18. PARKER, J.B. (ed). "DICE Mk V. The preparation of Nuclear Data into a Form Suitable for Monte Carlo Calculations using an Electronic Computer" UKAEA Report AWRE O-27/66 (1966).

19. ARONSON, A.L., Brookhaven National Laboratory, Personal Communication (January 1973).

20. MUIR, D.W., Los Alamos Scientific Laboratory, Personal Communication (January 1973).

21. CONN, R. and STACEY, W.M. Jr. "Variational Methods for Controlled Thermonuclear Reactor Blanket Studies". Argonne National Laboratory, AP/CTR/T M-3 (1972).