CALCULATIONAL MODEL AND DATA FOR
CTR NEUTRONICS AND PHOTONICS

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**CALCULATIONAL MODEL AND DATA FOR
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exclusive of data**
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I Introduction

The design of the nuclear island of a fusion reactor involves a large number of technical studies and trade offs in arriving at even an acceptable system, let alone an optimal one. In spite of this, the coupling between various aspects of the design may be rather simple. For example, the plasma produces the neutron flux which drives the nuclear-thermal system including the blanket and shield, but there is little or no physics coupling of this subsystem back on the plasma. There is of course an economic coupling through the magnet costs.

Coupling of different aspects of the design problem are of two types, physical and economic. The economic coupling is very important in the optimization of the system, but influence the design calculations in only a minor way. When physical coupling is strong and operates in both directions between two or more subsystems or disciplines, it becomes difficult or impossible to separate the calculations. The coupling can be strong in one direction without seriously complicating matters. This is particularly true if the coupling is essentially linear. This is basically the case in the way the plasma couples to the blanket and shield.

The plasma provides a source of neutrons of about 14 MeV energy (see Muir¹ regarding the spread of energies). The transport and nuclear reaction rates are linear in the source strength except for a minor, in most cases negligible (however, see Gerstl²) temperature dependence of the cross sections. The plasma also provides

a flux of electromagnetic radiation and charged particles to the first wall. These sources also produce linear effects. The reaction of the blanket and shield back on the plasma occurs through the sputtering of wall particles and reradiation of electromagnetic energy. The sputtering may have important consequences for the plasma and may justify a divertor system, the coating of the wall with a low "Z" material, or even the choice of wall materials. However, it has only a small impact on the neutron and photon fluxes or reaction rates and has little influence on the other design studies required for the blanket and shield.

Thus on the input side the plasma in a first approximation provides a source normalization and in a less important way the exact geometry of the source. On the output end of any nuclear effects are the reaction rates for thermal, materials, chemical, cryogenic, environmental, and safety analyses. These have almost no effect on the nuclear analysis. Even the design trade offs made in meeting functional requirements such as tritium breeding, energy production, and coolant flow rates are relatively easy accommodations in most instances for both the nuclear and thermal designers. This means that most nuclear design features and details can be worked out with only a rather general understanding with the thermal and mechanical designers, with final optimization and accommodation being superimposed late in the design process. Calculations may be done almost entirely independent of others. Finally, the nuclear responses which are the inputs for other analyses are essentially linear in both the neutron and gamma fluxes and the number densities of the materials. This makes the specification of the results easy.

II Results Required for CTR Design and Analysis

The nuclear analysis provides the input for a number of other analyses. These inputs are in the form of a number of weighted integrals (or functionals, of the neutron and gamma fluxes). Introducing the scalar product notations

$$(f, g) = \int_V dV \int_0^\infty dE \int_{4\pi} d\Omega f(\vec{r}, E, \vec{\Omega}) g(\vec{r}, E, \vec{\Omega}),$$

and

$$(\vec{F}, \vec{G})_N = \sum_u \int_{t_0}^T dt F_u(t) G_u(t),$$

the quantities of interest can be written concisely and are given in Table I. Here the volume is that of the reactor, E the neutron energy, $\vec{\Omega}$ the neutron direction, and $\vec{r}$ the position vector. "u" represents the set of numbers indicating the element, mass, and isomeric state, and the sum is over all nuclides. $\vec{F}$ and $\vec{G}$ are vectors, each component referring to a different nuclide. t_0 is the initial time and T is greater than any time of interest. Table I gives 11 functionals of the fluxes which is a rather complete list of the required results. The first eight are linear in the fluxes and thus do not need to be repeated for a simple change of power level. The last three are in principle non-linear in the fluxes. In practice they may sometimes be practically linear and in any case only the last stage of the calculations need be repeated on a change of flux magnitude. The first column is a descriptive title of the design rate, and the second column states the analysis for which it is required. The symbols assigned in the third column are used for convenient reference here, but in general are not at this time very standardized in the literature. The last column gives the scalar product

which must be evaluated numerically in obtaining the required results.

The quantities occurring in these products are defined in Table II.

In carrying out sensitivity studies of these quantities to various changes in the data or system, several quantities bilinear in the fluxes and the adjoint fluxes occur. However, these are internal to the calculations and should not be added to the list in Table I.

III Computational Methods and Computer Programs

In order to evaluate the integrals and sums described in the previous section and to find the sensitivity of these results to various system and data changes, a set of computer programs, data libraries, and fluxes are required along with the input describing the particular system. The determination of the fluxes in turn requires a set of computer programs and data libraries with a specific system input. The data libraries, which must be in a suitable form for immediate use in turn require processing procedures usually in the form of computer programs to take basic nuclear data and produce the required libraries. Thus, there are two levels of data and three levels of calculations as indicated in the flow diagram designated Figure 1.

Figure 1
Basic Information Flow in Nuclear Calculations

The last three levels starting at the right will be described in this section. The first three levels will be taken up in the next section with the middle section appearing partly in both to tie the discussion together. The output calculations fall into three categories, the flux calculations into two and these collectively draw on five data libraries.

The situation is shown schematically in Figure 2. The three blocks on the right in this figure describe the calculation of three types of quantities. The first is concerned with the calculation of the linear responses of the system to the neutron source, i.e., the first eight responses of Table I. The second calculational block is devoted to the perturbation calculations of the sensitivity of the responses of Table I to the variation of data and system parameters. The third block is concerned with the number density of various nuclides produced by the flux and by decay processes, and the effects of these nuclides.

The two blocks of the middle column in Figure 2 are both concerned with the calculation of the neutron and gamma fluxes. In both cases, the calculations must be multigroup in energy and high order transport approximations as has been shown earlier.³ The one dimensional methods are of importance in survey studies while the two or three dimensional methods should be used for such special purposes as estimating homogenization effects and leakage from ports.

The left hand column represents the data libraries required in various calculations. The data are divided here into five libraries, all of which must be in a suitable multigroup format which is the end result of processing raw data into a form for immediate use. The first

library is the library of neutron cross sections needed in determining the neutron angular flux. The second library contains the gamma production cross sections in multigroup to multigroup format. On multiplication by the neutron flux, the source of gamma photons for gamma transport calculations results. The third contains the gamma multigroup transport cross sections for determining the gamma flux. The fourth library is a response library containing kerma space factors, reaction cross sections, and other cross sections for the important design quantities. They must have a group structure which is the same as or compatible with that used in determining the fluxes. The last library contains the data for calculating the number densities of all nuclides and their decay effects, except that the neutron transmutation rate per nuclide, which is flux dependent, must be provided separately.

The implementation of the calculational program is pictured schematically in Fig. 3. There are existing and adequate computer programs and libraries in most cases, but some areas are handled only by in-house methods at the various labs and schools, and in some instances the work has probably not been implemented fully on a computer.

The flux calculations are generally carried out with readily available programs which are well documented. One dimensional (i.e., slab, infinite cylinder, and sphere) calculations have mostly been on the basis of the discrete ordinates transport approximation. There is no reason to pursue other approximations here. The Oak Ridge program ANISM is indicated in this block because of its ready availability from RSIC. The essentially equivalent Los Alamos program DTF4 could be used equally well. Multidimensional transport studies are

indicated as being carried out with the Morse program. This is an ORNL Monte Carlo program which uses combinatorial geometry for great flexibility in handling configurations of interest. It has the further merit of accepting the same data as ANISN, thus eliminating a potential source of confusion. This program is also available from RSIC. There are other Monte Carlo programs from ORNL, LASL, and LLL which are comparable, but offer no overriding advantages for the purpose at hand. There are in addition, two dimensional S_n programs which could be useful in some instances. The pressure to pursue detailed multidimensional studies has been very slight and only a few Monte Carlo studies have resulted.^{4,5} To date, toroidal geometry effects have not been studied and no program or even formulation of this problem has appeared. There will undoubtedly be a flux tilt from the inside to the outside of the torus. Eventually, this must be investigated, but it is not a high priority item.

The fluxes produced by ANISN or MORSE or similar programs must be weighted and summed to give the various required results. Some reaction rates could be edited directly from these programs. However, the variety of results required has resulted in separate programs to provide these results at different installations. At Brookhaven this program is called TRITON and at the University of Wisconsin it is called LINK. The programs are relatively simple but are necessary for efficient and flexible use of the results.

Sensitivity studies, which are extremely important at this stage in CTR work, are implemented by perturbation programs like ORNL's SWANLAKE and the University of Wisconsin's VARIED. SWANLAKE is currently available and documented; thus it is the recommended program for this task.

The calculation of transmutation chains and activation effects is not carried out with any standard accepted program or library; but is based on local methods and data at each installation at the present time. The Brookhaven system for carrying out these calculations is currently being implemented. Earlier studies have been based primarily on the activity of the direct transmutation products.

The data libraries for these calculations vary considerably in adequacy and convenience. Here, the libraries will be described briefly with a more complete discussion reserved for the next section. The DLC-2D library is available from RSIC and is based on the basic files in ENDF/B3. It is in a 100 group form used earlier in the GAM libraries (the group structure described in the University of Wisconsin report FDM-68)⁶. The group structure is generally deemed more than adequate, but if group collapsing is carried out, the high energy groups should be retained due to their importance for many processes. The library is generally regarded as satisfactory although this has not been analysed thoroughly. In any case it is easily updated as later versions of ENDF/B are made available. For example, a DLC-2E library based on ENDF/B4 should be available from RSIC soon.

The gamma production data in ENDF has been missing for many materials. Thus some neutron group to gamma group libraries have used mixed sources for their data. In addition, the libraries are incomplete and as a consequence of these inadequacies, they have not been given formal names. The library currently available employs 100 neutron energy groups and 43 gamma energy groups.

The multigroup gamma transport library has been called SMUGLIB here since it was generated by the program SMUG. It is a theoretically based 43 group library and is rather complete. It should be documented and released soon as a standard library by RSIC.

The library MACKLIB is a documented (ORNL TM3995) partial reaction and neutron kerma factor library for a large selection of materials. It can easily be updated and will probably be released in an ENDF/4 version at some point. Contrary to the simplified flow chart of the figures, some of the response data is not currently available in this library (in particular the displacement cross sections and the gamma kerma factors). The gamma kerma factors are actually located in SMUGLIB.

The final secondary library has not been assembled at this time.

IV Nuclear Data and Its Processing

The secondary libraries described briefly above are highly specialized in both purpose and form. The basic nuclear data as it appears in the literature from experiments or calculations is very diverse in form and quality. A large amount of processing of the data is necessary to bridge this gap. A substantial amount of processing has taken place in preparing the evaluated nuclear data files ENDF/B. These high quality files are used wherever possible and the basic data will be divided into two categories, ENDF/B and other sources. The transition between these two sources is shown as a basic information flow on Figure 4. A processing program is required to prepare each of the five secondary libraries. The arrows generally show the flow of data. This is very general and

greater detail is brought out by considering the implementation of this chart. This is described by Figure 5.

Generally speaking, the data situation is not as good as the calculational. However, the ENDF/B files have improved in quality and versatility with each issue. It is quite possible that in about two years when ENDF/B5 appears, that it will be unnecessary to use any other data source and that processing programs will be available for all secondary libraries. This would leave us with only the question of acceptable tolerances on the data. At present ENDF/B4 is essentially complete, but secondary libraries have not yet been prepared from it. Thus most secondary libraries are based on ENDF/B3 and supplemental data. These supplemental sources include ENDF/A, CSISRS, The Table of Isotopes, and nuclear model codes, as indicated in Figure 5.

The multigroup neutron transport library can be obtained from the ENDF/B files with a number of processing programs. The DLC-2D package was generated with the ORNL program SUPERTOG. This may be used to generate later versions of DLC-2, but the more recent processing program MINX may be used instead. In any case, RSIC is expected to provide a DLC-2 type library and it should not be necessary for most users to use SUPERTOG or MINX. The processing program LAPHOR of LASL or its ORNL version LAPHINGAS can produce a gamma production library from ENDF/B data. This has been done in cases where the data is available in ENDF/B3. In addition, there is an ORNL program POPOP4 which contains its own basic library and processes the data. This has been used for several additional materials. Nevertheless, our library is very incomplete and

contains the group to group data for C, O, Pb, H-1, and Al in 100 neutron groups to 43 gamma groups. The 43 group structure is described in UW-FDM68. This data was obtained from M. Abdou at Wisconsin and he has transmitted some further data. The other data transmitted has limitations which make its use very questionable. Since ENDF/B4 is now out and is much more complete than ENDF/B3 with regard to the gamma files, either ORNL or LASL could produce a better and more complete library on a short time scale if absolutely essential. On a longer time scale (of the order of six months) M. Abdou expects to complete at Argonne a more complete processing program to supercede MACK and include a comprehensive gamma production capability.

The SMUGLIB library of multigroup gamma transport cross sections is produced by the ORNL program SMUG. SMUG is based on the well developed theory of Compton Scattering, Pair Production, and the Photoelectric Effect. Other interactions of gammas with matter are justifiably ignored. Since tests of the data against theory indicate the theory is very accurate (except at the lowest energies which are unimportant) these results are unlikely to change. The 43 group structure should also be adequate for the purposes under study. The library is fairly comprehensive, but if another element is required, it can readily be obtained from SMUG, RSIC might provide this without the necessity of getting the program operational at Brookhaven.

The program MACK was originally written at Wisconsin and made operational at ORNL. It was intended as a program to compute neutron kerma factors, but was easily modified to generate the partial reaction cross sections required for a number of responses of the system. The

data input is from ENDF/B and is limited by the availability of data in the files. The MACKLIB library is based on ENDF/B3. It is not a complete library of response quantities as the gamma kerma factors are in SMUGLIB and the displacement cross sections are not included. Some displacement cross sections are given in UW-FIM68, Chapter 6. These are based on the work of Doran and are the best to date. Displacement cross sections can also be obtained from the ORNL program RICE. However, this program has some notable limitations in its theory and in its internal data library. As mentioned earlier, M. Abdou is going to ANL and will work on an extended version of MACK. This extension will include gamma production, neutron kerma factors, and displacement cross sections in a self consistent manner and will thus produce all responses except gamma kerma factors. Some results should be obtainable within 6 months and the complete package within about a year.

In the area of transmutation and activation calculations, no processing program exists to prepare secondary libraries and until ENDF/B4 there was very little of the required data in the ENDF files. Thus there is no documented and readily available library for these calculations. Steiner at ORNL and Vogelsang and Sung at U.W. have hand prepared libraries of undetermined accuracy. In the future, fission product libraries will be processed from data that has been added to ENDF/B4. This data will not suffice for CTR activation studies, but some data will be available and the processing program should be adaptable to our needs. By the time ENDF/B5 appears the data may be reasonably complete.

In the meantime, much of the decay data can be obtained from "The Table of Isotopes" and transmutation cross sections from MACKLIB or from processing with MACK the output of nuclear model codes like FASCRO.

TABLE I

<u>Design Quantity Rates</u>	<u>Type of Analysis Needed For</u>	<u>Symbol</u>	<u>Expression For</u>
Tritium Production	Chemical	T	$(\sum_n, T, \psi)$
Displacement Production	Materials	D	$(\nu_D \sum_{PK}, \psi)$
Charged Particle Production	Materials	C_H	$(\sum_H, \psi)$
		C_{He}	$(\sum_{He}, \psi)$
Transmutation	Materials	M_{XY}	$(\sum_X^Y, \psi)$
Energy Production	Thermal	P	$\sum_R (Q_R \sum_R, \psi)$
Neutron Energy Deposition	Thermal	H_n	$\sum_R (K_R, \psi)$
Gamma Energy Deposition	Thermal	H_γ	$\sum_R (K_\gamma, \psi_\gamma)$
Energy Leakage	Cryogenics	J_E	$(\mu, \psi) + (\mu, \psi_\gamma)$
Activity Production	Chemical	A	$(\bar{\lambda}, \underline{N})$
Decay Heat	Safety	H_D	$(\bar{E}\bar{\lambda}, \underline{\underline{N}}_{\underline{N}})$
Biological Hazard Potential Production	Environmental	BHP	$(\underline{bhp}\lambda, \underline{N})_{\underline{N}}$

TABLE II

$\psi(\vec{r}, E, \vec{\Omega})$	Neutron angular flux distribution
$\psi_\gamma(\vec{r}, E, \vec{\Omega})$	Gamma angular flux distribution
Σ_{Tr}	Tritium production cross section $N_{Li6} \sigma_{Li6}(n, T) + N_{Li7} \sigma_{Li7}(n, n'T)$
Σ_{PK}	Primary knock on cross section from radiation damage theory
$\nu_D(E_{PK})$	Number of displacements per primary knock-on of energy EPK
Σ_p	Hydrogen production cross section $\sum_u N_u [\sigma_u(n, p) + \sigma_u(n, D) + \sigma_u(n, T)]$
Σ_{He}	Helium production cross section $\sum_u N_u [\sigma_u(n, He^3) + \sigma_u(n, He^4)]$
Σ_X^Y	Transmutation cross section from nuclide Y to nuclide X
Σ_R	Cross section for reaction R
Q_R	Q value for reaction R
K_R	Kerma factor for reaction R
K_γ	Kerma factor for gamma rays
μ	Direction cosine $\vec{\Omega} \cdot \vec{n}$ where $\vec{n}$ is a unit normal vector to the surface
λ_u	Decay constant of unstable nuclide "u"
$\bar{E}_u \lambda_u$	Product of the average decay energy with the decay constant
$(bhp)_u \lambda_u$	Product of the biological hazard potential with the decay constant

References for Calculational Model and Data for
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