MACK: A Program to Calculate Neutron Energy Release Parameters and Multigroup Neutron Reactions Cross Sections from ENDF/B

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UNIVERSITY OF WISCONSIN

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M. Abdou, C.W. Maynard

Fusion Technology Institute
University of Wisconsin
1500 Engineering Drive
Madison, WI 53706

http://fti.neep.wisc.edu

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Calculation of the heat-generation and dose rates due to interaction of nuclear radiation with matter is of prime importance in practically any nuclear system. A theoretical model and computational techniques were developed[1] for calculation of the neutron fluence-to-kerma factors[2] from nuclear data in ENDF/B[3] format.

For the purposes of the calculation, the heating rate due to neutron reactions is conveniently divided into two types of contribution. The first type is heat generated by charged particles (and recoil nuclei) emitted in neutron reactions, and the second is heat generated by the secondary gamma radiation produced by these reactions. The heating rate by the first type of contribution can be expressed as

$$H(\vec{r}) = \int \phi_n(\vec{r},E) \sum_j N_j k_j(E)dE \qquad (1)$$

where

$$k_j(E) = \sum_i k_{ij}(E) = \sum_i \sigma_{ij}(E)E_{ij}(E) \qquad (2)$$

and $\phi_n(E)$ is the neutron flux for neutrons of energy E, N_j is the nuclide density for element j, σ_{ij} is the microscopic cross section for reaction i in element j, E_{ij} is the energy release per reaction, and k denotes the microscopic fluence-to-kerma factor. The analytic expressions for E_{ij} for all possible nuclear reactions for E less than 20 MeV were obtained from a solution of the kinematics equations f. the nuclear reactions. The anisotropy of elastic and inelastic scattering is included and the competition between gamma and charged particles emission is adequately treated. The MACK program[1] was written to calculate pointwise neutron kerma factors at an arbitrary energy mesh from nuclear data in ENDF[3] format. The program processes all reactions significant to heat deposition and recognizes all of the multiplicity of data formats currently allowed by ENDF/B. The limit on the accuracy of kerma factors calculations is set only be the adequacy and availability of the required nuclear data.

In addition, the MACK program calculates energy group kerma factors and group cross sections by reactions averaged over an arbitrary input weighting function or any of several "built-in" functions for any desired energy group structure. An efficient treatment of the resonance region was built into the code to calculate the contribution to cross sections from the resolved and unresolved resonance parameters including the Doppler effect. A calculational flow chart of the MACK program is given in figure 1 from which the general features and algorithm of the program follow.

The contribution to energy deposition from radioactive decay of the residual nucleus is also calculated. Fermi[1] Theory of β-decay was used to calculate the average kinetic energy of a β^- or β^+ particle for a given endpoint energy, E_o, of the β-spectrum and atomic number, Z, of the residual nucleus. The results are in excellent agreement with the experiment and show that the ratio, R, of the average to maximum kinetic energy for β^- varies from about 37% to 48% for E_o from 1 MeV to 10 MeV. For β^+, R is about 90% for low E_o, decreases to a minimum of about 44% at ~1 MeV, and then increases again. R depends strongly on E_o and Z for small E_o. The results are quite different from that commonly used in literature[4], namely R=30% for β^- and 40% for β^+. Although the effect may be small on the total heating rate in the nuclear system, it is very important in decay heating calculations.

The pointwise cross sections, pointwise kerma factors, energy group cross sections and kerma factors can be printed, punched, and saved on tape for individual reactions and the sum as selected by input. The pointwise kerma factors by reaction and sum can be used for inclusion in the ENDF/B evaluation for the nuclide with MT numbers in the 300's series.[4] The output group kerma factors and partial cross sections are in a form suitable for use as "activity cross section tables" in the present transport codes[5,6,7] (one-, two-, or three-dimensional) for calculation of heating rates and reaction rates of interest (e.g. helium and hydrogen production).

The program has proven to be extremely useful in providing the basic input for heat transfer and radiation damage analysis of fusion reactor blankets and magnet shields at the University of Wisconsin[8].

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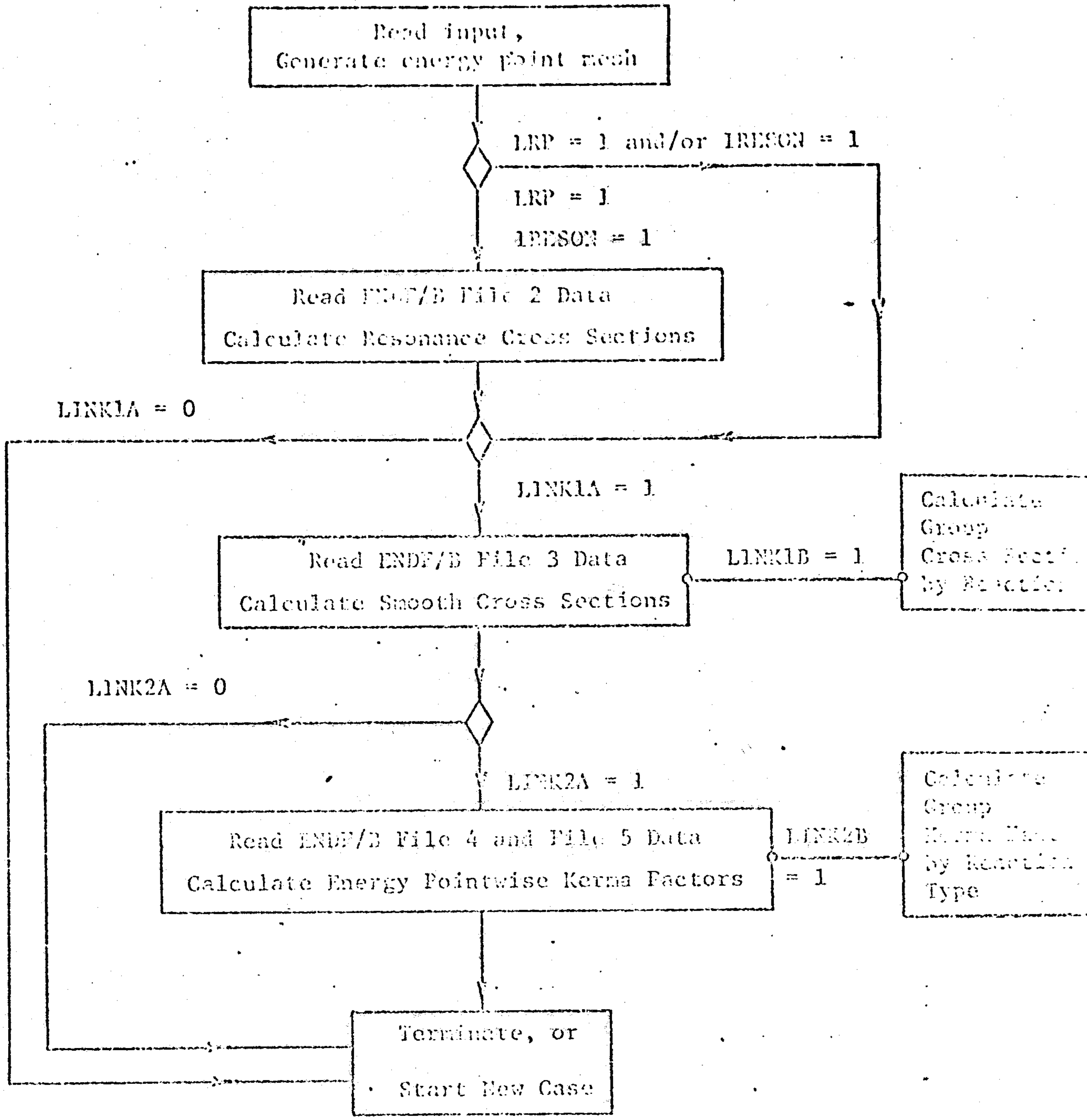

Figure 1 - Calculational Flow Chart for MACK