AAEC/E583

AUSTRALIAN ATOMIC ENERGY COMMISSION

RESEARCH ESTABLISHMENT

LUCAS HEIGHTS RESEARCH LABORATORIES

EXTENSION OF THE AUS REACTOR NEUTRONICS SYSTEM FOR APPLICATION TO FUSION BLANKET NEUTRONICS

G.S. ROBINSON

March 1984

ISBN 0 642 59789 8

AUSTRALIAN ATOMIC ENERGY COMMISSION
RESEARCH ESTABLISHMENT
LUCAS HEIGHTS RESEARCH LABORATORIES

EXTENSION OF THE AUS REACTOR NEUTRONICS SYSTEM FOR APPLICATION TO FUSION BLANKET NEUTRONICS

by

G.S. ROBINSON

ABSTRACT

The AUS modular code scheme for reactor neutronics computations has been extended to apply to fusion blanket neutronics. A new group cross-section library with 200 neutron groups, 37 photon groups and kerma factor data has been generated from ENDF/B-IV. The library includes neutron resonance subgroup parameters and temperature-dependent data for thermal neutron scattering matrices. The validity of the overall calculation system for fusion applications has been checked by comparison with a number of published conceptual design studies.

National Library of Australia card number and ISBN 0 642 59789 8

The following descriptors have been selected from the INIS Thesaurus to describe the subject content of this report for information retrieval purposes. For further details please refer to IAEA-INIS-12 (INIS: Manual for Indexing) and IAEA-INIS-13 (INIS: Thesaurus) published in Vienna by the International Atomic Energy Agency.

A CODES; BREEDING BLANKETS; COMPUTER CALCULATIONS; CROSS SECTIONS; KERMA; NEUTRON REACTIONS; NUCLEAR DATA COLLECTIONS; PHOTONS; THERMONUCLEAR REACTIONS; TRITIUM

CONTENTS

1. INTRODUCTION

The AUS scheme [Robinson 1975] for reactor neutronics computations was developed during the early 1970s as a code system for application to all fission reactor types, both fast and thermal. The main group cross-section library AUS.ENDFB [Robinson 1977] contained 128-group neutron cross sections derived mainly from ENDF/B-IV [Garber 1975] and featured subgroup representation of resonances for both actinides and resonance scatterers. For the AUS system to be applied to fusion blanket neutronics, it was necessary to extend the system to allow coupled neutron-photon calculations. It was also necessary to include kerma factor (the product of cross section and energy release) data for calculations of heat production and to provide a more detailed representation of neutron reactions at energies up to about 14 MeV.

A new AUS group cross-section library AUS.ENDF200G, containing 200 neutron and 37 photon groups, has been generated from ENDF/B-IV. The neutron group structure is essentially the same as that of ENDFB at low energies but the number of high energy groups has been greatly increased. A description of the library and the methods of generation is given in Section 2. Although the library has been generated for fusion applications, it is intended that it cover the widest possible range of neutronics calculations and this has influenced its development. Modifications to existing AUS modules were relatively minor and only one editing module has been added to the system. These developments are described in Section 3.

A one-dimensional model of the STARFIRE design [Baker et al. 1980] was chosen for an investigation of energy, spatial and angular mesh requirements in a typical fusion blanket, and of methods for an efficient computation within the AUS system. This investigation is described in Section 4. One way of checking the validity of the system of calculations is by comparison with published results for well-defined calculations. Comparisons with one-dimensional calculations based on ENDF/B-IV data for a number of conceptual designs are given in Section 5.

2. THE GROUP CROSS-SECTION LIBRARY AUS.ENDF200G

2.1 Library Structure

The format of data in an AUS cross-section data pool which is used for neutron cross-section libraries has been given by Robinson [1975]. The library includes group scatter matrices with all energy transfer mechanisms (except fission) combined, group cross sections, and subgroup parameters for the resonance treatment. All relevant data may be temperature-dependent and the outscatters from a group may be dependent on potential scattering. The group cross sections given are transport, absorption, υ-fission, scattering, total, fission, and two reactions at the discretion of the library compiler.

To include photon data, this structure has been modified by the addition of a block of data for photon production and another block for photon interaction. The production block gives for each neutron group the cross section for photon production in each photon group. To allow for shielding, separate (n,γ) and (n,f) multiplicity matrices may be given where a resonance treatment is adopted. The photon interaction block has the same structure as that for temperature-independent, non-resonance neutron cross sections. The cross sections given are transport, absorption, zero, Compton scattering, total, zero, photo-electric and pair production.

The kerma factor has been added as one or more additional cross sections. Separate factors for elastic scattering, (n,γ), (n,f) and everything else allow resonance shielding where required.

2.2 Library Contents

The current contents of the library are given in Table 1. All the data come from ENDF/B-IV except the photon production data for zirconium which have been obtained from the EPR group library [Ford et al. 1976], and the decay energy data to be included in the kerma factor, for which the values of Abdou and Roussin [1974] were adopted. The actual values of decay energy used after the weighting of isotopes are given in Table 2.

The scattering expansion used was P_3 for neutrons and P_5 for photons, except for some nuclides at neutron energies above 142 keV where P_7 data were included. The resonance treatment of

resonance scatterers has been applied for neutron energies from 1.35 MeV to 750 eV, whereas for actinides it has been applied over the ENDF/B-IV resonance range.

Data for uranium isotopes, which are for neutrons only, have been included at this stage as this is the minimum requirement for testing the library against fission reactor integral experiments. Further actinide data will have to be included in the library for hybrid studies, for which the extended AUS system is ideal.

The neutron group structure given in Table 3 is the same as the 128-group library AUS.ENDFB below 1.2 keV, apart from a minor adjustment from 3 eV to 10.7 eV, but has a much increased number of groups at high energy. The groups have uniform lethargy width over a number of energy ranges as given in the following table:

Energy Range	Lethargy Width
15.5 - 12.8 MeV	0.03125
12.8 - 0.14 MeV	0.0625
140 - 1.2 keV	0.125
1200 - 3 eV	0.25
3 - 0.0125 eV	0.1
0.0125 - (0.001) eV	0.5

The photon group structure (Table 4) is the same as that of VITAMIN-E [Weisbin et al. 1979].

The number of thermal groups and the attention paid to the resonance treatment is probably excessive for fusion blanket requirements. However, it is hoped that in the future this library will be the basis for all neutronic calculations within the AUS system.

2.3 Library Generation Methods

2.3.1 General

A number of different codes have been used to generate the various types of data included in the library. This is an unfortunate procedure as it involves repetition of processing, particularly for neutron cross sections. However, the same weighting function has been used throughout and care has been taken to renormalise where possible the output of the various codes to the most accurate neutron cross sections. The weighting spectra used for four ranges of neutron energy were as follows:

Energy Range	Weighting Spectra
0 - 0.126 eV	300 K Maxwellian
0.126 eV - 674 keV	1/E
674 keV - 10 MeV	fission spectrum of temperature 1.27 MeV
10 - 20 MeV	1/E

The weighting spectrum used for photon cross sections was constant in energy.

2.3.2 Most neutron cross sections

Most of the neutron cross sections have been generated with a modified version [Robinson 1981] of the XLACS2 code which is a module of the AMPX-II code system [RSIC 1978]. The major modification was made to the section of the code which generates thermal scattering matrices. This section was extensively re-written to provide a smooth join of epithermal and thermal matrices. A semi-analytic free gas treatment, sufficiently quick to be applied to all nuclides, was included.

Thermal scattering treatment was applied for neutron energies below 61 eV. The resonance treatment was an infinite dilution calculation at the lowest thermal scattering temperature. Default values were used for all options except for the number of angles employed in the calculation of elastic scattering, for which 384 were used for hydrogen and 64 for all other nuclides.

2.3.3 Neutron resonance cross sections

For those nuclides given a resonance treatment, the resonance data have been generated by a set of AAEC programs, following the general procedure given by Robinson [1977] for AUS.ENDFB. In outline.

- a point cross section file was generated,
- the neutron slowing-down equation was solved numerically for a range of mixtures of the resonance nuclide and hydrogen,
- the results were edited to provide group resonance integrals and P_0 elastic scattering matrices and,
- the resonance integrals were fitted to subgroup parameters.

A number of detailed improvements have been made to these methods. In particular, the unresolved resonance range is now treated by first selecting a ladder of resonances which reproduces the infinitely dilute group cross sections, then proceeding as for resolved resonances.

2.3.4 Photon production and kerma factor data

Both photon production and kerma factor data have been generated using the MACK-IV code [Abdou et al. 1978], thus ensuring as much consistency of the two sets of data as is possible using ENDF/B-IV. A number of modifications were made to MACK-IV, mainly in sections relating to output. The changes were made to allow the production of separate photon production data for (n,γ), (n,f) and the remaining reactions, and separate kerma factor data for these reactions and elastic scattering. In this way it is possible to use approximate calculations of neutron cross sections in MACK-IV, renormalise the output to XLACS2 cross sections and provide for resonance shielding within AUS.

A low-grade resonance calculation at zero temperature (in K) was adopted and the standard set of energy points used for the points at which the code calculates data before forming group averages. This standard set has three ranges with equal lethargy intervals between points in each range (energy range 10^{-5} eV, 1 eV, 1 MeV, and 17.4 MeV; number of points per range 19, 580 and 400).

A major option within MACK-IV is the use of a direct path which employs ENDF/B-IV photon production data in the calculation of neutron kerma factors or an indirect path. The indirect path had to be used for D, ^{11}B and Zr, because ENDF/B-IV has no photon production data for them. An option was included to use the indirect path for (n,γ) kerma factors but retain the direct path for other reactions. This option was adopted for all ENDF/B-IV materials which are mixtures of isotopes (except Pb) because the use of a single Q-value for each reaction type makes the calculation of the small recoil energy of the nucleus from the difference of the available energy and the photon energy completely inaccurate. For Pb, the direct path was retained because separate (n,γ) photon data are not included in ENDF/B-IV.

2.3.5 Photon interaction

Photon interaction data were calculated using the SMUG module of the AMPX-II system.

3. AUS MODULE DEVELOPMENT

3.1 General

The programs used to generate the cross-section library which were discussed in Section 2 are not included as modules in the AUS system. AUS modules are those programs related to neutron (and photon) transport calculations which are based on the use of an AUS cross-section library and make use of AUS data pools. The module development required to incorporate photon transport was relatively minor. Most modules work with cross-section data pools in which no distinction is made between neutrons and photons. Modifications to existing modules were necessary only for those modules working with the main cross-section library. An additional edit module was added to provide quantities of interest in fusion blanket calculations.

AUS includes a multi-dimensional diffusion capability but only one-dimensional transport modules. Multi-dimensional transport calculations are performed by producing card-image cross sections for such standard codes as DOT [Rhoades and Mynatt 1973] and MORSE [Emmett 1975].

3.2 MIRANDA Module

MIRANDA [Robinson 1977], which serves as the cross-section preparation module of AUS, was the only module requiring major modification. MIRANDA accesses the cross-section library and produces as output a cross-section data pool appropriate to the system under study in which the data have been resonance shielded, temperature dependence eliminated, and the number of energy groups reduced. The normal MIRANDA output cross sections are in the form in which photons and neutrons are not distinguished. The module incorporates a multi-region resonance calculation and a homogeneous spectrum calculation.

Resonance shielding of the photon production and neutron kerma data has been included in the MIRANDA resonance treatment. As the components of these data are included in the library, it was simply necessary to shield these components using the same factors as the appropriate cross sections.

The number of photon groups may be reduced in MIRANDA by group collapsing over a constant-in-energy spectrum, an input spectrum, or the spectrum from a P_0 or B_ℓ calculation identical to that for neutrons in which the photon source may be the photon production from the neutron spectrum calculation.

3.3 BEDIT - A Fusion Blanket Edit Module

The AUS system includes a module EDIT [Pollard 1975] for general purpose editing of one-dimensional flux calculations. Rather than modify EDIT to distinguish between neutrons and photons, a new module BEDIT has been written which produces as printed output those quantities of interest in fusion blanket studies. The standard output from BEDIT is one-group reaction rates (such as neutron and photon kerma, photon production, neutron and photon absorption) for each material in the system and for each of its component nuclides, plus reaction rate scans to provide detailed spatial distributions. Tritium production in ^{6}Li and ^{7}Li, including spatial distributions, is normally produced.

4. MESH REQUIREMENTS FOR A FUSION BLANKET CALCULATION

4.1 Choice of Model

A one-dimensional S_N transport calculation of a reference design for the STARFIRE concept [Baker et al. 1980] was chosen for an investigation of the energy, spatial and angular mesh required for accurate calculations. Although the results are sensitive to the materials used in blanket, some more general principles can be derived which are particularly applicable to any design with a water-cooled first wall.

The material densities used in all STARFIRE calculations in this report were taken from Table 10-26 of Baker et al. [1980] and are reproduced in Table 5. The zone layout and volume fractions used in the mesh investigation are given in Table 6. An enrichment of 60 per cent ^{6}Li was used. Unless otherwise stated, all S_N calculations in this report were performed using the ANAUSN module [Clancy 1982] in cylindrical geometry, with a free outer boundary and a spatially uniform source in the plasma.

4.2 Spatial and Angular Mesh

An investigation of the spatial and angular mesh was performed using a set of cross sections in 20 neutron and 5 photon groups. The results are given in Table 7. As well as presenting integral quantities, the distribution of tritium production in ^{6}Li is represented by the value adjacent to the second wall and also by the value at the much smaller peak adjacent to the reflector. The peak energy deposition in the breeder, which occurs adjacent to the second wall, is given. The photon energy deposition in the outer 3 cm of the reflector is included as a convenient measure of the photons entering the shield (not represented in the model).

It can be seen that the integral quantities are not sensitive to the range of parameters considered (except for a 0.5 per cent change in tritium production between S_4 and S_8) but that the distributions are sensitive. The following conclusions have been drawn:

- the S_N order require is at least 8;
- a P_3 scattering expansion is adequate;
- a relatively coarse mesh is adequate except in the breeder;
- mesh intervals of about 3 cm are adequate in the interior of the breeder; and
- the mesh intervals at the boundary of the wall and breeder need to be chosen on the basis of the definition required in the energy deposition.

Concerning the last point, a relatively coarse mesh (0.2 cm) gave the average energy deposition over that interval quite well (0.2 per cent accuracy when comparing Cases 2 and 3 — see Table 7). The 0.1 cm interval of the 43-mesh set was chosen quite arbitrarily. The problem at the boundary between the wall and breeder is that there is a significant thermal flux component and the macroscopic thermal cross section in the breeder is about 10 cm^{-1}.

4.3 Energy Groups

The investigation of energy groups dealt with the number of groups required and the most effective spectra to be used in group collapsing. The results of two approaches are presented in Table 8. The straightforward method used condensation over one or more spectra in MIRANDA to reduce the number of groups to that of the final S_N calculation. In the indirect method, a preliminary condensation in MIRANDA was followed by a coarse mesh S_4P_0 calculation to provide region-dependent spectra for condensation to the final number of groups.

The spectra used in MIRANDA were for slowing down in an infinite medium with a volume source given by the fusion neutrons. The mixed' spectrum was from a zero-dimensional calculation of a mixture of wall, multiplier and breeder materials chosen to give a spectrum similar to that at the second wall. The '3 zone' spectra used a thickness weighted mixture of wall and multiplier materials to define one spectrum, but the breeder and reflector were condensed over their own spectra. The first S_N calculation was S_4P_0 with mesh intervals of 253, 20, 1, 2 of 2.5, 1, 0.1, 2.2, 6.9, 3 of 9.2, 6.9, 2.3, 3, 2 of 6 cm. The EDIT module was used to condense each material zone over the appropriate spectrum. The breeder was divided into five zones of thickness 0.1, 2.2, 16.1, 25.3 and 2.3 cm in each of which a different spectrum was used. The final S_N calculation was S_8P_3 for the 43-mesh set of Table 7. The coarse and fine group sets were chosen after preliminary calculations indicated the large spectrum changes involved, and the importance of neutrons slowing down in the walls to the peak tritium production in the breeder.

In Table 8, Case 1 is the benchmark. Cases 2 and 3 demonstrate the advantage of the indirect method. If Case 4 is compared with Case 3, there is negligible effect from varying the spectra in the preliminary condensation. Case 5 shows, much better than Case 2, the errors that may be introduced by condensing to a reasonable number of groups over reasonable spectra. Case 6 indicates the large errors arising from condensation over an inappropriate spectrum.

The indirect method, using 25 groups, provides results comparable with those obtained by a direct calculation in 141 groups at a fraction of the computing time. It was necessary to retain a thin ($\sim$ 0.1 cm) spectrum defining zone in the breeder at the wall interface in order to calculate the peak energy deposition accurately.

4.4 Application

The results of this investigation may be applied more widely than the particular STARFIRE model considered. The required spatial mesh is quite sensitive to the particular blanket configuration, but angular mesh and energy condensation should be much less so. All the calculations described in the following section included a preliminary condensation to 115 neutron plus 26 photon groups, a coarse mesh S_4P_0 calculation to provide spectra for condensation to 20 neutron plus 5 photon groups and a final S_8P_3 calculation. The STARFIRE calculations used the coarse mesh and 43-mesh intervals given above with only minor variations in the void region and with the breeder zone compressed.

5. COMPARISON WITH PUBLISHED RESULTS

5.1 STARFIRE

The STARFIRE design [Baker et al. 1980] was chosen as the major study for which a comparison with published results should be made. Baker et al. included extensive documentation of a range of one-dimensional scoping studies of the blanket. They also gave results for a one-dimensional model of the reference design which included results for energy release and leakage into the shield as well as tritium breeding. It is believed that the group cross section in these calculations came from VITAMIN-C [Roussin et al. 1980] and the nuclear response functions from MACKLIB-IV [Gohar and Abdou 1978], both of which are based on ENDF/B-IV.

Comparisons have been made for the reference design with either a Zr_5Pb_3 or Be multiplier. The atom densities were taken from Table 10-26 of Baker et al. and are reproduced in Table 5. The thickness and composition by volume of the various zones were taken from Table 10-43 and are reproduced in Table 9. Additional data not given explicitly by Baker et al. were

- a uniform source corresponding to a plasma temperature of 24 keV extending over a 214 cm radius,
- a first wall inner radius of 214 cm,
- cylindrical geometry with a free outer boundary condition,
- a temperature of 600 K throughout.

No reasonable variation in these additional data affected the results significantly except the assumption of a uniform source inside the first wall. However, a source which peaked near the origin decreased the tritium breeding ratio. The assumption made for this comparison is that which gives the maximum tritium breeding ratio.

A comparison of the results using the AUS scheme with those given in Table 10-44 of Baker et al. is given in Table 10. All quantities in the table are per fusion neutron. The comparison is rather poor when it is considered that the same basic nuclear data have been used and the differences should result only from cross-section processing and methods of calculation.

The difference in tritium breeding ratio was the most surprising. Tritium breeding depends only on the well-established neutron component of the calculation and it was seen, in Section 4, that results for integral quantities in the STARFIRE blanket are not sensitive to details of the calculation. A comparison of tritium breeding with a number of other published results was therefore undertaken.

5.2 INTOR-EC

Pelloni et al. [1982] have used a European community designed blanket (INTOR-EC) for INTOR in a comparison of different cross-section libraries. Their specifications for a blanket using Li_2SiO_3 and another using $Li_{17}Pb_{83}$ are reproduced in Tables 11 and 12 respectively. They also specified cylindrical geometry with an albedo of 0.3 on the external boundary of the reflector. To conform with this boundary condition, the final S_N calculations were performed in the ANISN code [Engle 1973] using an S_8P_3 approximation. A plasma temperature of 10 keV and a blanket temperature of 300 K were used in the AUS calculations.

The results given by Pelloni et al. for 171 group calculations using VITAMIN-C data for three of their cases have been chosen for comparison. The results are given in Table 13. The agreement obtained is very satisfactory.

5.3 CTR Standard Blanket

The CTR standard blanket problem specified by Steiner [1973] is a rather dated concept which has Nb as the structural material, an Li (94 per cent Li, 6 per cent Nb) breeder, and a graphite reflector. The use of infinitely dilute Nb cross sections is one of the specifications. Results using VITAMIN-C data have been reported by Roussin et al. [1978] and are compared with AUS results in Table 14. The agreement is satisfactory.

5.4 DEMO

DEMO [Abdou et al. 1982] is a conceptual design for a demonstration fusion reactor. It is more recent than the commercial reactor design STARFIRE in the series of conceptual design studies performed at Argonne National Laboratory. The DEMO documentation includes a large number of scoping studies using either three-dimensional Monte-Carlo or one-dimensional S_8P_3 calculations in ANISN. The cross-section libraries were VITAMIN-C and MACKLIB-IV. Three of the one-dimensional cases have been chosen for a comparison of tritium breeding.

The atom densities, based on those of Table 7-9 of Abdou et al., are given in Table 15. The zone layout and composition for the three cases are given in Table 16. In addition, Abdou et al. specified a uniform source over a plasma of radius 208 cm and a 16.5 cm thick scrape-off zone. Additional data used in the AUS calculations were an 8.4 keV plasma temperature and a 550 K blanket temperature. The results for the three cases are given in Table 17. The agreement is quite reasonable.

There is a larger discrepancy between ANL and AUS results for a $LiAlO_2$ breeder with a Be multiplier for STARFIRE than with the same breeder and multiplier for DEMO. Hence a series of calculations was undertaken in the course of which the DEMO model was progressively altered to that used for STARFIRE. The calculated tritium breeding ratios are given by

- exact DEMO
- change to natural Li
- 46 cm thick breeder with reflector
- changes to wall and multiplier
- change to breeder volume fractions
- exact STARFIRE

This is to be compared with ANL results of 1.19 and 1.217 for DEMO and STARFIRE, respectively. It would appear that the results given by Baker et al. for the one-dimensional models of the reference design for STARFIRE are not consistent with ENDF/B-IV data.

5.5 Summary

In these comparisons, all the published results were obtained using ENDF/B-IV data in the group data libraries VITAMIN-C and MACKLIB-IV. Quite reasonable ($\sim$ 1 per cent) agreement for tritium breeding ratio was obtained except for STARFIRE, the only design for which other calculated quantities were available. Agreement to about 6 per cent was obtained for the total energy release in the STARFIRE blanket.

A wide range of cases was considered. In particular, the thermal neutron component of tritium breeding given in Table 18 shows great variation. It is of interest that the VITAMIN-C data, which contain no thermalisation treatment, are in good agreement with AUS for the well thermalised systems. It is unlikely that such good agreement would be obtained for all thermal systems or for thermal neutron distributions.

6. CONCLUSION

The AUS system, which had previously been applied chiefly to fission reactor core calculations, has been extended for fusion neutronics computations. Relatively minor modifications to existing modules were required to include photons in the calculations, but the main extension was the development of a new cross-section library AUS.ENDF200G, with 200 neutron groups, 37 photon groups and kerma factor data, which was generated from ENDF/B-IV. The extended scheme is also well suited to calculations of fast and thermal fission reactor cores, fusion-fission hybrids, shielding and many other nuclear applications. Although application of the new library to fission calculations will require the inclusion of more actinide data, the use of a single general-purpose library has many advantage.

The attempt to validate AUS calculations of fusion blankets by comparison with published results which used ENDF/B-IV data has had limited success. Except for the STARFIRE design which

included the only suitable results for energy release, good agreement on tritium breeding was found. The use of design studies for code verification is not very satisfactory. The establishment of an international benchmark model is most desirable to check the many features of fusion blanket neutronics which are not amenable to experimental verification. Comparison of AUS with integral experiments on tritium breeding is intended.

7. REFERENCES

Abdou, M.A. and Roussin, R.W. [1974] - MACKLIB. ORNL-TM-3995.

Abdou, M.A., Gohar, Y. and Wright, R.Q. [1978] - MACK-IV, a new version of MACK: a program to calculate nuclear response functions from data in ENDF/B format. ANL/FPP-77-5.

Abdou, M.A. *et al.* [1982] - A demonstration tokamak power plant study (DEMO). ANL/FPP/82-1.

Baker, C.C. *et al.* [1980] - STARFIRE - a commercial tokamak fusion power plant study. ANL/FPP-80-1.

Clancy, B.E. [1982] - ANAUSN - a one-dimensional multigroup S_N transport theory module for the AUS reactor neutronics system. AAEC/E539.

Emmett, M.B. [1975] - The MORSE Monte Carlo radiation transport code system. ORNL-4972.

Engle, W.W. [1973] - A users' manual for ANISN - a one-dimensional discrete ordinates transport code with anisotropic scattering. K-1693 (revised).

Ford, W.E., Santoro, R.T., Roussin, R.W. and Plaster D.M. [1976] - Modification number one to the coupled 100 n-21 cross-section library for EPR calculations. ORNL-TM-5249.

Garber, D. [1975] - ENDF/B summary documentation. ENDF-201.

Gohar, Y. and Abdou, M.A. [1978] - MACKLIB-IV - a library of nuclear response functions generated with the MACK-IV computer program from ENDF/B-IV. ANL/FPP-TM-106.

Howerton, R.J. [1975] - The Lawrence Livermore Laboratory evaluated nuclear data library (ENDL) translated into ENDF/B format. UCID-16727.

Pelloni, S., Stepanek, J. and Dudziak, D. [1982] - Comparison of different fusion nuclear data libraries using the European INTOR blanket design. EIR-479.

Pollard, J.P. [1975] - AUS module EDIT. AAEC unpublished report.

Rhoades, W.A. and Mynatt, F.R. [1973] - The DOT III two-dimensional discrete ordinates transport code. ORNL-TM-4280.

Robinson, G.S. [1975] - AUS - The Australian modular scheme for reactor neutronics computations. AAEC/E369.

Robinson, G.S. [1977] - AUS module MIRANDA - a data preparation code based on multiregion resonance theory. AAEC/E410.

Robinson, G.S. [1981] - Notes on the AAEC version of XLACS II. ORNL/RSIC/PSR-182.

Roussin, R.W., Weisbin, C.R., White, J.E., Greene, N.M., Wright, R.Q. and Wright, J.B. [1980] - VITAMIN-C: the CTR processed multigroup cross-section library for neutronics studies. ORNL/RSIC-37.

Roussin, R.W. *et al.* [1978] - Experience in developing and using the VITAMIN-C 171-neutron, 36-gamma-ray group cross-section library. ORNL/RSIC-41.

RSIC [1978] - AMPX-II modular code system for generating coupled multigroup neutron-gamma-ray cross-section libraries from data in ENDF format. ORNL/RSIC/PSR-63.

Steiner, D. [1973] - Analysis of a benchmark calculation of tritium breeding in a fusion reactor blanket: the United States contribution. ORNL-TM-4177.

Weisbin, C.R., Roussin, R.W., Wagshal, J.J., White, J.E. and Wright, R.Q. [1979] - VITAMIN-E: an ENDF/B-V multigroup cross-section library for LMFBR core and shield, LWR shield, dosimetry and fusion blanket technology. ORNL-5505.

TABLE 1
CONTENTS OF AUS.ENDF200G AT 1/8/83

Nuclide	Photon and Kerma Data	Resonance Treatment	Temp. (K)	Additional Reactions	Neutron P_ℓ Order*	Notes
ZZ999	No	No	-	-	-	(a)
CH2	Yes	No	296	n,γ n,2n	7	(b)
H2O	Yes	No	1000,600,450,296	n,γ n,2n	7	(b)
D20	Yes	No	1000,600,450,296	n,γ n,2n	7	(b),(f)
C	Yes	No	1600,1000,600,296	n,γ n,2n	7	(b)
BE	Yes	No	1000,600,296	n,γ n,2n	7	(b)
O	Yes	No	3000,2000,1000,600 450,296	n,γ n,2n	7	
HE3	No	No	300	n,p n,d	3	
LI6	Yes	No	300	n,α -	7	
LI7	Yes	No	300	n,α -	7	
B10	Yes	No	300	n,α n,2n	3	
B11	Yes	No	300	n,γ n,2n	3	(g)
N	Yes	No	300	n,γ n,p	3	
F	No	No	300	n,γ n,2n	3	
NA	Yes	Yes	300	n,γ n,2n	7	
AL	Yes	Yes	300	n,γ n,2n	7	
SI	Yes	No	300	n,γ n,2n	7	
CA	Yes	No	300	n,γ n,2n	7	
TI	Yes	No	300	n,γ n,2n	3	
V	Yes	No	300	n,γ n,2n	3	
CR	Yes	Yes	300	n,γ n,2n	7	
MN	Yes	No	300	n,γ n,2n	3	
Fe	Yes	Yes	300	n,γ n,2n	7	
Fe54D	No	No	-	n,p -	-	(c)
NI	Yes	Yes	300	n,γ n,2n	7	
CU	No	No	300	n,γ n,2n	3	
ZR	Yes	No	300	n,γ n,2n	7	(d)
NB	Yes	No	300	n,γ n,2n	3	
MO	Yes	No	300	n,γ n,2n	3	
CD	No	No	300	n,γ n,2n	3	
I	No	No	300	n,γ n,2n	3	
W182	Yes	No	300	n,γ n,2n	3	
W183	Yes	No	300	n,γ n,2n	3	
W184	Yes	No	300	n,γ n,2n	3	
W186	Yes	No	300	n,γ n,2n	3	
PB	Yes	No	300	n,γ n,2n	3	
U234	No	Yes	300	n,γ n,2n	3	(e)
U235	No	Yes	2100,900,300	n,γ n,2n	7	
U236	No	Yes	300	n,γ n,2n	3	(e)
U238	No	Yes	2100,900,300	n,γ n,2n	7	

*Scattering expansion. 7 implies P_7 for neutron energies above 142 keV and P_3 below that.

(a) ZZ999 is a 1/v absorber with a cross section of 1 barn at 0.0253 eV.

(b) S(α, β) from ENDFB was used for thermal scattering.

(c) From ENDFB-IV dosimetry file. Only (n,p) is given.

(d) Photon production data taken from the EPR library [Ford et al. 1976] in which the Zr data were processed from the ENDL library [Howerton 1975].

(e) The cross sections were not re-processed from ENDFB but were expanded in a simple manner from the previous 128-group library AUS.ENDFB [Robinson 1977].

(f) Does not include photon production from deuterium.

(g) Does not include photon production data.

TABLE 2
DECAY ENERGY USED IN AUS.ENDF200G IN MeV

Reaction / Nuclide	n,2n	n,n'p	n,γ	n,p	n,d	n,t	n,α
	MeV						
BE	0.095			6.24			1.56
O				2.6924			
LI6				1.56			
LI7		1.56	9.31		1.56		
B10						0.095	
B11			6.42	4.86			9.31
NA			0.557	1.909			
AL			1.2448	0.7055			0.557
V			1.07	0.934			0.210
CR	0.0007	0.0288		1.07			
FE				0.651			
NI	0.0459						
NB							0.931
W183				0.2085			
W184			0.1309	0.428			0.1233
W186	0.1309		0.3113	0.885			0.8135
PB			0.01213				

TABLE 3
NEUTRON GROUP BOUNDARIES

Group	Lower Energy MeV	Lethargy	Group	Lower Energy MeV	Lethargy
0	15.488	-0.4375			
1	15.012	-0.40625	33	2.375	1.4375
2	14.550	0.375	34	2.231	1.5
3	14.102	-0.34375	35	2.096	1.5625
4	13.668	-0.3125	36	1.969	1.625
5	13.248	-0.28125	37	1.850	1.6875
6	12.840	-0.25	38	1.738	1.75
7	12.062	-0.1875	39	1.632	1.8125
8	11.332	-0.125	40	1.534	1.875
9	10.645	-0.0625	41	1.441	1.9375
10	10.000	0.0	42	1.353	2.0
11	9.394	0.0625	43	1.271	2.0625
12	8.825	0.125	44	1.194	2.125
13	8.290	0.1875	45	1.122	2.1875
14	7.788	0.25	46	1.054	2.25
15	7.316	0.3125	47	0.990	2.3125
16	6.873	0.375	48	0.930	2.375
17	6.456	0.4375	49	0.874	2.4375
18	6.065	0.5	50	0.821	2.5
19	5.698	0.5625	51	0.771	2.5625
20	5.353	0.625	52	0.724	2.625
21	5.028	0.6875	53	0.681	2.6875
22	4.724	0.75	54	0.639	2.75
23	4.437	0.8125	55	0.600	2.8125
24	4.169	0.875	56	0.564	2.875
25	3.916	0.9375	57	0.530	2.9375
26	3.679	1.0	58	0.498	3.0
27	3.456	1.0625	59	0.468	3.0625
28	3.247	1.125	60	0.439	3.125
29	3.050	1.1875	61	0.413	3.1875
30	2.865	1.25	62	0.388	3.25
31	2.691	1.3125	63	0.364	3.3125
32	2.528	1.375	64	0.342	3.375

TABLE 3 (Continued)
NEUTRON GROUP BOUNDARIES

Group	Lower Energy keV	Lethargy	Group	Lower Energy eV	Lethargy
65	321.4	3.4375	99	10333.0	6.875
66	302.0	3.5	100	9119.0	7.0
67	283.7	3.5625	101	8047.0	7.125
68	266.5	3.625	102	7102.0	7.25
69	250.3	3.6875	103	6267.0	7.375
70	235.2	3.75	104	5531.0	7.5
71	220.9	3.8125	105	4881.0	7.625
72	207.5	3.875	106	4307.0	7.75
73	195.0	3.9375	107	3801.0	7.875
74	183.2	4.0	108	3354.0	8.0
75	172.1	4.0625	109	2960.0	8.125
76	161.6	4.125	110	2613.0	8.25
77	151.8	4.1875	111	2306.0	8.375
78	142.6	4.25	112	2035.0	8.5
79	125.9	4.375	113	1796.0	8.625
80	111.1	4.5	114	1585.0	8.75
81	98.03	4.625	115	1398.0	8.875
82	86.52	4.75	116	1234.0	9.0
83	76.35	4.875	117	961.1	9.25
84	67.38	5.0	118	748.5	9.5
85	59.46	5.125	119	582.9	9.75
86	52.48	5.25	120	454.0	10.0
87	46.31	5.375	121	353.6	10.25
88	40.87	5.5	122	275.4	10.5
89	36.07	5.625	123	214.5	10.75
90	31.83	5.75	124	167.0	11.0
91	28.09	5.875	125	130.1	11.25
92	24.79	6.0	126	101.3	11.5
93	21.87	6.125	127	78.89	11.75
94	19.30	6.25	128	61.44	12.0
95	17.04	6.375	129	47.85	12.25
96	15.03	6.5	130	37.27	12.5
97	13.27	6.625	131	29.02	12.75
98	11.71	6.75	132	22.60	13.0

(Continued)

TABLE 3 (Continued)
NEUTRON GROUP BOUNDARIES

Group	Lower Energy eV	Lethargy	Group	Lower Energy eV	Lethargy
133	17.603	13.25	167	0.2056	17.7
134	13.710	13.5	168	0.1860	17.8
135	10.677	13.75	169	0.1683	17.9
136	8.315	14.0	170	0.1523	18.0
137	6.475	14.25	171	0.1378	18.1
138	5.043	14.5	172	0.1247	18.2
139	3.928	14.75	173	0.1128	18.3
140	3.059	15.0	174	0.1021	18.4
141	2.768	15.1	175	0.0924	18.5
142	2.505	15.2	176	0.0836	18.6
143	2.266	15.3	177	0.0756	18.7
144	2.050	15.4	178	0.0684	18.8
145	1.855	15.5	179	0.0619	18.9
146	1.679	15.6	180	0.0560	19.0
147	1.519	15.7	181	0.0507	19.1
148	1.375	15.8	182	0.0459	19.2
149	1.244	15.9	183	0.0415	19.3
150	1.125	16.0	184	0.0376	19.4
151	1.018	16.1	185	0.0340	19.5
152	0.921	16.2	186	0.03075	19.6
153	0.834	16.3	187	0.02782	19.7
154	0.754	16.4	188	0.02518	19.8
155	0.683	16.5	189	0.02278	19.9
156	0.618	16.6	190	0.02061	20.0
157	0.559	16.7	191	0.01865	20.1
158	0.506	16.8	192	0.01688	20.2
159	0.458	16.9	193	0.01527	20.3
160	0.4140	17.0	194	0.01382	20.4
161	0.3746	17.1	195	0.01250	20.5
162	0.3389	17.2	196	0.00758	21.0
163	0.3067	17.3	197	0.00460	21.5
164	0.2775	17.4	198	0.00279	22.0
165	0.2511	17.5	199	0.00169	22.5
166	0.2272	17.6	200	0.00001	27.6

TABLE 4
PHOTON GROUP BOUNDARIES

Group	Lower Energy MeV	Group	Lower Energy keV
0	20.0		
1	14.0	20	1000
2	12.0	21	800
3	10.0	22	700
4	8.0	23	600
5	7.5	24	512
6	7.0	25	510
7	6.5	26	450
8	6.0	27	400
9	5.5	28	300
10	5.0	29	200
11	4.5	30	150
12	4.0	31	100
13	3.5	32	70
14	3.0	33	60
15	2.5	34	45
16	2.0	35	30
17	1.66	36	20
18	1.5	37	10
19	1.33		

TABLE 5
STARFIRE MATERIAL DENSITIES

Material	Nuclide	Atom Density 10^{-24} cm^{-3}
$LiAlO_2$	Li	0.03106
	Al	0.03106
	0	0.06211
Be	Be	0.1236
Zr_5Pb_3	Zr	0.0234
	Pb	0.0140
H_2O	H_2O	0.0335
PCA Steel	Fe	0.05486
	Cr	0.01266
	Ni	0.01282
	Mo	0.0009793
	Mn	0.001710
	Ti	0.0002942
	Si	0.0008384
	C	0.0001961
	N	0.00003358
C	C	0.08023

TABLE 6
MODEL USED IN MESH INVESTIGATIONS

Zone	Outer Radius cm	Composition as Volume %
Plasma	253	Void
Scrape-off	273	Void
First wall	274	50% PCA, 27% H_2O
Multiplier	279	100% Zr_5Pb_3
Second wall	280	35% PCA, 17% H_2O
Breeder	326	6.55% PCA, 3.26% H_2O, 52.16% $LiAlO_2$
Reflector	341	5% PCA, 5% H_2O, 90% C

TABLE 7
EFFECT OF SPATIAL AND ANGULAR MESH

Case Description				Tritium Production per Fusion Neutron				Kerma per Fusion Neutron		
Case	S_N	P	Mesh Points (see below)	Total ^6Li	Total ^7Li	*Peak ^6Li 10^{-6} cm^{-1}	**Edge ^6Li 10^{-6} cm^{-1}	Total MeV eV cm^{-1}	*Peak eV cm^{-1}	†Boundary eV cm^{-1}
1	4	3	32	1.0975	0.0230	137.4	7.31	16.74	919	1.529
2	4	3	40	1.0968	0.0230	137.4	7.45	16.74	919	1.547
3	4	3	49	1.0970	0.0230	170.7	10.10	16.74	1088	1.546
4	4	3	43	1.0969	0.0230	155.8	8.76	16.74	1013	1.543
5	8	3	43	1.1019	0.0233	154.6	8.35	16.79	1020	1.345
6	12	3	43	1.1028	0.0234	152.9	8.19	16.80	1014	1.321
7	8	2	43	1.1010	0.0234	154.4	8.33	16.80	1018	1.343

* At first breeder mesh interval. ** At last breeder mesh interval
† Photon kerma only for outer 3 cm of the reflector.

32 mesh - 253, 10, 10, 1, 4 of 1.25, 1, 0.2, 0.4, 0.6, 1.1, 2.3, 8 of 4.6, 2.3, 1.1, 0.6, 0.4, 0.2, 5 of 3.

40 mesh - as 32 mesh but 8 of 4.6 became 16 of 2.3

49 mesh - 253, 10, 10, 1, 4 of 1.25, 1, 0.05, 0.075, 0.11, 0.17, 0.25, 0.38, 0.57, 0.695, 1, 1.3, 2, 2.6, 9 of 3.06667, 2.6, 2, 1.3, 1, 0.695, 0.57, 0.38, 0.25, 0.17, 0.11, 0.075, 0.05, 1, 2, 3 of 3, 2, 1

43 mesh - 253, 10, 10, 1, 4 of 1.25, 1, 0.1, 0.16, 0.25, 0.40, 0.65, 0.74, 1, 1.3, 2, 2.6, 9 of 3.06667, 2.6, 2, 1.3, 1, 0.74, 0.65, 0.40, 0.25, 0.16, 0.10, 5 of 3.

TABLE 8
EFFECT OF ENERGY GROUP CONDENSATION

Case	Case Description: MIRANDA Spectra	Group Structure: 1st S_N n+γ	Group Structure: 2nd S_N n+γ	Tritium Production per Fusion Neutron: Total ^6Li	Total ^7Li	*Peak ^6Li 10^{-6} cm^{-1}	**Edge ^6Li 10^{-6} cm^{-1}	Kerma per Fusion Neutron: Total MeV	*Peak eV cm^{-1}	†Boundary eV cm^{-1}
1	Mixed	-	115+26	1.0991	0.0234	162.4	8.88	16.87	1061	1.370
2	Mixed	-	20+5	1.0995	0.0229	167.9	8.81	18.67	1099	3.054
3	Mixed	115+26	20+5	1.0997	0.0233	160.4	8.76	16.86	1051	1.370
4	3-zone	115+26	20+5	1.0996	0.0233	159.3	8.75	16.87	1045	1.370
5	3-zone	-	20+5	1.1232	0.0230	158.8	9.05	17.33	1046	1.417
6	Breeder	-	20+5	1.0951	0.0234	143.6	7.28	16.74	964	1.265

* At first breeder mesh interval. ** At last breeder mesh interval
† Outer 3 cm of the reflector.

Group Structures:

115 groups - 15.5, 14.55, 14.1, 13.7, 13.2, 12.8 MeV, then 0.125 Δu groups to 1.23 keV, 0.25 Δu to 3 eV, 0.5 Δu to 0.0125 eV, 0 eV.

20 groups - 15.5, 12.8, 10 MeV, then 1.0 Δu groups to 3 eV, 0.414 eV, 0.056 eV, 0 eV.

26 groups - 20, 10, 8, 7.5, 7, 6.5, 6, 5, 4, 3, 2.5, 2, 1.66, 1.5, 1.33, 1, 0.7, 0.512, 0.51, 0.4, 0.3, 0.2, 0.15, 0.10, 0.06, 0.03, 0.01 MeV

5 groups - 20, 6, 3, 1, 0.51, 0.01 MeV.

TABLE 9
SPECIFICATION FOR STARFIRE REFERENCE DESIGN

Zone	Thickness cm	Composition as Volume %
First wall	1	50% PCA, 27% H_2O
Multiplier	5	100% Zr_5Pb_3 or 70% Be
Second wall	1	35% PCA, 17% H_2O
Breeder	30	80% $LiAlO_2$*, 10% PCA, 5% H_2O
Reflector	15	90% C, 5% PCA, 5% H_2O

* Natural Li for the Be multiplier, enriched to 60% ^6Li for the Zr_5Pb_3 multiplier.

TABLE 10
COMPARISON OF STARFIRE RESULTS

Multiplier	Zr_5Pb_3		Be	
	Baker et al.	AUS	Baker et al.	AUS
^6Li tritium production	1.186	1.107	1.142	1.070
^7Li tritium production	0.020	0.023	0.075	0.075
Tritium breeding ratio	1.206	1.130	1.217	1.145
Energy release (MeV)	17.44	16.31	19.87	19.06
Neutron leakage	0.019	0.023	0.038	0.043
Neutron energy leakage (MeV)	0.041	0.055	0.057	0.068
Gamma-ray energy leakage (MeV)	0.036	0.041	0.085	0.087
Total energy leakage (MeV)	0.077	0.097	0.142	0.155

TABLE 11
SPECIFICATION FOR INTOR-EC Li_2SiO_3 CONCEPT

Zone	Component	Outer Radius cm
1	Plasma	220
2	Vacuum	250
3	First wall	251.3
4	Multiplier	260.4
5	Breeder	266.6
6	Breeder	272.8
7	Breeder	279.0
8	Reflector	291.0

Zone	3	4	5	6	7	8
Nuclide	Atom Density 10^{-24} cm $^{-3}$					
Ni	7.40-3*	7.40-4	8.29-4	8.21-4	8.14-4	7.40-3
Cr	1.77-2	1.77-3	1.98-3	1.96-3	1.95-3	1.77-2
Fe	6.06-2	6.06-3	6.79-3	6.73-3	6.67-3	6.06-2
Pb		1.99-2				
D_2O		2.68-3				
H_2O			7.40-3	9.35-3	9.95-3	
O			1.45-2	1.235-2	6.25-3	
Si			4.83-3	4.13-3	2.08-3	
^6Li			7.16-4	5.68-4	3.08-4	
^7Li			8.93-3	7.65-3	3.84-3	

* 7.40×10^{-3}, etc.

TABLE 12
SPECIFICATION FOR INTOR-EC $Li_{17}Pb_{83}$ CONCEPT

Zone	Component	Outer Radius cm
1	Plasma	220
2	Vacuum	250
3	First wall	253
4	Breeder	293
5	Reflector	305

Zone	3	4	5
Nuclide	Atom Density 10^{-24} cm^{-3}		
Ni		9.88-4*	7.40-3
Cr		1.37-3	1.77-2
Fe		5.76-3	6.06-2
H_2O	6.70-3	3.35-3	
Al	4.82-2		
Pb		2.19-2	
^6Li		3.33-4	
^7Li		4.16-3	

* 9.88×10^{-4}, etc.

TABLE 13
COMPARISON OF TRITIUM BREEDING FOR INTOR-EC

Case		Tritium Breeding Ratio	
		Pelloni et al.	AUS
Li_2SiO_3 blanket	^6Li	1.006	1.013
	^7Li	0.016	0.017
	Total	1.023	1.030
$Li_{17}Pb_{83}$ blanket	^6Li	1.162	1.166
Natural Li	^7Li	0.017	0.018
	Total	1.179	1.184
$Li_{17}Pb_{83}$ blanket	^6Li	1.316	1.324
90% ^6Li	^7Li	0.002	0.002
	Total	1.318	1.326

TABLE 14
COMPARISON OF TRITIUM BREEDING FOR THE CTR STANDARD BLANKET

	Tritium Breeding Ratio	
	Roussin et al.	AUS
^6Li	0.969	0.959
^7Li	0.575	0.574
Total	1.544	1.533

TABLE 15
DEMO MATERIAL DENSITIES

Material	Nuclide	Atom Density 10^{-24} cm^{-3}
$LiAlO_2$	Li	0.03106
	Al	0.03106
	O	0.06211
Li_2O	Li	0.04058
	O	0.08115
Be	Be	0.1236
H_2O	H_2O	0.0335
PCA steel	B	0.00002188
	C	0.0001971
	N	0.0000338
	Al	0.00005264
	Si	0.0008427
	Ti	0.0002965
	V	0.00009292
	Cr	0.01274
	Mn	0.001723
	Fe	0.05499
	Ni	0.01290
	Cu	0.0000149
	Nb	0.00001529
	Mo	0.0009868
Fe1422	C	0.002309
	N	0.00006487
	Si	0.0003916
	Cr	0.001848
	Mn	0.01219
	Fe	0.06953
	Ni	0.00158

TABLE 16
SPECIFICATIONS FOR DEMO MODELS

Case	Zone	Thickness cm	Composition as Volume %
1	Armour	1	100% PCA steel
	First wall	1	65% PCA steel, 35% H_2O
	Breeder	68	63% Li_2O*, 5% PCA steel, 5% H_2O
	Shield	30	90% Fe1422, 10% H_2O
2	Armour	1	100% PCA steel
	First wall	0.34	100% PCA steel
		0.3	100% H_2O
		0.3	100% PCA steel
	Multiplier	8	100% Be
	Breeder	58.5	63% Li_2O^+, 5% PCA steel, 5% H_2O
	Shield	30	90% Fe1422, 10% H_2O
3	Armour	1	100% PCA steel
	First wall	0.34	100% PCA steel
		0.3	100% H_2O
		0.3	100% PCA steel
	Multiplier	6	100% Be
	Breeder	58.5	63% $LiAlO_2$**, 5% PCA steel, 5% H_2O
	Shield	30	90% Fe1422, 10% H_2O

* Natural Li †Li enriched to 30% ^6Li ** Li enriched to 60% ^6Li

TABLE 17
COMPARISON OF TRITIUM BREEDING FOR DEMO

No.	Case		Tritium Breeding Ratio	
			Abdou et al.	AUS
1	Li_2O	^6Li	0.916	0.907
	Natural Li	^7Li	0.315	0.314
		Total	1.231	1.221
2	Be/Li_2O	^6Li	1.249	1.255
	30% ^6Li	^7Li	0.109	0.108
		Total	1.358	1.363
3	Be/$LiAlO_2$	^6Li		1.185
	60% ^6Li	^7Li		0.024
		Total	1.19*	1.209

This result was taken from Figure 6.7 of Abdou et al. which was assumed to have been reversed with Figure 6.9

TABLE 18
THERMAL COMPONENT OF TRITIUM BREEDING RATIO

Case		^{6}Li Enrichment %	Tritium per Fusion Neutron for Neutrons <0.4 eV
STARFIRE	Zr_5Pb_3	60	0.022
STARFIRE	Be	nat.	0.170
INTOR-EC	Li_2SiO_3	nat.	0.489
INTOR-EC	$Li_{17}Pb_{83}$	nat.	0.514
INTOR-EC	$Li_{17}Pb_{83}$	90	0.076
CTR	standard blanket	nat.	0.067
DEMO	Li_2O	nat	0.014
DEMO	Be/Li_2O	30	0.168
DEMO	$Be/LiAlO_2$	60	0.111