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ABSTRACT

MCRP is a Monte Carlo computer program for tracking neutrons slowing down in single rod and rod cluster lattices. The code is intended for calculations of resonance absorption in reactor fuel nuclides using cross sections at 124 000 energy points below 20 keV. The only intrinsic assumptions are that scattering is both elastic and isotropic in the centre of mass system.

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MONTE CARLO METHOD; NEUTRONS; FUEL RODS; REACTOR LATTICES; M CODES; RESONANCE ABSORPTION; ELASTIC SCATTERING; CENTRE-OF-MASS SYSTEM; NEUTRON SLOWING-DOWN THEORY; SLOWING-DOWN

CONTENTS

1. INTRODUCTION

One of the most basic problems in reactor physics is that of calculating the resonance absorption of neutrons slowing down in reactor lattices. The use of the Monte Carlo method allows a treatment from which all approximations may be removed. The MCRP computer code has been designed for benchmark calculations against which the approximations used in a lattice code may be checked. MCRP uses actinide cross sections at 124 000 points in the range 19.3 keV to 0.07 eV in the format specified by Chiarella [1971]. These actinide data files are common to MCRP and the collision probability code PEARLS [Chiarella 1971], and have been used to generate the resonance data employed in the MIRANDA module [Robinson 1977] of the AUS neutronics scheme. This enables checks to be made between the three methods for the same data base.

The assumption that neutron scattering is elastic and isotropic in the centre of mass system has been made in MCRP to simplify the treatment of cross sections. This assumption is quite good in the energy range considered and, in any case, can also be made in checks against the MCRP benchmark results.

2. GENERAL

MCRP is very similar to the MOCUP code of Bannister *et al.* [1968] but is written in FORTRAN for an IBM3033 computer. At present, cluster geometry is the only available option. The outer moderator boundary is assumed to be reflecting and may be cylindrical (white), square or hexagonal. Single rod calculations can be performed, though not optimally, because the tracking routine is unnecessarily complicated for simple annular geometry. The program is written in modular form and extensions to other geometries will not be difficult. Tracking speeds on the IBM3033 computer vary from a maximum of 100 000 collisions per minute for some simple two-region calculations to 50 000 collisions per minute for a 37-rod cluster with cans and tubes.

The possible energy range over which neutrons can be tracked is from 19.3046 keV to 0.0719413 eV (or lethargy 6.25 to 18.75). A neutron history begins with a neutron crossing a nominated starting energy and tracking ceases when the neutron energy falls below a specified cutoff. Printed output consists of escape probability for the cell and reaction rates per source neutron, region by region, over a multigroup energy structure which is specified in the input data. Results are printed after all batches are completed and optionally after each batch.

Two different cross section representations are available. In the simpler representation, the cross sections are independent of energy. This is normally used to represent a classical moderator with $\sigma_a = 0$ and constant σ_s. The detailed representation includes 124 000 points giving energy-dependent capture, fission and total cross sections in the structure specified by Chiarella [1971]. The constant lethargy tabulation has been retained, despite the inconvenience that this causes in Monte Carlo, to ensure compatibility with PEARLS calculations. Linear interpolation is used between points. The best available data have been generated from ENDF/B-IV [Garber 1975] using the methods outlined by Robinson [1977, 1984]. Data for ^{235,238}U and $^{239-242}$Pu are available at temperatures of 300, 900 and 2100 K.

The program strategy is similar to that for MOCUP, with the total number of neutron histories being divided into batches, each comprising a fixed number of neutrons. The energy range is divided into 775 groups - one group for each 160 points of the PEARLS tabulation. As each group is considered, the cross-section data appropriate to the group is read from the disc. Each neutron with energy within the group is tracked until its energy after collision has fallen below the group; its current coordinates are then stored. When all neutrons in a batch with energies within the group have been processed, the procedure is repeated for the next group. A bit pattern sort routine described by Mason [1971] is used to select the neutrons with energies in each group. Results are collected on completion of each batch and may optionally be printed. Single precision 32-bit floating point arithmetic is used to track the neutrons but results are accumulated in double precision to avoid the accumulation of round-off error. With this strategy and dynamic storage allocation, the program occupies only a little core and is ideal for use with a multi-processing operating system.

3. DETAILED DESCRIPTION

The only energy degradation process treated by the program is elastic scattering, which is assumed to be isotropic in the centre of mass system. Let A be the mass (in neutron masses) of the scattering nuclide and θ and ψ the scattering angles in centre of mass and laboratory frames respectively. Define the following

quantities:

$$\alpha = (A-1)^2/(A+1)^2 \tag{1}$$

$$\mu = cos\theta \tag{2}$$

$$\mu_L = cos\psi \tag{3}$$

Isotropic scattering in the centre of mass system implies that the probability $P(\mu)\, d\mu$ of obtaining a cosine in the interval $d\mu$ about μ is simply

$$P(\mu)\, d\mu = \frac{1}{2}\, d\mu \quad . \tag{4}$$

The cosine μ is obtained during sampling by selecting a random number η from (0,1) and setting

$$\int_{-1}^{\mu} P(\mu)\, d\mu = \eta \quad , \tag{5}$$

giving

$$\mu = 2\eta - 1 \quad . \tag{6}$$

If the energy before collision is E, the energy E′ after collision is found from the relation

$$E' = 0.5\, [(1+\alpha) + \mu(1-\alpha)]\, E \quad . \tag{7}$$

The laboratory scattering angle cosine μ_L satisfies

$$\mu_L = (A\mu + 1)/(A^2 + 2A\mu + 1)^{1/2} \quad . \tag{8}$$

Given μ_L, the direction cosines (λ', μ', ν') relative to the old direction of travel (α, β, γ) can be obtained by rejection techniques.

First,

$$\lambda' = \mu_L \quad . \tag{9}$$

If η_1, η_2 are, respectively, a random cosine and sine obtained by rejection

$$\mu' = \eta_1 \ (1-\mu_L^2)^{1/2} \quad , \tag{10}$$

$$\nu' = \eta_2 \ (1-\mu_L^2)^{1/2} \quad . \tag{11}$$

To obtain the direction cosines (λ, μ, ν) relative to the usual x, y, z laboratory frame we define a set of axes at the collision point with the following direction cosines:

$$(\ell_1, m_1, n_1) = (\alpha, \beta, \gamma) \tag{12}$$

$$(\ell_2, m_2, n_2) = (\alpha\gamma/(\alpha^2 + \beta^2)^{1/2},\ \beta\gamma/(\alpha^2 + \beta^2)^{1/2},\ -(\alpha^2 + \beta^2)^{1/2}) \tag{13}$$

$$(\ell_3, m_3, n_3) = (-\beta/(\alpha^2 + \beta^2)^{1/2},\ \alpha/(\alpha^2 + \beta^2)^{1/2},\ 0) \tag{14}$$

Then (λ, μ, ν) are given by the relations

$$\lambda = \ell_1\lambda' + \ell_2\mu' + \ell_3\nu' \quad , \tag{15}$$

$$\mu = m_1\lambda' + m_2\mu' + m_3\nu' \quad , \tag{16}$$

$$\nu = n_1\lambda' + n_2\mu' + n_3\nu' \quad . \tag{17}$$

Each neutron begins its history with unit weight which is reduced at every collision. Suppose that the collision takes place in a material consisting of several nuclides with number densities N_i and microscopic scattering and absorption cross sections σ_{si} and σ_{ai} respectively. The macroscopic cross sections for the material are

$$\Sigma^T = \sum_i N_i\, (\sigma_{si} + \sigma_{ai}) \quad , \tag{18}$$

$$\Sigma^S = \sum_i N_i\, \sigma_{si} \quad . \tag{19}$$

The probability of absorption in the material is simply $(1 - \Sigma^S/\Sigma^T)$. If the weight of the neutron before collision is w, then $w(1 - \Sigma^S/\Sigma^T)$ is scored as absorption in the region and the scattered neutron is given the weight $w\,\Sigma^S/\Sigma^I$. The choice of scattering nuclide is determined from a cumulative probability distribution defined as follows:

$$F_o = 0 \quad , \tag{20}$$

$$F_j = F_{j-1} + N_j \sigma_{sj}/\Sigma^S \quad . \tag{21}$$

A random number η is selected from (0,1) and the neutron is assumed to scatter from nuclide j if $F_{j-1} < \eta < F_j$. To optimise the selection process, the nuclides comprising a material should be specified in order of decreasing $N_j\ \sigma_{sj}$, although this will make little difference to the overall calculation time.

Tracking continues until the energy of the neutron falls below the energy range of interest. As there is no upscattering mechanism, it is not necessary to employ 'Russian roulette' to terminate neutron histories. Neutrons of low weight are retained since even these make a significant contribution to reaction rates at the bottom of the resonance region. The tracking method employed for cluster geometry is similar to that described by Doherty [1970]. Any number of annular subdivisions of either rods or coolant and moderator regions can be specified in the input data, and reaction rates in a specified group structure will be printed by the program. All reaction rates are normalised to one source neutron passing the nominated starting energy.

The source distribution is based on the assumption that the flux above the starting energy E_o is spatially flat with an energy variation

$$\phi(E) = \phi_o/E \quad . \tag{22}$$

The average logarithmic energy decrement ξ of a nuclide with mass A is

$$\xi = 1 + \frac{\alpha}{1-\alpha}\, ln\, \alpha \quad . \tag{23}$$

where α is defined in equation 1. The rate at which neutrons are produced at energy $E\ (\leq E_o)$ by scattering with nuclide j at energies $E'\ (\geq E_o)$ is

$$p_j(E) = \int_{E_o}^{E/\alpha_j} dE'\, N_j\, \sigma_{sj}\ \phi_o/[(1-\alpha_j)(E')^2]$$

$$= N_j\ \sigma_{sj}\ \phi_o\ [1/E_o - \alpha_j/E]/(1-\alpha_j) \quad . \tag{24}$$

The total number T_j produced in the interval $(E_o, \alpha_j E_o)$ is simply

$$T_j = \int_{\alpha_j E_o}^{E_o} p_j(E)dE \tag{25}$$

$$= N_j\ \sigma_{sj}\ \xi_j \phi_o \quad .$$

For each region we define a total integral R which is the sum over nuclides in the region,

$$R = \sum_j^{sum}\ N_j\ \sigma_{sj}\ \xi_j \quad . \tag{26}$$

The cumulative probability distribution for the region is defined as usual by

$$F_o = 0 \quad , \tag{27}$$

$$F_j = F_{j-1} + N_j \sigma_{sj}\ \xi_j/R \quad .$$

Thus if a neutron is to be born in the region, the nuclide j with which it collides is selected by $F_{j-1} <$ random $\eta < F_j$.

The selection of region is based on a similar cumulative probability distribution. If k is a region index, we define

$$S = \sum_k^{sum}\ V_k\ R_k \tag{28}$$

where V_k is the volume of region k and R_k is defined by equation 26.

With

$$F_o = 0 \quad , \tag{29}$$

$$F_k = F_{k-1} + V_k R_k / S \quad , \tag{30}$$

the region k is selected by the condition $F_{k-1} < \eta < F_k$.

In this way, the region and scattering nuclide of the source neutron are determined. Within the region, the starting coordinates are selected from a uniform volume distribution, and the starting direction cosines uniformly from the unit sphere. The only remaining variable is the energy which is obtained by a rejection technique. The probability $P_j(E)\,dE$ of obtaining an energy in the interval dE about E after a collision above E_o with nuclide j is

$$P_j(E)\,dE = p_j(E)\,dE/T_j \tag{31}$$

$$= A_j - B_j/E \quad ,$$

where

$$A_j = 1/[\xi_j(1-\alpha_j)E_o] \quad , \tag{32}$$

$$B_j = \alpha_j/[\xi_j(1-\alpha_j)] \quad . \tag{33}$$

We select η_1, η_2 from (0,1) and evaluate

$$z_1 = E_o - \eta_1 E_o (1-\alpha_j) \tag{34}$$

$$z_2 = A_j - B_j/z_1 \tag{35}$$

$$z_3 = \eta_2 (A_j - B_j/E_o) \tag{36}$$

If $z_2 > z_3$, we accept z_1 as the starting energy. Otherwise we select another pair η_1, η_2 and repeat the procedure. The efficiency of the algorithm is $\xi_j/(1 - \alpha_j)$.

4. INPUT DESCRIPTION

Input data to MCRP are in free format and read with the SCAN input routine [Bennett and Pollard 1967]. The first set of numbers specify the dimensions assigned to the arrays.

MAXISO the maximum number of nuclides in the cell.

MAXGP maximum number of groups in edit.

MAXMAT maximum number of materials.

MAXCON maximum number of nuclides per material.

MAXNUT maximum number of neutrons per batch.

MAXANN maximum number of annular subdivisions.

MAXSUB maximum number of rod subdivisions.

MAXTCH maximum number of rod pitches.

MAXROD maximum number of rods.

MAXTAP maximum number of nuclides using full 124 000 energy point representation.

The problem data then follows.

TITLE card (read and printed 20 A4).

IBCA type of outer boundary - 0 circular, 4 square, 6 hexagonal.

NANN number of annuli.

(ANN(I), I = 1, NANN) outer radius of each annulus, the outermost being the volume equivalent radius for square and hexagonal boundaries.

(MANN(I), I = 1, NANN) material number of the material within each annulus.

NPITCH number of pitch circles on which rods are placed.

NROD (I) number of rods on pitch circle I.

PROD (I) radius of pitch circle I.

QROD (I) angular displacement in radians of the first rod from an arbitrary axis y = 0 drawn through the centre of the cluster.

MROD (I) number of radial subdivisions of the rods on pitch circle I.

(RAD(J,I), J=1, MROD(I)) the radial subdivisions of the rods on pitch I.

(MRADK (J,I), J = 1, MROD(I)) the materials in the subdivisions.

Repeat for each pitch from NROD(I).

NMAT number of materials.

NNMAT (I) number of nuclide constituents.

(MAT(J), CMAT(J), J = 1, NNMAT(I)) nuclides and concentration in atoms per barn cm.

Repeat for each material from NNMAT(I).

NISO number of nuclides.

ISOTY(I) nuclide type of nuclide I.
For ISOTY (I) = 1, a constant cross section nuclide, data consist of the following:

AMU (I) mass in a.m.u. of nuclide (neutron mass is taken as 1.008665);

SIGS (I) scattering cross section in barns;

SIGA (I) absorption cross section in barns.
For ISOTY (I) = 3, a nuclide for which a 124 000 point library is to be used, data consist of the following:

IENTRY (I) the unit number (>11) on which the library is located. A DD card must be supplied for each nominated unit.

Repeat for each nuclide from ISOTY(I).

NGROUP number of groups for which output will be printed.

IDATA indicates the units for subsequent data:
= 1 group boundaries in lethargy;
= 2 group boundaries in MeV;
= 3 group boundaries in eV.

(GROUPB (I), I=1, NGROUP+1) group boundaries in increasing lethargy or descending energy order.

NBATCH number of batches.

MBATCH number of neutrons per batch.

BEGIN starting energy for neutron histories in units fixed by IDATA.

FINIS finishing energy for neutron histories in units fixed by IDATA.

(NPRINT(I), I = 1, MAXREG) output type:
= 1 details for region I are not printed;
= 2 details for region I are printed at the end of the run;
= 3 details for region I are printed at the completion of each batch;

where MAXREG = the number of regions in the calculation. Each annulus is a region. Each rod subdivision on each pitch is a region. All rods on the same pitch are treated as the same rod for output purposes.

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