COMPUTER CODES INCORPORATING PRE-EQUILIBRIUM DECAY

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ABSTRACT

A. Theoretical Description

After establishing the need to describe the high-energy particle spectrum which is evident in the experimental data, the various models used in the interpretation are presented.

This includes the following:

a) Cascade Model
b) Fermi-Gas Relaxation Model
c) Exciton Model
d) Hybrid and Geometry-Dependent Model

B. Workshop (Problem Session)

The codes description and preparation of input data for STAPRE was presented (Dr. Strohmaier). A simulated output was employed for a given input and comparison with experimental data substantiated the rather sophisticated treatment.

Selected Computer Codes for the Calculation of Neutron Reaction Cross Sections Combining Compound and Pre-Compound Reaction Mechanisms

A. Introduction

1.0 Purpose and Nature of Physical Problem (Pre-Equilibrium Model)

There are two extremes that are encountered in the energy distribution of nucleons resulting from a nuclear reaction mechanism. The high-energy end is usually described in terms of a combined direct (discrete) and compound nuclear process while the low end is explained in terms of the statistical theory where the Bohr independence hypothesis is assumed.

In between these extremes there exists a wide spectrum of intermediate stage processes characterized by what is commonly called a pre-equilibrium resulting from the sharing of the incoming energy with a small number of nucleons.

In order to explain these phenomena, several models based on classical and semi-classical ideas have evolved during the past few years.

The various methods range from rather simple to very complex treatments, with the basic assumption that the system in its decaying mechanism proceeds through a phase having relatively few degrees of freedom to a higher order configuration where equilibrium is reached.

During this time-dependent process, the emission of both particles and gamma-rays is possible with the mean energy of the particles being greater for emission from the pre-equilibrium configuration.

The time-dependent classical representation of particle emission may be expressed as

$$\frac{d^2\sigma_\nu}{d\Omega\, dE} = \sigma_r \sum_Q \int_0^{E_{max}} dE \int_0^\infty W(E,Q,t)\,\lambda(\nu,\varepsilon,\theta\,|\,E,Q,t)\,dt \quad (1)$$

where δ_R = reaction cross-section,

W (E,Q,t) = probability per unit energy that the reaction may be expressed in terms of the excitation energy E, in a state Q at a time t,

$\lambda(\nu, \varepsilon, \theta / E,Q,t)$ = probability per unit time that the system in such a state will emit a particle of type ν at an angle θ with a kinetic energy ε.

The quantity Q is rather general and its interpretation depends upon the particular model that is used, subject to the condition that

$$\sum_Q \int W(E,Q,t)\,dt = 1 \quad (2)$$

Several review articles have appeared which go into great detail concerning the various models and their application in interpreting pre-equilibrium processes.[1-5]

2.0 General Description

2.1 Cascade Model

In this model the interaction is consistent as a quasi-free scattering process where the target nucleus is taken to be a Fermi gas. The mean free paths and energy transfers are based on nucleon-nucleon experimental scattering cross sections and angular distributions, with collisions between two particles with energy less than the Fermi energy being forbidden by the Pauli principle.

A Monte-Carlo simulation treatment of Eq. (1) by sampling many intra-nuclear cascades defines the momenta and coordinates of each nucleon involved in the cascade.

Bertini [6] developed a code in which the fastest moving particle in each cascade is followed from collision to collision, while the Brookhaven-Columbia group [7-9] followed the evolution of the intra-nuclear cascade in time.

In both cases the collisions are followed until all particle energies are below some prescribed minimum.

By following the reaction process explicitly, both equilibrium and pre-equilibrium spectra may be calculated. The angular distributions of emitted particles are also predicted.

2.2 Fermi-Gas Relaxation Model

This model encompasses another approach to the solution of the "master equation" Eq. (1) and is commonly referred to as the Harp-Miller-Berne Model.[10,11]

In this approach the single particle levels are computed with a Fermi gas spacing. The energy scale is divided into bins having a certain width (e.g. 1 MeV) and the number of available single particle levels in each bin is calculated and stored. The change in the population of states occurs as the result of two nucleons, which are in different single particle states, being scattered. The fractional change in each bin is calculated as a function of time.

The evolution process is carried out sequentially in units of time which are short compared to the nucleon-nucleon collision time.

An advantage of this model is that nuclear structure effects may be reproduced when a realistic set of single particle levels are used. However, the angular distribution of emitted particle cannot be met.

2.3 Exciton Model

This model is a phenomenological one and was proposed by Griffin [12,13]. The status of the system is classified according to the number of particles (p) and holes (h) that it contains. In this model a nucleon is assumed to enter the nucleus forming a one-particle (1p) zero-hole (0h) state. Upon interaction with one of the target nucleons a 2p - 1h state is formed. Further collisions create more particle-hole pairs (e.g. 3p - 2h, 5p - 4h, etc.).

The interaction of these excitons with the other nuclear particles permits various states to exist. For each group of states there is a certain number that can undergo particle emission. Therefore, a nuclear cascade is initiated which ends when statistical equilibrium is reached for a particular exciton number. The spectrum may then be calculated for each class of states.

The evolution of the system is described in terms of a set of coupled differential (master) equations, which have the form[14]

$$\frac{dP(n,t)}{dt} = P(n-2,t)\lambda_+(n-2,E) + P(n+2,t)\lambda_-(n-2,E) - P(n,t)\left[\lambda_+(n,E) - \lambda_-(n,E) + \sum_\nu \int_0^{E-B_\nu} W_\nu(n,\varepsilon)d\varepsilon\right] \quad (3)$$

There is one equation for each permissible n. The following quantities are defined:

p(n,t)	is the occupation probability of an n-exciton state at time t,
$\lambda^+(n,E)$	is the transition rate for the transition of an n-exciton state to an (n+2)-exciton state,

$\lambda^{-}(n,E)$ is the transition rate for the transition of an n-exciton state to an (n-2)-exciton state,

$w_{\nu}(n,\varepsilon)d\varepsilon$ is the emission rate for a particle ν with energy between ε and $\varepsilon+d\varepsilon$, for emission to the continuum from an n-exciton state,

E is the excitation energy,

B_{ν} is the binding energy of particle ν in the composite nucleus,

The pre-equilibrium spectrum for a particle ν is given by

$$N_{\nu}(\varepsilon) = \sigma_c(\varepsilon_{\alpha}) \sum_{\substack{n=n_0 \\ \Delta n=2}} w_{\nu}(n,\varepsilon) \int_0^{T_{eq}} P(n,t)\,dt \qquad (4)$$

where $\sigma_c(\varepsilon_{\alpha})$ is the formation cross section for the composite nucleus. The pre-equilibrium cross section is obtained by integrating the spectrum over an appropriate energy range.

The emission rate of particles of type β with p_{β} nucleons and energy ε may be expressed as

$$W_{\beta}(\beta,\varepsilon,p,h)\,d\varepsilon = \frac{(2S_{\beta}+1)}{\pi^2 \hbar^3}\mu_{\beta}\,\varepsilon\,\sigma_{\beta}(\varepsilon) R_{\beta}(p)(p_{\beta})! \times \frac{W(p-p_{\beta},h,U)}{W(p,h,E)}\,d\varepsilon \qquad (5)$$

where μ_{β} is the reduced mass, $\sigma_{\beta}(\varepsilon)$ the cross section for the inverse process, S_{β} the spin of the emitted particle. $R_{\beta}(p)$ is the probability of finding a particle of type β among the p particles, while $W(p,h,E)$ is the density of the initial exciton state and $W(p-p_{\beta},h,U)$ is the density of the residual nucleus with an excitation energy U.

Several methods have been proposed for solving the master equations; they are reviewed in Refs. 2 & 4.

Recently a more unified approach has been made in which equilibrium is approached via a pre-equilibrium process, thus the evaporative component is a natural consequence of the method.

By using an exact matrix method to solve the set of master equations, the artificial time division between the pre-equilibrium and equilibrium processes is eliminated.

2.4 Hybrid and Geometry - Dependent Hybrid Model

The hybrid model [16,17] combines the features of the Fermi gas relaxation model and the exciton model. The excited particle populations during equilibrium are calculated assuming equally-spaced single particle states as in the exciton model. The states are classified according to the number of particle of holes they contain, and the intranuclear transition rates were determined by calculating the mean free paths of the nucleus in nuclear matter.

A further refinement in which nuclear geometry effects were considered led to the development of the "geometry-dependent Hybrid Model."[18]

The pre-equilibrium emission probability is given as

$$P_x(\varepsilon)d\varepsilon = \sum_{\substack{n=n_0 \\ \Delta n=2}}^{\bar{n}} \left[n_{P_x} \frac{\rho_{p,h}(U,\varepsilon)\,g\,d\varepsilon}{\rho_{p,h}(E)} \right] \left[\frac{\lambda_c(\varepsilon)}{\lambda_c(\varepsilon)+\lambda_{+}(\varepsilon)} \right] D_n$$
$$= \sum_{\substack{n=n_0 \\ \Delta n=2}}^{\bar{n}} {}_nP_x(\varepsilon)d\varepsilon \qquad (6)$$

where n_{P_x} is the number of particles of type x (neutrons or protons) in the n-exciton state.

$\rho_{p,h}(U,\varepsilon)$ is the density of states with n-excitons such that if one is emitted, it would have an energy ε.

$\rho_{p,h}(E)$ is the density of n-exciton states and excitation energy E. $\lambda_c(\varepsilon)$ is the emission rate into the continuum of a particle with channel energy ε; g is the single particle level density of the composite nucleus.

$\lambda_{+}(\varepsilon)$ is the transition rate of a particle at energy ε+ V (V=real potential well depth).

The multiplication factor D_n is the fraction of reaction cross sections surviving decay from simpler states.

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B. Workshop (Problem Session)

The following codes have been chosen as examples of calculating reaction cross sections and particle spectra resulting from both equilibrium and pre-equilibrium conditions.

STAPRE: M. Uhl and B. Strohmaier
OVERLAID ALICE: M. Blann

Abstracts and general information on other codes that also handle cross sections and particle spectra are given for the following codes:

GNASH: (A Multi-purpose Statistical Model Code) (Unpublished) P. G. Young and E. D. Arthur, LASL, U.S.A.

TNG: (A Two-Step Hauser-Feshbach Code with Precompound Decays and Gamma-Ray Cascades) (Unpublished) C. Y. Fu, ORNL, U.S.A.

MODESTY: W. Matthes, Ispra, Italy.

1. STAPRE

A detailed description of this code is given in the lecture by B. Strohmaier and M. Uhl on "STAPRE – a statistical model code with consideration of pre-equilibrium decay" delivered at this Course.

Name of Code: STAPRE (A computer code for particle induced activation cross sections and related quantities).

Authors: M. Uhl and B. Strohmaier

Institution: Institute for Radium Research and Nuclear Physics, Vienna, Austria.

Nature of Problem Solved: STAPRE is a statistical model code for calculating particle-induced cross sections using discrete (Hauser-Feshbach) evaporation and pre-equilibrium (exciton model) formalisms. Gamma decay is described by means of a cascade model.

Program Language: FORTRAN IV.

Program Size: CDC Cyber 61,400 words.

2. OVERLAID ALICE

Name of Code: OVERLAID ALICE

Author: M. Blann

Institution: Univ. of Rochester, Rochester, New York, USA

Documentation: COO-3494-29, 1975
COO-3494-32 (Revised) 1976

Nature of Problem Solved: Evaporation cascade including fission plus pre-equilibrium emission based on Hybrid Model using neutrons, protons, and deuterons as projectiles.

Program Language: Fortran H

Size of Program: 180K bytes - IBM 360/75
In overlay mode the code is designed to run with less 140k bytes of core.

OVERLAID ALICE

Types of Calculation

This computer code can perform several types of calculations and combinations of these types:

(1) a standard Weisskopf-Ewing evaporation calculation [1,2] with multiple particle emission. Emitted particles may be either neutrons; n and p; n, p, and α; or n, p, α and d. Excitation energies of the compound nucleus up to 200 MeV can be considered. Residual nuclei (evaporation residue yields) of a grid 11 mass units wide by 9 atomic numbers deep may be calculated as the code is presently dimensioned. Particle spectra may also be selected in the output.

The inverse reaction cross sections may either be read in from cards, or by default are computed by the optical model subroutine. The latter means that ∿ 95% of the total computation time is used in generating the inverse cross sections. For this reason the σ(inv)results are punched on cards for possible future use, unless the punching is suppressed.

The evaporation cascade is computed with 1 MeV bin width with the method previously described in the literature [2].

(2) An s-wave approximation [3,4] may be selected, which gives an upper limit to the enhancement of γ-ray deexcitation due to angular momentum effects. In this option the calculation of (1) is performed but for every partial wave in the entrance channel. In this approximation it is assumed that the rotational energy for each partial wave is irrevocably committed to rotational motion and therefore unavailable for particle emission. The rotational energy versus J may be selected either as the rigid rotor value, or from the equilibrium deformed rotating liquid drop model of Cohen et al.[5] The transmission coefficients for the partial waves to be used in the computation may be read in from cards or by default will be provided by the parabolic model[6] routine (projectile atomic number ≥ 2) or by the optical routine (n,p,d).

(3) The evaporation calculation can include fission competition according to the Bohr-Wheeler approach, using angular momentum dependent ground state and saddle point energies[7]. The latter values come from the Cohen et al[5] rotating liquid drop calculations. The calculations may be performed at every partial wave or by bins or partial waves which differ by 1 MeV in rotational energy. Default gives calculation over all partial waves, however, upper and lower limits on angular momentum may be selected (i.e. the calculation may be limited to an angular momentum 'window'). Provision is made in input to modify the liquid drop fission barrier by some factor, as well as the a_f/a_n ratio (default = 1). An option exists by which it is assumed that neutron emission carries an average of 2ħ in angular momentum from the emitting nucleus, and proton emission 3ħ [7].

(4) Provision is made to permit precompound emission via the hybrid model[8] for the first neutron or protom emitted. Input for this aspect (including the geometry-dependent approach) is discussed in greater depth in report

COO-3494-27[9]. When this option is selected in conjunction with fission, the author has assumed that the fast precompound process will precede fission with no competition. As excitation energies increase and fission and evaporation widths increase, this assumption may become invalid. However, it should also be noted that the basic criteria of the compound nucleus model are not met, and the fission and evaporation calculations are of questionable theoretical validity. 'Let the buyer beware'!

The actual input variables are described on the comments cards preceding the main program. The CALL ERRSET subroutines in MAIN are overflow and underflow instructions (largest number and continue, zero and continue) and should be replaced by the hardware or software of the computer to be used.

The treatment of angular momentum is approximate.

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3. GNASH

A Multipurpose Statistical Theory Code

CODE NAME: GNASH (Gamma-ray, Neutron, and Asserted Particle Spectra from Neutron-Induced Reactions on Heavy Nuclei).

AUTHORS: P.G. Young and E.D. Arthur

COMPUTER: CDC 7600

CAPABILITY: GNASH calculates level activation cross section, discrete gamma-ray cross sections, isomer ratios, and neutron, gamm-ray and charged-particle spectra from almost any combination of neutron-induced reactions up to 20 MeV or higher. The code handles de-excitation of up to ten nuclei in the decay sequence, and each decaying nucleus can emit up to six types of radiation (neutrons, gamma-rays, protons, alphas, etc.). A maximum of 50 discrete levels can be included for each residual nucleus formed in the calculation, which provides great flexibility in calculations of activation cross sections, isomer ratios, etc. Examples of reactions that can be handled in a single calculation are (n,γ), (n,n'γ), (n,γn'), (n,pγ), (n,npγ), (n,αnγ), (n,2nγ), (n,3nγ), (n,4nγ), etc.

METHOD: The calculation follows closely the statistical theory described by Uhl[1]. Widths for particle decay are computed from externally calculated optical model transmission coefficients. Gamma-ray widths are calculated using either the Weisskopf single-particle approximation[2] or the Brink-Axel giant dipole resonance model.[3] Gamma-ray emission by electric and magnetic dipole or quadrupole transitions are allowed, and gamma-ray cascades are followed in detail. The Gilbert and Cameron[4] form of level density function is used and is matched with inputted discrete data for up to 50 low-lying states per residual nucleus. A simple pre-equilibrium model is used to correct particle spectra and level excitation cross sections for semi-direct processes.

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4. TNG

Name of Code: TNG (A Two-Step Hauser-Feshbach Code with Precompound Decays and Gamma-Ray Cascades)

Author: C.Y. Fu, ORNL

Computer for which Code is Designed: IBM 360/75 and 360/91

Nature of Physical Problems Solved: The code is designed for calculating nuclear reaction cross sections below 20 MeV. Binary-reaction, tertiary-reaction and gamma-ray-production cross sections such as (n,γ), (n,p), (n,2n), (n,n'γ), (n,αγ) may be calculated. Energy distributions of secondary particles and gamma rays may be output in ENDF/B formats. Angular distributions of the first outgoing particles may be output in terms of Legendre coefficients.

Method of Solution: The Hauser-Feshbach formula[2] for compound binary reactions is extended to include tertiary reactions. Sequential decays without correlation between the two outgoing particles are assumed. Transmission coefficients needed for each step of the sequential decays are calculated with an in-house optical model without spin-orbit coupling. Binary-reaction part of the code, including width-fluctuation corrections, is based on the ORNL Hauser-Feshbach code HELENE.[3] A precompound model[4] may be included as a correction to the energy distributions of the first outgoing particles. Gamma-ray competition with the second outgoing particles and the gamma-ray-cascades calculations are spin- and parity-dependent, thus sensitive to the angular momentum effects of the Hauser-Feshbach method. Gamma-ray branching ratios, if not available experimentally, are estimated from the tails of electric giant dipole resonances.[5] The parity selection rule of electric dipole transitions may be partially relaxed as a means of including magnetic dipole transitions.

Restriction on Complexity: Present dimensioning restricts a maximum of three types of binary particles and three types of tertiary particles.

Representative running time: The running time is roughly proportional to $(E \times \Delta E)^2$ where E is the incident neutron energy and ΔE the continuum bin width. For E = 14 MeV, ΔE = 0.2 MeV and a case that includes (n,n'x), (n,px) and (n,αx) with x = γ, n, p, or α, and gamma-ray-cascades for every residual nucleus, the running time would be roughly two minutes on IBM 360/91.

Related or Auxiliary Programs: Collective excitation cross sections from measurements and/or calculations may be input to TNG so that the collective effects are included in the calculated gamma-ray-production cross sections.

Status: In use at ORNL.

Machine Requirements: 300 K bytes of core.

Materials available: Complete code package will be available by July 1, 1975 from the Radiation Shielding Information Center at the Oak Ridge National Laboratory.

Acknowledgements: Work funded by the Defense Nuclear Agency and the Atomic Energy Agency under contract with the Union Carbide Corporation.

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5. MODESTY

Name of Code: MODESTY (Calculation of Nuclear Reaction Cross Sections with the Statistical Model) EUR 5722.e (1977)

Author: W. Matthes

Establishment: Joint Research Centre, Ispra, Italy

Nature of Problem Solved: Code MODESTY calculates all energetically possible reaction cross sections and particle spectra within a nuclear decay chain.

It is based on the statistical nuclear model following the method of Uhl [1] where the optical model is used in the calculation of partial widths and the Blatt-Weisskopf single particle model for γ decay.

The program is designed in the "modular concept in that all necessary nuclear data are automatically searched for from an external (tape or disc) library of fundamental data.

Plans are underway to modify the code to include pre-equilibrium effects and a more sophisticated treatment of γ-decay by including the Brink-Axel model.

Program Language: PL/1 (IBM 360/75)

Size: 130k bytes

Ref.

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