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A-UR -07-3337

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TITLE: NEUTRON SECONDARY-PARTICLE PRODUCTION CROSS SECTIONS AND THEIR
INCORPORATION INTO MONTE-CARLO TRANSPORT CODES

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ABSTRACT -- Realistic simulations of the passage of fast neutrons through
tissue require a large quantity of cross-sectional data. What are needed
are differential (in particle type, energy and angle) cross sections.

A computer code is described which produces such spectra for neutrons
above ~14 MeV incident on light nuclei such as carbon and oxygen.
Comparisons have been made with experimental measurements of double-
differential secondary charged-particle production on carbon and oxygen at
energies from 27 to 60 MeV; they indicate that the model is adequate in this
energy range.

In order to utilize fully the results of these calculations, they
should be incorporated into a neutron transport code. This requires (1)
defining a generalized format for describing charged-particle production,
(2) putting the calculated results in this format, (3) interfacing the
neutron transport code with these data, and (4) charged-particle transport.
The design and development of such a program is described.

INTRODUCTION

The use of high-energy ($\leq$65 MeV) neutron radiotherapy is in progress at many centers. To a first approximation, treatment planning at such facilities may be accomplished by interpolation and smoothing of measured depth-dose data. However, when variations in the radiation quality are of interest, it is necessary to use neutron transport calculations to characterize fully the field. This, firstly, enables the variations in response to a neutron dosemeter with position to be understood. Secondly, the charged-particle information allows the calculation of microdosimetric parameters. Finally, using a biological model, it allows assessment of the biological effectiveness of the radiation as a function of position.

For such tasks it is necessary to use a Monte-Carlo neutron transport code with the following features: First it must have an energy range up to ~65 MeV; secondly, it must use reliable neutron cross sections for hydrogen, carbon, and oxygen; thirdly, it must characterize and, ideally transport all the secondary charged particles produced by the neutrons. We describe here some progress towards such a goal.

CALCULATION OF NON-ELASTIC CROSS SECTIONS

In the range 15-65 MeV detailed neutron cross sections on carbon and oxygen are not well known. Much data are needed -- total cross sections are not sufficient and absolute double-differential (energy/angle) secondary particle spectra are needed over the whole energy range. Such large quantities of data cannot practically be measured, thus it becomes necessary to calculate them, subject to validation by whatever measured data are available.

As has been discussed elsewhere[1,2], the nature of the light nuclei

carbon and oxygen is such that their unique nuclear structures must be taken into account in any model calculation -- they have too few nucleons to allow a purely statistical treatment of their reactions. In addition, both nuclei show extensive alpha-particle clustering. Such considerations preclude the use of "general purpose" statistical nuclear reaction models such as the pre-equilibrium model[3] or the evaporation model[4], where simple forms are necessarily used to represent the density of states.

A more appropriate nuclear model for light nuclei has been described elsewhere[2,5,6]. It considers outcoming particles to be due to two consecutive processes: First, a direct stage in which the incident neutron collides with individual nucleons and clusters, which in turn may undergo futher collisions or may acquire enough energy to escape from the nuclous. In the second "equilibrium" stage, the remaining energy is statistically distributed and results in the emission of low-energy particles.

The first process is modelled with an intranuclear cascede code. In brief, it has the following principal features: Firstly, the nucleus is represented by an ensemble of nucleons and alpha particles with appropriate spectroscopic factors. Secondly, the calculation is time-dependent in that binding and separation energies are adjusted as particles leave the nucleus. Thirdly, a simple pickup reaction is allowed to compete with the intra-nuclear cascade.

De-excitation of the compound nucleus is accomplished using the "Fermi-breakup" model[7] in which channel probabilities and outgoing particle energies are assumed to occur with frequencies proportional to their statistical weights. Perhaps the most significant feature of this code is that particle-unstable states are allowed as intermediates in a sequential series of decays. In addition, two-body (the most common) breakups use an

appropriate Coulomb barrier penetration factor and are restricted to conserve parity and isospin, and by a neutral-particle angular-momentum barrier. Up to seven-body breakup is permitted.

More details of the codes are described elsewhere[2,5,6], as well as extensive comparisons with experiments. This latter aspect is of utmost importance as only with such comparisons can the nuclear model be extrapolated with confidence to regions where there are no data. A typical comparison between theory and experiment for oxygen at 40 MeV is shown in Figure 1. The agreement for the protons, deuterons, and alphas (the main contributors to the dose) is quite satisfactory.

INTERFACE BETWEEN CROSS SECTIONS AND TRANSPORT CODES

The cross-sectional output from the computer codes needs to be put in a standard format that is usable by a transport code. The standard format for neutron cross-sectional data is the so-called ENDF (Evaluated Nuclear Data File) system. The current, fifth, version of this system[8] does not allow for the specification of secondary particle spectra (other than neutrons and photons). However, preliminary specifications[9] have been drawn up for the sixth version of ENDF, in which secondary charged-particle production cross sections and their energy-angle correlations may be specified. In essence, the cross section for production of secondary particle "i" at angle θ_i and energy E_i is represented by

$$\sigma_i(E_n,E_i,\theta_i) = \sigma(E_n)Y_i(E_n)f_i(E_n,E_i,\theta_i)/2\Pi$$

where $\sigma(E_n)$ is the reaction cross section, $Y_i(E_n)$ is the yield of particle "i", and f_i is a normalized distribution function, which may be specified in several different formats.

CURRENT COUPLED NEUTRON/CHARGED-PARTICLE TRANSPORT CAPABILITIES

A prototype for a coupled neutron/charged-particle transport capability is now operational[10], and may be considered a first prototype for such a system. It does not utilize cross sections appropriate for light nuclei, but instead uses the physics models internal to the general Monte-Carlo transport code HETC[11]. (Cross sections generated by HETC have been compared[12] to double-differential secondary charged-particle production cross sections on carbon of the type shown in Figure 1; the agreement is rather poor.) A schematic flow diagram of the code linkages and data flow is shown in Figure 2. In essence, all charged particles and all neutrons above 20 MeV are transported using the HETC code. At each interaction, details of the emitted particles are stored on an event "history file" for subsequent analysis. If a neutron with energy below 20 MeV is generated in HETC, it is stored in a file which will be used as input to the neutron transport code MCNP[13]. This code, which accesses ENDF-V cross sections (which exist below 20 MeV), then transports the neutrons down to any energy; in principle it makes an event "history file" in the same format as the charged-particle history file, for subsequent analysis. In fact, as discussed above, as ENDF-V cross sections do not yield secondary charged-particle spectra, this capability is of limited use for the present application.

Thus, the main limitations of the system described in Figure 2 are: Firstly, cross sections above 20 MeV are generated using a model that is inappropriate for light nuclei; secondly, below 20 MeV no secondary charged-particle spectra are generated by neutrons; finally, no charged particles (other than electrons) are transported below 20 MeV. In the final section, we discuss a system without these limitations.

OPTIMIZED COUPLED NEUTRON/CHARGED-PARTICLE TRANSPORT CAPABILITY

A flow diagram for an optimized system is shown in Figure 3. ENDF-VI is not restricted to cross sections below 20 MeV: Using our cross-section generating codes discussed above, cross sections (including double-differential secondary particle spectra) may be generated in ENDF-VI format that may be accessed by MCNP.

High-energy protons may also induce nuclear reactions -- a 50-MeV proton will have ~3% probability of inducing such a reaction in tissue. Therefore, it is desirable to treat these reactions in MCNP. This may be accomplished by firstly having a set of reaction cross sections for protons in ENDF-VI format, analogous to those for neutrons; these have been calculated with the same codes as described above. Secondly, these protons may be transported in MCNP. This latter requires range/stopping-power information to be accessible to MCNP as the protons will, of course, lose energy by electronic collision in between nuclear collisions. Lower-energy protons and heavier charged particles -- which do not undergo a significant number of nuclear collisions -- may either be slowed down in MCNP using stopping-power tables, or their energy simply recorded on the history file for subsequent analysis. The former option is useful when the incident neutron spectrum (and thus the secondary charged-particle spectra) changes significantly over the range of the charged particles.

The resulting "history file" from MCNP essentially would contain all the charged-particle information in the field. It may thus be used for subsequent dosimetric, microdosimetric, or biological-model analyses.

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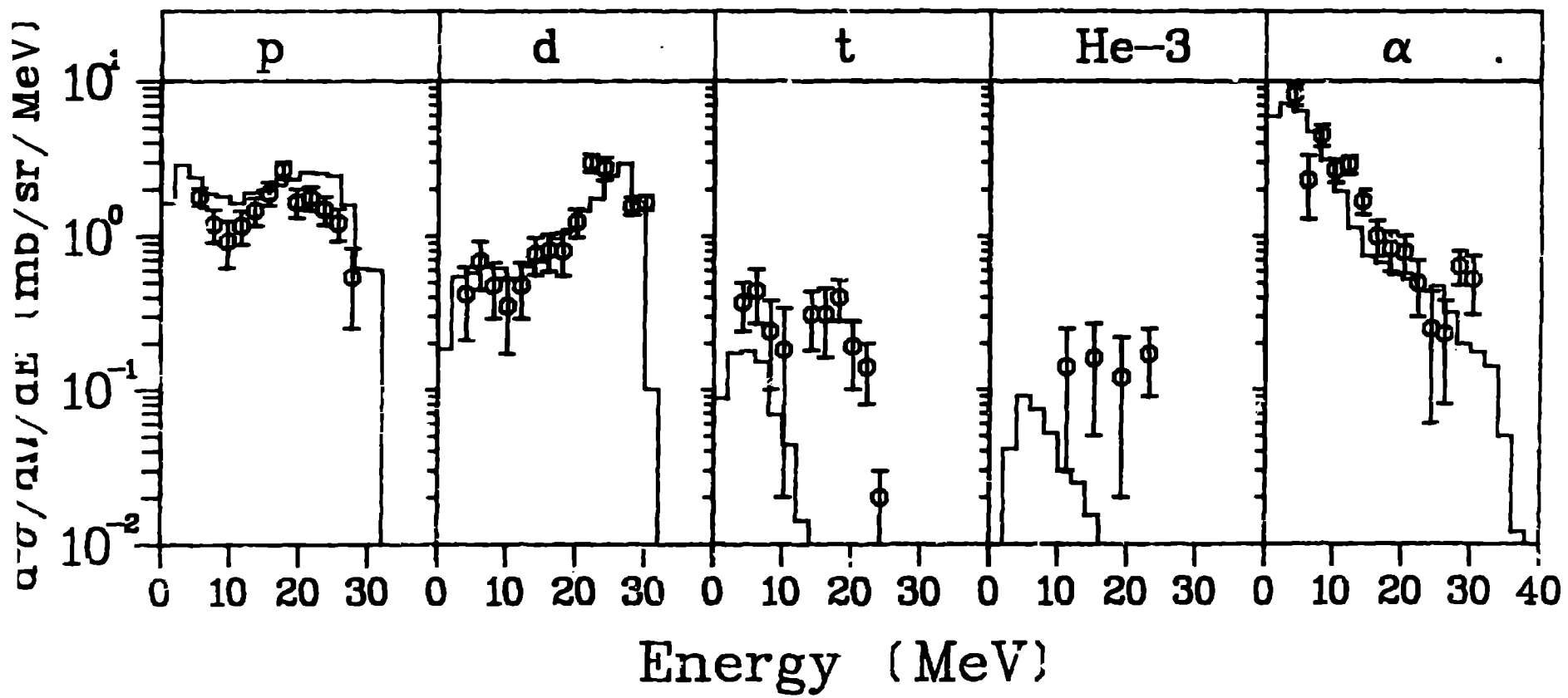9. MacFarlane, R.E., private communication (1987).

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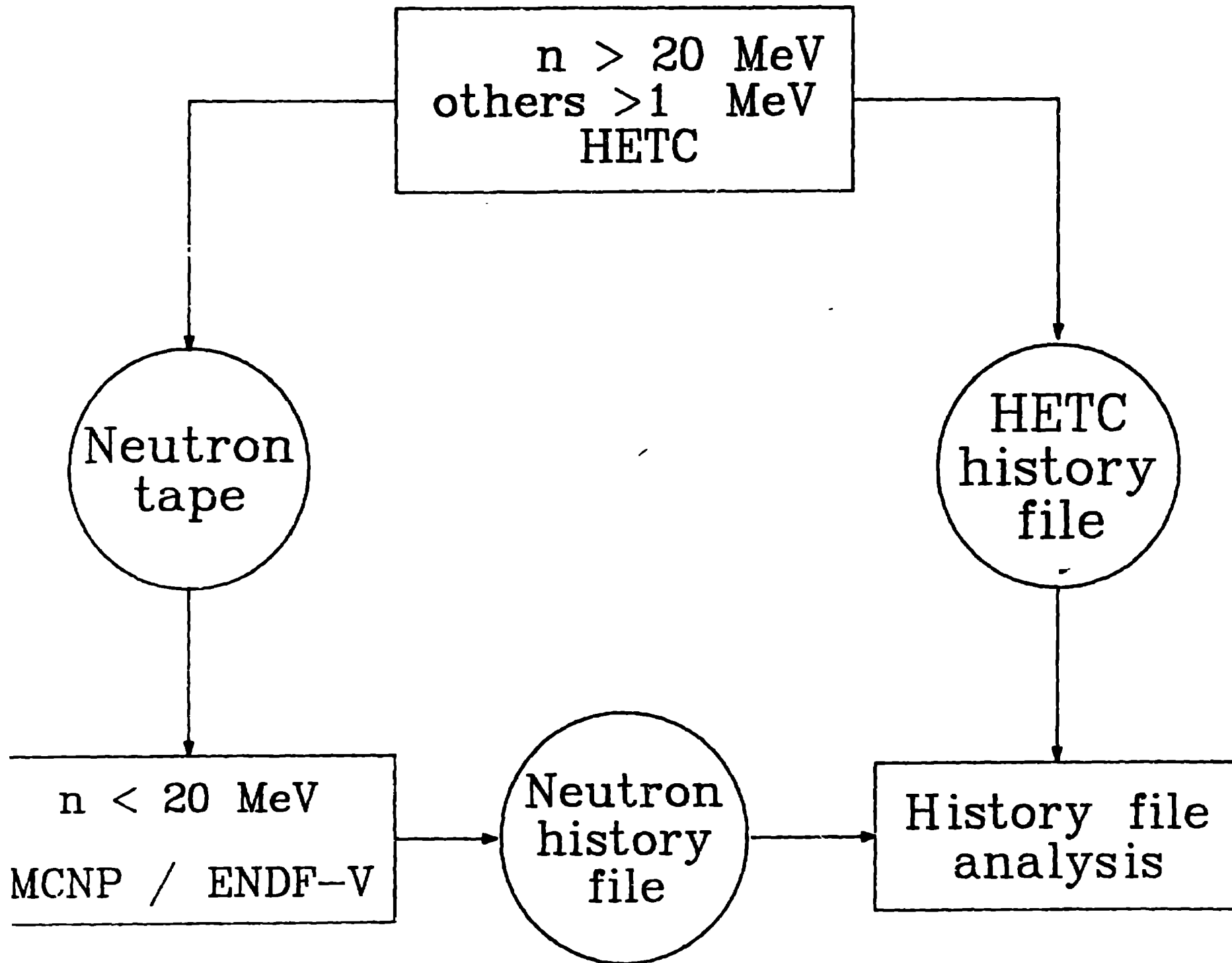
FIGURE CAPTIONS

FIG. 1. Cross sections for the production of hydrogen and helium isotopes
at 20° by 40 MeV neutrons incident on oxygen. The data are taken from
Subramanian et al.[6]

FIG. 2. Flow diagram of code linkages and data flow in current HETC/MCNP
system.

FIG. 3. Flow diagram of code linkages and data flow for optimized
neutron/charged-particle transport in light elements below 100 MeV.

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+-------------------------+          +----------------+
|  n    0→100  MeV        |          | History  file  |
|  p  10→100  MeV         | History  | analysis       |
|                         | ( file )  |                |
|  MCNP / ENDF-VI         |          |                |
+-------------------------+          +----------------+
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