

# **Present Methods for Physics Calculations of Hybrid Fast Systems at PSI**

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## **Abstract**

At the Paul Scherrer Institute (PSI), hybrid systems with a fast neutron spectrum are extensively investigated. The high-energy particle interaction is treated using the Monte Carlo method. For the transport of neutrons at low energies a deterministic approach is adopted, together with modern nuclear data libraries.

## **Méthodes de Calcul Appliquées aux Systèmes Hybrides à Spectre Rapide**

## **Résumé**

A l'Institut Paul Scherrer (PSI), les systèmes hybrides à spectre rapide font l'objet d'études très approfondies. La méthode Monte Carlo est utilisée pour traiter les interactions de particules à haute énergie. Pour le transport des neutrons à basse énergie une approche déterministe est adoptée ainsi que l'utilisation de bibliothèques de données nucléaires des plus modernes.

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# 1 Introduction

This paper gives a general description of the calculational methods and associated nuclear data for the analysis of hybrid fast systems presently used at the Paul Scherrer Institute (PSI) [1].

Codes and data are either available on VAX/VMS at PSI or on Zürich CRAY-YMP and Lausanne PASCAL-M94 computers.

Section 2 describes the nuclear data and their processing scheme, Section 3 presents the codes most frequently used. Section 4 reports on the methods for fuel recycling and toxicity calculations. The overall computational scheme is shown in Figure 1.

## 2 Nuclear Data

### 2.1 Nuclear Data and Methods above 20 MeV

Particle transport calculations above 20 MeV are carried out using the PSI version of the HETC Code [2] [3]. The HETC code allows the study of the transport of high-energy nucleons and mesons in the energy region above 15 MeV for nucleons and 2.2 MeV for mesons. The upper energy limit for the code is not fixed, the lower energy limit is indistinct but somewhat below 50 MeV. Traditionally, 15 MeV is selected for neutrons as being somewhat below the upper limit of neutron cross-section data sets, thereby easing the transition to fast neutron transport codes. It should be noted that the region from 15 MeV to 50 MeV (where the interaction can be considered to be changing from “full” compound to “full” Serber) is not well treated.

An input data-set is required by HETC, for the intra-nuclear cascade part of the code and the evaporation calculation. The input data arrays for the intra-nuclear cascade calculations are in the form of Fermi energies, nucleon-nucleon differential cross sections and single pion-nucleon cross sections [4]. The nuclear data used in the evaporation model consist of pre-computed functions, pairing energies, and mass excess values based on the 1983 mass tables [5].

### 2.2 Nuclear Data below 20 MeV

The nuclear data libraries available are primarily from the JEF-2.2 evaluation. For some important nuclides such as  $^{237}\text{Np}$  additional data were taken from the ENDF/B-VI, JENDL-3, and CENDL-2 evaluations. We could access, retrieve, and process these data using the on-line nuclear data services located at the NEA Data Bank in Paris, IAEA in Vienna, and Brookhaven National Laboratory in the USA.

In the following paragraphs a description of these libraries is given and their processing scheme is illustrated.

### 2.2.1 Processing Scheme

Pointwise and groupwise cross sections were generated using the code system NJOY from Los Alamos (Edition 89.62) [6]. A newer version of NJOY (Edition 91.91) has recently been installed and extensively tested on both the CRAY-YMP and PASCAL-M94 computers. No substantial discrepancies were found in the fast data sets produced with these two editions of NJOY.

NJOY includes sophisticated methods of reconstruction of zero temperature pointwise cross sections using various resolved resonance formalisms, Doppler-broadening by the accurate point-kernel method, group-to-group thermal scattering matrices, flux-weighted fission-fraction vectors, and a weighting flux produced by a pointwise solution of the slowing-down problem which accurately accounts for broad and intermediate resonance effects in the epithermal region.

Pointwise cross sections were processed in the usual way into an ENDF/B like format (PENDF) using the NJOY modules RECONR, BROADR, UNRESR, and THERMR.

193 neutron group cross sections up to  $P_3$  (GENDF files) were generated from the PENDF and ENDF files using the NJOY module GROUPT. Hereby a suitable weighting spectrum for fast breeder calculations (IWT=7 in the NJOY terminology) was used, and the cross sections were shielded with the narrow-resonance flux model. The 193 groups include 92 fast energy groups below 14.92 MeV, mostly equally spaced in lethargy.

### 2.2.2 MICROX-2 Libraries

GENDF and PENDF data were edited into the FDTAPE and GARTAPE data files for the spectrum cell code MICROX-2 [7] using a PSI version (Edition 2) of the original coupling and reformatting module MICROR [8].

The FDTAPE data file contains over 300 data sets for almost all JEF-2.2 isotopes including actinides, structural materials, fission products and light nuclides. It consists of 92 group dilution- and temperature- dependent cross sections in the fast energy range, and individual fission spectra for the actinides. The temperature ranges from 293 to 2200 K and the sigma zeros of the highly resonant nuclides from 1 to  $10^{10}$  barns.

The GARTAPE data file contains about 60 data sets for the most important actinides, structural material and light nuclides, and consists of detailed pointwise temperature-dependent resonance cross sections in the resolved and unresolved resonance regions: 24362 energy points equally spaced in velocity between 2 eV and 8.0072 keV have been generated. The temperature ranges from 293 to 2200 K.

## 3 Codes

For the analysis of hybrid fast systems we mainly use deterministic methods:

In this section a brief description of the spectrum cell code MICROX-2 is given, and the treatment of fission products is illustrated. In addition, the transport-theory code TWODANT [9], the methodology for generating the required multigroup, multiregion fixed neutron source below 20 MeV, the transport-theory burn-up code 2DTB, and the perturbation-theory code PERT-V [10] for the determination of kinetic parameters are described.

### 3.1 The Spectrum Cell Code MICROX-2

MICROX-2 is an integral transport theory spectrum code from General Atomics which solves the neutron slowing down and thermalization equations on a detailed energy grid for a two region lattice cell. MICROX-2 was developed for the efficient and rigorous preparation of neutron broad group cross sections for poorly moderated systems such as fast breeder reactors in addition to well moderated thermal reactors such as light water and high temperature reactors. The fluxes in the two regions are coupled by transport corrected collision probabilities for the generation of the regionwise transfer probabilities in the fast- and resonance-energy ranges. The computation of the collision probabilities is based upon the spatially flat neutron emission approximation and the transport approximation of anisotropic scattering. The collision probability calculation also uses an energy dependent Dancoff correction factor algorithm and is performed on the ultra-fine energy grid available on the GARTAPE data file. A second level of heterogeneity can be treated: The inner region may include two different types of particles. MICROX-2 accounts explicitly for overlap and interference effects between different resonance levels in both the resonance and thermal energy ranges; it allows for the simultaneous treatment of leakage and resonance self-shielding in doubly heterogeneous lattice cells. A semilogarithmic Bondarenko-interpolation between sets of temperature- and dilution-dependent FDTAPE data is available for energies larger than an input value, the upper energy for the pointwise resonance calculation. Up to  $P_3$  in the fast energy range and  $P_1$  order of scattering in the thermal range are used. The neutron leakage is determined by performing fine group and hyperfine point  $B_1$  slowing down in the fast and resonance-energy ranges and  $P_0$  plus  $DB^2$  thermalization calculations in the thermal range, in each region. Energy-dependent bucklings (positive, zero, or negative) can be supplied. A buckling search as a solution of the collapsed two group  $B_1$  equations can be performed. Zonewise fission spectra are generated as linear combinations of fission spectra for various fissionable actinides available on the FDTAPE data file. The detailed neutron flux and current spectra are used for collapsing the basic neutron cross sections into cell-averaged and region-averaged broad-group cross sections and scattering transfer arrays up to  $P_1$ . Broad group  $P_2$  and  $P_3$  scattering transfer arrays are determined with  $P_2$  and  $P_3$  weighting spectra obtained from an extended transport approximation.

When using the most recent PSI version of MICROX-2 (Edition 14) the resulting broad group microscopic and macroscopic cross sections can be used in TWODANT and 2DTB via a card image, material ordered, output format XSLIB [9].

## 3.2 Fission Products

For each actinide the XSLIB fission product cross sections are lumped into additional, problem dependent "pseudo fission product" cross sections using the PSI code PSD. The "pseudo fission product" cross sections compensate for too low absorption as a result of missing fission product data on the XSLIB file. PSD sums up suitably weighted fission product cross sections. The auxiliary PSI code RUSR generates the weighting factors from the independent yields available on the fission product yield data library (MF=8, MT=454 in ENDF terminology).

## 3.3 The Transport-Theory Code TWODANT

TWODANT is a modular computer program from Los Alamos designed to solve the two-dimensional, time-independent, multigroup discrete-ordinates form of the Boltzmann transport equations in x-y, r-z, and r- $\theta$  geometries. Both regular and adjoint, inhomogeneous fixed source and homogeneous problems subject to vacuum, reflective, periodic, white, or inhomogeneous boundary flux conditions are solved. General anisotropic scattering is allowed and anisotropic homogeneous sources are permitted. The diamond-difference scheme is used for space-angle discretization. Negative fluxes are eliminated by a local set-to-zero-and-correct algorithm. A standard inner (within group) iteration, outer (energy-group-dependent source) iteration technique is used. Both inner and outer iterations are accelerated using the diffusion synthetic acceleration method. The diffusion solver uses the multigrid method and Chebychev acceleration of the fission source.

Simple problems can be easily run and many of the code options can be ignored by the casual user. At the same time numerous options for selective and sophisticated executions are available to the more advanced user.

The modular construction of the code package separates the input processing, the transport equation solving and the post-processing, or edit, functions into distinct, independently executable code modules, connected to one another solely by means of binary interface files.

## 3.4 Neutron Source Modelling Below 20 MeV

HETC writes the results, describing the individual events which occurred during the cascade initiated by the source particles, in a very detailed form on a history tape. The history tape contains all the information to reconstruct the "physics", it is therefore very large (> 25 MBytes) and very cumbersome to handle. Hence, a first code module, ANALYZ2, was developed and linked to HETC, which writes the neutron source in a condensed form as a saveset. The saveset contains the energy, direction of travel, position and statistical weight of each neutron to be transported. A second code module, 2DBTPC, analyses the saveset for the position and spectrum of the neutrons and finally outputs the results as a multigroup spatially distributed heterogeneous source in the format required by the 2DTB and TWODANT codes.

### 3.5 The Burn-Up Code 2DTB

The code 2DTB, which can use both transport- and diffusion-theory options, is a PSI extension of the original diffusion code 2DB from General Atomics [11].

In the new transport-theory option the original 2DB burn-up capability is used in connection with fluxes produced with TWODANT: The input file for a TWODANT run is automatically generated at each burn-up step. The original 2DB limitation to a maximum number of 50 neutron groups has been removed and variable dimensions have been extensively introduced. A new option for the power normalization has been implemented to be used in external fixed source problems, and a new subroutine has been written for reading the XSLIB cross section format. The burn-up calculation can be restarted if the results from the previous step were saved; an input file for MICROX-2, which accounts for the fission product composition, is automatically written for burn-up dependent cell calculations.

### 3.6 The Perturbation-Theory Code PERT-V

The PERT-V code at PSI is based on a Los Alamos modification of the original Battelle-Northwest Laboratory code. PERT-V is a diffusion theory first-order perturbation theory code designed to compute reactivity worth components for specified spatial positions, effective delayed neutron fractions, neutron generation times, the inhour/ $\delta k$  conversion factor, and reaction rates for specified spatial positions, especially for fast reactor analysis. The leakage components of the reactivity coefficients are computed with a mesh-centered diffusion theory finite-difference approximation. The other components of the reactivity coefficients, the effective delayed neutron fraction, the neutron generation time, the inhour/ $\delta k$  conversion factor, and the activities are computed directly from the broad-group direct and adjoint fluxes from TWODANT and XSLIB format cross sections.

## 4 Fuel Recycling and Toxicity Calculations

For detailed analyses of transmutation concepts [12] [13], out-of-pile cooling of fuel and fuel reloading in successive cycles have to be considered as well.

Cooling of the target material after irradiation is handled by the ORIHET code. ORIHET is a PSI adaptation of the Oak Ridge Isotope GENERATION and depletion code ORIGEN [14], which uses the matrix-exponential method to study the buildup and decay of activity in reactor cores. The code calculates the concentrations after given time intervals and can output various derived quantities: activity, mass, power dissipation, gamma spectra, etc.

Reprocessing and reloading of the spent fuel is handled by the code module RELOAD. Several reprocessing strategies are envisaged depending on the type of fuel used. The toxicities resulting from the reprocessing stage (reprocessing losses, fission products, etc.) are calculated by the ORIHET code.

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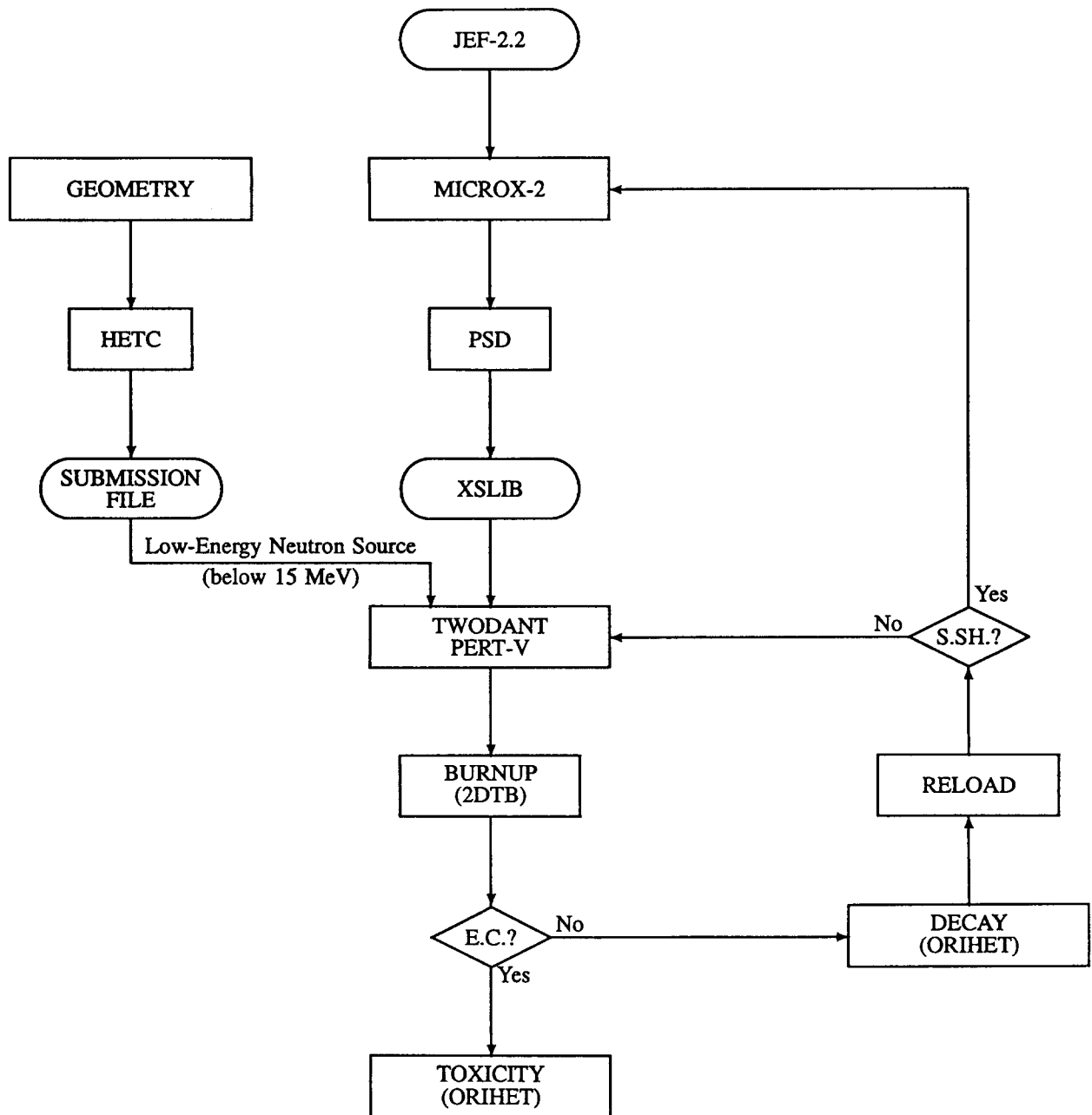


Figure 1. The code package used for transmutation system calculations