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HETC/KFA-1, AN UPDATED VERSION OF HETC FOR HIGH-ENERGY SPALLATION PHYSICS CALCULATIONS

T.W. Armstrong*, P. Cloth, B.L. Colborn*, D. Filges, G. Sterzenbach

Institut für Reaktorentwicklung, Kernforschungsanlage Jülich GmbH
Postfach 1913, D-5170 Jülich, Germany
*KFA Consultant, P.O. Box 2807, La Jolla California 92038, USA

ABSTRACT

Several modifications have been made to the high-energy radiation transport code HETC in conjunction with model validation and SNQ target station design calculations being carried out at KFA. The updated features of the new version of the code, designated HETC/KFA-1 are summarized.

1. INTRODUCTION

The High-Energy Transport Code (HETC), Ref. /1/, is being used at KFA for various predictions related to SNQ target station investigations, and basic physics experiments to check the accuracy of the models incorporated in HETC are also being carried out. Several modifications have been made to HETC in conjunction with this work, and others are in progress and planned.

Modifications to the code which have been incorporated and documented to date as a new code version designated HETC/KFA-1 are summarized below in Section 2. The documentation for this version of the transport code, awell as for a general analysis code for transport results called SIMPEL, is contained in Ref. /2/.

In addition, several other modifications to HETC have been implemented, but not yet documented or fully tested; these are summarized in Section 3.

2. CODE MODIFICATIONS INCORPORATED AS HETC/KFA-1

2.1 Updated Nuclear Mass Data

In the evaporation model calculations, atomic masses are needed to determine binding energies for various types of particle emissions. In the standard version of HETC, the evaluated 1964 Atomic Mass Table values are used. These input data have been updated to use the 1977 Atomic Mass Evaluation values of Wapstra and Bos /3/.

Spallation collisions often produce residual nuclei outside of the A and Z range covered by these input mass data (e.g., Figure 1), in which case the Cameron semi-empirical mass formula is used. In computing mass differences, unrealistic values can sometimes be obtained if the table values are used for the starting nuclide and the semi-empirical formula used for the ending nuclide. A change was made to use the mass formula for both nuclides if either one is outside the input table range, which provides a more consistent treatment.

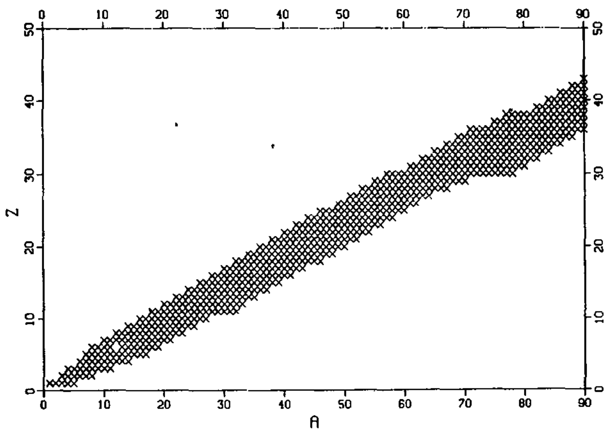

Figure 1 Nuclide A and Z range covered by updated input data for evaporation model. The symbols denote nuclides for which data are available and stored on the input tape. (Only data for A < 90 shown)

2.2 Level Density Option

The level density formulation used in HETC for the evaporation model is $a = (A/B_0)(1 + Y(A-2Z)^2/A^2)$ with $Y = 1.5$, or $a \approx A/B_0$. The parameter B_0, which has an important influence on neutron production, is set to 8 MeV in the standard version of HETC for all nuclei.

An option has been added to allow B_0 to vary with A. The values used are those compiled by Baba /4/ from experiments on nuclear level spacing (Figure 2).

2.3 Angular Distribution of Evaporation Particles

In the standard version of HETC, emitted evaporation particles are usually assumed isotropic in the laboratory system. Dr. R. Prael of Los Alamos has made the kinematic modifications to take into account the recoil direction of the residual nucleus during evaporation, and these changes have been incorporated into HETC/KFA-1. In this procedure, the evaporation particle directions are selected from an isotropic center-of-mass distribution, and this angle and the recoil direction are transformed to provide non-isotropic angular distribution in the laboratory system.

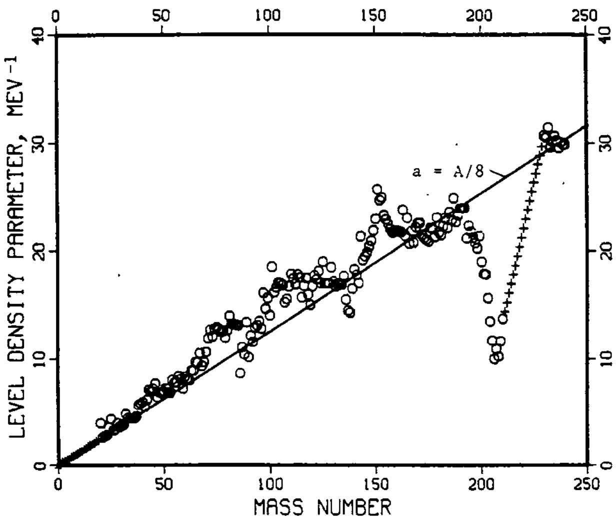

Figure 2 Level density parameters (circle symbols measured data, cross symbol interpolated values) incorporated as a "variable B_0" option in the HETC/KFA-1 code. (The linear dependence of A/8 is usually assumed in the HETC code).

2.4 High-Energy Fission Option

An option for allowing high-energy fission using the Rutherford and Appleton Laboratory (RAL) model written by F. Atchison /5/ has been incorporated into HETC/KFA-1. A series of calculations to check this model against experimental data and the ORNL fission model for both thick and thin targets has been carried out at KFA. Some of these results have been reported at previous ICANS meetings, and all of the comparisons made are included in a recently issued KFA report /6/.

2.5 Low-Mass Heavy Ion Beams

In addition to the standard source particles allowed by HETC (which are p, n, π^+, and μ^+), modifications are incorporated into HETC/KFA-1 to include beam particles with masses up to A = 10. The basic procedure is to represent the projectile ion as a cluster of nucleons, and then treat ion-nucleus non-elastic nuclear collisions as the sum of individual nucleon-nucleus collisions using the standard intranuclear-cascade-evaporation model contained in HETC.

2.6 Miscellaneous

Other updates included in HETC/KFA-1 include range straggling for primary beam particles, different transport energy cutoffs for ionization and nuclear collisions, modifications to the Coulomb scattering treatment, and a procedure for obtaining the spectra of γ-rays from spallation collisions.

3. OTHER UPDATES

The HETC code has also been extended to include elastic scattering and importance sampling, as summarized below. However, these modifications have not as yet been fully tested, so they are not included in the version HETC/KFA-1.

3.1 Elastic Scattering

Updates have been made to allow elastic scattering for neutrons in the energy range from 15 MeV to 20 GeV and protons from 100 MeV to 20 GeV, for target nuclei of arbitrary A.

For elastic cross sections up to the 150 MeV, we have used values from the ORNL HILO cross section library /7/, which are based on optical model calculations. While this library extends to 400 MeV, the values above 150 MeV are too large, as shown for iron, for example, in Figure 3. Thus, in the energy range from 150 MeV to 20 GeV values are taken from the estimates of Wilson and Costner /8/, which are referred to in Figure 3 as the NASA library.

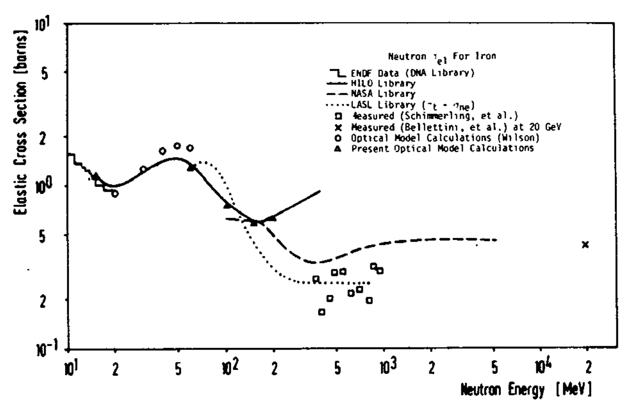

Figure 3 Comparison of neutron elastic cross sections for iron from various sources.

The angular distribution of elastically scattered particles is selected from an approximate optical model expression:

$$f(x) \quad (J_1(x)/x)^2$$

$$\cos\theta = 1-1/2x^2 \; (aA^{1/3} \; (E(E+1878))^{1/2}+1)^{-2}$$

where J_1 is a first kind, first order Bessel function and $a = 7.095 \times 10^{-3}$.

3.2 Importance Sampling

The HETC code has been modified to incorporate the following variance reduction techniques for improved statistical accuracy: (a) collision biasing, where particle splitting and Russian roulette are allowed for cascade particles emerging from collisions, (b) boundary biasing, where splitting and Russian roulette are allowed for particles crossing geometry/media boundaries, and (c) the exponential transform, where path lengths can be biased according to the "importance" of the particle direction. These importance sampling techniques have been programmed in such a way that the degree of biasing can be specified according to various types of criteria that depend on particle parameters, material properties, and target geometry.

4. References

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