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Methods and computer codes for nuclear systems calculations

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Abstract. Some numerical methods for reactor cell, sub-critical systems and 3D models of nuclear reactors are presented. The methods are developed for steady states and space–time calculations. Computer code TRIFON solves space-energy problem in (X, Y) systems of finite height and calculates heterogeneous few-group matrix parameters of reactor cells. These parameters are used as input data in the computer code SHERHAN solving the 3D heterogeneous reactor equation for steady states and 3D space–time neutron processes simulation. Modification of TRIFON was developed for the simulation of space–time processes in sub-critical systems with external sources. An option of SHERHAN code for the system with external sources is under development.

Keywords. Reactor; neutron; sub-critical; computer code.

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1. Introduction

Some numerical methods for reactor cell, sub critical systems and 3D models of nuclear reactors are presented. Some features of neutron transport in sub critical systems with external sources (accelerator-driven systems) are considered. For reactors, the approach is based on the extension of Landau–Pomerantchuk–Galanine–Feinberg heterogeneous reactor theory [1] – an advanced method of heterogeneous reactor theory [2] that includes:

- general formulation of few-group heterogeneous reactor equation,
- its transformation from matrix to a different form with the presentation of axial dependencies by finite Fourier expansions,
- development of a consistent theory for the characteristics of reactor cell – few-group boundary conditions.

On the basis of these theoretical achievements two computer codes were developed: TRIFON, Version 2.1 for reactor cell calculations [3] and SHERHAN for 3D heterogeneous reactor calculations [4]. Modifications of TRIFON code for sub-critical systems with external source were performed.

2. Numerical methods for ADS

Some features of neutron transport in sub critical systems with external sources (accelerator-driven systems) are described below. Generally the eigenvalue problem for critical systems (solutions of uniform systems of equations for eigenfunctions and eigenvalues) should be replaced for source problem (solutions of non-uniform systems of equations with a fixed neutron source).

2.1 *Main equation*

The neutron transport in a sub critical system with an external source may be described by the equation:

$$F = H(\Sigma_{\mathrm{s}} F + Q),$$

where Σ_{s} is the macroscopic scattering cross-section; the source for group i is composed of three parts:

$$Q^i = Q^i_{\mathrm{s}} + Q^i_{\mathrm{f}} + S,$$

where Q^i_{s} is due to neutron scattering from upper groups $j > i, Q^i_{\mathrm{s}} = \sum \Sigma^{ij} F_j$, where F_j is the neutron flux in the group $j; \Sigma^{ij}$ is the macroscopic cross-section of scattering from group j to group i. The source

$$Q^i_{\mathrm{f}} = \theta^i S_{\mathrm{f}}; \quad S_{\mathrm{f}} = \nu \Sigma_{\mathrm{f}} F$$

is due to fissions, Σ_{f} is the macroscopic fission cross-section and ν is the number of secondary neutrons per fission. Here θ is the energy distribution of neutrons and corresponds to the fission spectrum. The source S_{f} for a given iteration is estimated by the distribution of fissions in the total energy interval. The external neutron source S has its own space-energy distribution, produced by proton beam in the target.

2.2 *Reaction rates and neutron balance*

In a multi-group presentation capture and fission reaction rates for every nuclide l in every physical region k are calculated from upper to a flow group i:

$$C^i_{kl} = V \sigma_k c_{kl} \sum_{j=1}^{i} F^j_k \sigma^j_{cl}; \quad F^i_{kl} = V_k c_{kl} \sum_{j=1}^{i} F^j_k \sigma^j_{fl};$$

$$\nu F^i_{kl} = V_k c_{kl} \sum_{j=1}^{i} F^j_k (\nu\sigma)^j_{fl}.$$

The current of neutrons across a fixed energy boundary is defined by the equality

$$\varepsilon^i_k = \sum_l \sum_{j \le i} \sum_{m > i} \Sigma^{jm}_k F^j_k.$$

Their total values (the sums over k and l) $C^i, F^i, \nu F^i, \varepsilon^i$ and the current of neutrons across the outer boundary of the system J^i up to a fixed group i (for every group below external source and fission spectrum boundaries) obey the following neutron balance equation:

$$C^i + F^i + \varepsilon^i + J^i = S + \nu F.$$

Similarly, for all ranges of energies (total number of captures and fissions plus neutron current across the outer boundary is equal to the number of neutrons produced by external source and the number of neutrons born in fissions),

$$C + F + J = S + \nu F; \quad Q_{\mathrm{r}} = \nu F.$$

For the source problem, multiplication factor is defined as

$$K_{\mathrm{s}} = \nu F/(S + \nu F) = \nu F/(C + F + J),$$

where all the values in the equation above are integrals over space and energy with neutron flux taken as the solution of non uniform system of equations with the source term. To take account of (n, xn) reactions the term F is to be replaced by

$$F + \sum_x (n, xn) \quad \text{and} \quad \nu F \quad \text{by} \quad \nu F + \sum_x x(n, xn).$$

2.3 *Calculation of concentrations corresponding to a given level of sub-criticality*

A necessary level of sub-criticality (and hence for a given neutron source the power level) may be found by a proper choice of fuel or absorber mass g, found as a root of the equation for a given K_{s}^0:

$$K_{\mathrm{s}}(g) = K_{\mathrm{s}}^0.$$

A set of fuel or absorber nuclides should have a prescribed composition.

2.4 *Continual feed with a constraint – constant power (sub-criticality) level*

For the systems with liquid fuel and carrier (molten salt) the effective flux is decreased, as it spends a part of time (t_2) outside the system (primary loop with heat exchanger) as the ratio $t_1/(t_1 + t_2)$.

Continual re-fueling is modeled as follows: If F_n is the number of fissions at time point t_n, then $F_{n+1} = F_n - DF_n$, where DF_n is the decrease of F due to burning of fissile material between points t_n and t_{n+1}. The amount of F_{n+1} recovered from the requirement is $F_{n+1} \to F_n - DF_n + dF_n = F_n = \ldots F_0 = \text{const}$, that is the term $dF_n = DF_n$ is added to account for injection of liquid fuel at time point t_{n+1}. Keeping total fission rate in the system constant means that the sub-criticality level ($K_{\mathrm{s}} < 1$) is constant due to one of the basic relations (see below).

2.5 *Basic relations*

The following basic relations may be useful for sub-critical systems with an external source. The total proton current J (number of protons, $\mathrm{cm}^{-2}\ \mathrm{s}^{-1}$) relates to electric current I (ampere A) by the equation

$$J = I\,(A)/e \text{ (Coulomb)}.$$

Reactor thermal power is equal to

$$P(MW) = nI(A)E_{\mathrm{f}}\ (\mathrm{MeV})/\nu(1/K_{\mathrm{s}} - 1),$$

where n is the number of neutrons produced by each particle (proton) in the target, ν is the mean number of neutrons emitted per fission; E_{f} (= 200–210 MeV for U, Pu) – energy released in fission.

The neutron balance equation is

$$\nu + S/F + (n, 2n)/F = 1 + \alpha + q + q_{\mathrm{FP}} + x + L',$$

where S is the external neutron source, F is the number of fissions, C is the number of captures in all the materials; α is the mean ratio of capture/fission in fissile materials; q is the ratio of parasitic capture to fission rate F; q_{FP} is the ratio of captures in fission products (produced in fissile materials) to F, x is the ratio of useful captures to fissions F (in transmuted nuclides), $L' = L(1 + C/F)$, where L is the leakage of neutrons.

It may be noted that the greater the inventory of fissile materials in the system, the less is the value of q and the leakage term, which usually leads to the increase of neutron utilization factor x and hence the productivity of the system. Besides, x may be higher in sub-critical systems with the external source compared to critical ones due to the term S/F in the left-hand side of the above equation. Usually high flux is not needed for the transmutation of long-lived radio nuclides, except for comparatively short-lived species like ^{90}Sr or ^{137}Cs.

The number of nuclei N_{f} undergoing fission per year is determined from the balance relation

$$E_{\mathrm{f}}\ (\mathrm{MeV})C_{\mathrm{f}}N_{\mathrm{f}} = P(\mathrm{MW})3600(\mathrm{sec})24(\mathrm{hours})365(\mathrm{days}),$$

where

$$C_{\mathrm{f}} = 1.60214 \times 10^{-19}\ (\mathrm{MW \cdot s/MeV}).$$

Thus the mass of material undergoing fission per year equals

$$G_{\mathrm{f}} = N_{\mathrm{f}}A_{\mathrm{t}}/0.6022142 \times 10^{24}\ \mathrm{g/year}; \quad (A_{\mathrm{t}} - \text{atomic mass}).$$

2.6 *The kinetics of sub-critical system with external source*

The kinetics of sub-critical system with external source differs from the kinetics of critical reactor. This may be demonstrated for a reactivity jump δk $(t > 0)$ by a transition of the system from one power level to another:

$$F_1(t) = F \cdot f(t); \quad t > 0; f(0) = 1;$$
$$F(\infty) = (1 - K_s)/(1 - K_s - \delta k)$$

though the function $f(t)$ is different if only the prompt or the prompt and delayed neutrons are taken into account.

2.7 *Delayed neutrons in systems with circulating fuel*

When liquid fuel moves across the core and the heat exchanger and returns back to the core, a part of the neutron emitters decays outside the core so that the effective value of delayed neutron fraction β is decreased. Let the time interval be divided into points $0, t_1, t_1 + t_2, 2t_1 + t_2, 2t_1 + 2t_2, \ldots$, where t_1, t_2 are residence time of fuel inside and outside the core respectively. Liquid fuel moves inside the core in time intervals of $[0, t_1], [t_1 + t_2, 2t_1 + t_2], [2t_1 + 2t_2, 3t_1 + 2t_2], \ldots, [nt_1 + nt_2, (n + 1)t_1 + nt_2], \ldots$. Let t' be the time point for the production of a precursor of delayed neutron (with fraction β and decay constant λ) and t is a relative time point inside the nth time interval for emitting neutrons by this precursor. Then the probability to emit neutrons around time point t is equal to

$$\lambda\beta \exp[-\lambda(t_1 - t' + n(t_1 + t_2) + t)]\mathrm{d}t.$$

The total probability is the sum of integrals over all time intervals $n = 0, 1, 2, \ldots$. Taking an average of the above expression over time interval $[0, t_1]$, we get the following value for the effective fraction of delayed neutrons:

$$\beta_{\text{eff}} = \beta \left[1 - \frac{[1 - \exp(-\lambda t_2)][1 - \exp(-\lambda t_1)]}{\lambda t_1 [1 - \exp(-\lambda t_2 - \lambda t_1)]}\right].$$

3. Computer code TRIFON, version 2.1

Computer: IBM PC, PENTIUM (language FORTRAN-90, Compiler: Microsoft Developer Studio 4.0)

Physical problems solved:

- Calculation of space-energy neutron distribution in a reactor cell with arbitrary isotopic composition.
- Simulation of neutron chain transformations (burn-up processes).
- Calculation of heterogeneous parameters of cells.

Input includes data on geometry and isotopic cell composition (initial for the case of burnup).

Method of solution

- Neutron transport in every group is evaluated by the collision probability method (or modified CPM).

- Multi-group energy presentation is used with fixed number of groups, extended to a higher number of groups for special treatment of resonance absorbing nuclides.
- Thermalization problem is solved for the thermal neutrons.

3.1 *Resonance absorption*

An effective direct treatment of resonances is used for prescribed nuclides. Subdivision of lethargy scale into n intervals in a given lethargy interval (U_0, U_n) corresponds to uniform division of F – image of the function $F(U)$, that roughly estimates the absorption by all resonance nuclides from U_0 to U. This leads to the accumulation of lethargy points near the centres of resonances (see figure 1). As a result only few lethargy intervals are needed to describe absorption by a given resonance.

3.2 *Heterogeneous few-group matrix parameters*

Few-group (G groups) heterogeneous parameters of a reactor cell – Λ-matrix – is defined as a $G \times G$ matrix of boundary conditions, giving the relation between G – vector-flux N and G – vector-current $J \sim (\mathrm{d}N/\mathrm{d}\rho)$,

$$\rho \mathrm{d}N/\mathrm{d}\rho = \Lambda N, \tag{1}$$

where ρ is the cell radius.

Λ-matrix is determined from $G + 1$ series of cell calculations with zero and non-zero linearly independent few-group currents on the cell boundary.

The collision probabilities are the same for $G + 1$ tasks and are calculated only once; the differences in these tasks are only in some scalar parameters.

The Λ-matrix is split into two parts:

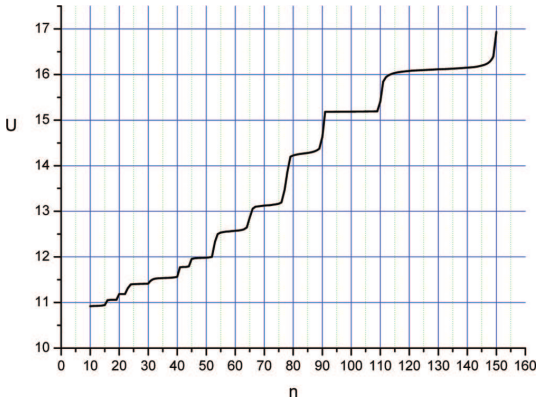

Figure 1. A typical non-uniform splitting of lethargy scale $U(n)$ for the PWR pin cell, n – number of groups.

$$\Lambda = \Lambda_1 + \Lambda_2, \quad \Lambda_1 = -\Lambda_1'/(1-\nu); \quad \Lambda_1' = \Lambda_2 N_0 \otimes q\Lambda_2;$$
$$\nu = k_0 - q\Lambda_2 N_0.$$

Λ_1' and ν linearly depend on the number of secondary neutrons released in fission, Λ_2 is a triangular matrix responsible for neutron absorption and slowing-down due to currents across cell's boundaries, k_0 is the multiplication factor, $N_0 - G$ is the vector of few-group fluxes on the cell boundary in the solution with zero currents, $q - G$ is the vector giving the contribution of neutron currents on the number of secondary neutrons released in fission, $\otimes$ is the tensor product. The reaction rate vectors RR are defined as

$$RR = RR_2 + H_0 \otimes q\Lambda_2/(1-\nu).$$

G-vector RR_2 depends on the absorption and slowing down of neutrons that leak in or out of the reactor cell, H_0 depends on the contribution of neutrons originated in fission for the case of the solution with zero currents across cell boundaries. Axial components of Λ-matrix are calculated by additional 'flux' determined by modified 'collision probabilities'. Λ-matrices and RR vectors are stored in exchange files as input data for 3D overall reactor calculations.

3.3 *Geometry*

- 1D multi-layer cylinder of finite height (CPM, an option-modified collision probability: neutron flux in each cylindrical layer is presented as a polynomial of arbitrary even power of space variable).
- 2D-(X, Y) systems of finite height composed of circular arcs and line segments (for example, clusters).

3.4 *Cross-section libraries*

ACMC system [5] addressing NJOY code to treat ENDF-B files has been developed. The processed libraries include multi-group cross-sections, resonance parameters, energy dependencies of cross-sections for thermal neutrons, transmutation chains for burnup calculations, fission product yields and energy release in fission. Cross-section library generation is possible with an arbitrary multi-group structure that may be changed to fine structure to account for resonance absorption for every specific variant. A system of special codes provides a possibility for the user to create and edit the language that is used for input data and the treatment of library and code instructions.

3.5 *Requirements for computer memory*

All arrays are described as allocate able and have changeable dimensions. Hence, the dimensions of solved problems actually depend on the computer memory only.

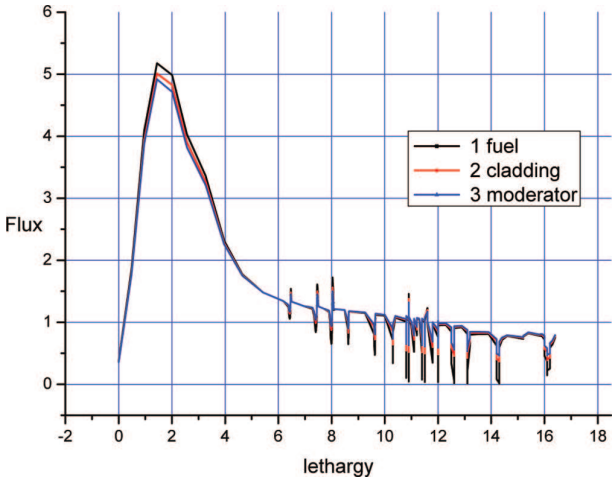

Figure 2. A typical flux distribution depending on lethargy (in 3 zones of PWR pin cell with MOX fuel) .

3.6 *Output of TRIFON*

- Space-energy distribution of neutron flux (depending on time if necessary).
- Reaction rates for all nuclides in all physical regions.
- Multiplication factor, leakage parameters.
- Few-group cross-sections.
- Λ-matrices, *RR*-vectors.
- Isotope mass balance as a function of burnup.

A typical flux distribution is shown in figure 2.

4. Computer code SHERHAN

The code is based on the advanced method of heterogeneous reactor theory (new formulation of heterogeneous reactor equations, their transformation from matrix to difference form and heterogeneous parameters of reactor cells). Effective multiplication factor, reaction rate distributions in 3D heterogeneous reactor with piece-wise non-uniform channels are calculated. Regular square or hexagonal lattice is allowed in a reactor of arbitrary shape in the x–y plane. The following heterogeneous reactor equation was derived:

$$N = (\nu + CFC^{-1}\gamma_1)N/k - CFC^{-1}\gamma_2 N; \quad F = K + IF;$$
$$\gamma_1 = CIC^{-1}\Lambda_1' + \gamma_2\nu; \quad \gamma_2 = C(IC^{-1}\Lambda_2 - \partial IC^{-1}), \tag{1}$$

where $K, I - (G \times K) \times (G \times K)$ is the $G - K$-diagonal matrix of the modified Bessel functions, $F - (G \times K) \times (G \times K)$ is the G-diagonal matrix of cell to cell

influence functions (modified Bessel functions, type K), C is a constant triangular matrix depending on moderator properties.

Operator-multiplicator

$$P_g : f_k \Longrightarrow (-\alpha_1\Delta_1 - \alpha_2\Delta_2 - \cdots + \beta\kappa^2\alpha^2)f_k; \quad \sum \alpha_i = 1,$$
$$\Delta_1 : f_k \Longrightarrow \sum_Q (f_{k+Qe_1} - 4f_k),$$

where $e_1 = (1, 0)$ is the unit vector and Q represents 0°, 90°, 180°, 270° turns 'cuts the terms of the full matrix F outside some fixed set of indices. Thus the product $R \approx P(\alpha, \beta)F$ becomes a local operator of a difference scheme'.

Then eq. (1) is transformed into an approximate difference equation:

$$P\varphi = P(\nu/k)\varphi + H(\gamma_1/k - \gamma_2)\varphi, \tag{2}$$

$$H = PD + R; \quad D = I^{-1}K.$$

For 3D problem the axial dependence is presented by finite Fourier expansion and eq. (2) symbolically remains the same.

The following procedures are included in SHERHAN code:

- determination of control rods positions bringing the reactor to critical state,
- flattening of radial power distribution based on:
  (1) parametric method of golden sections (GS),
  (2) a method incorporating the determination of influence functions depending on the reactivity introduced by movement of control rods using linear programming procedure (LP) to estimate,
- reactivity effects and control rod's worth,
- reaction rates balance,
- burnup simulation for a fixed set of time steps with reactor core elements reloading (interchange) or removal.

In the process of 3D burnup simulation the changing power distributions and position of control rods are shown in figure 3.

5. Testing of codes

The codes were tested by comparing the calculated results with other methods (including Monte-Carlo) and by comparing the results of critical experiments (VENUS-2). In the NEA/OECD benchmark for PWR pin-cell burnup simulation [6], the comparison of TRIFON results with the results of Iwasaki and Takano has shown that even for a burnup of 50 GWd/tHM the difference in isotope's number densities did not exceed 2–4%.

The results of TRIFON calculation of VENUS-2 experiment [7]: $K_{\text{eff}} = 0.9933$ and 0.9996 by TRIFON and SHERHAN respectively [8].

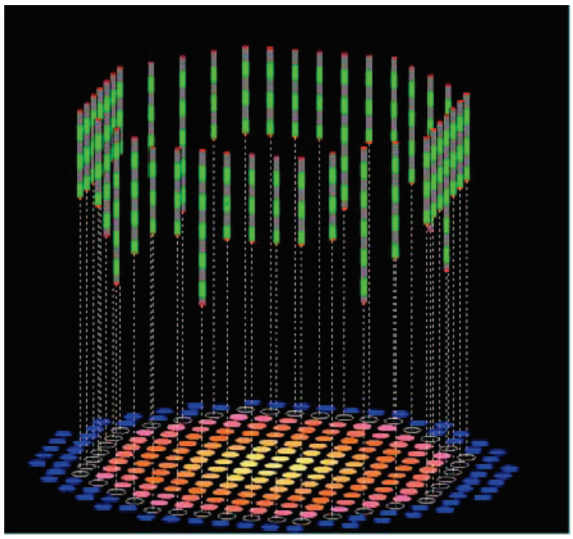

Figure 3. An example of power distribution and CR positions in the process of 3D burnup simulation (a model of fast lead-cooled reactor).

6. Conclusions

Some numerical methods for reactor cell, sub critical systems and 3D models of nuclear reactors are presented. The methods developed are for steady states and space-time calculations. Computer code TRIFON solves space-energy problem in (X, Y) systems of finite height and calculates heterogeneous few-group matrix parameters of reactor cells. These parameters are used as input data in the computer code SHERHAN solving the 3D heterogeneous reactor equation for steady states and 3D space-time neutron processes simulation. Modification of TRIFON was done for the simulation of space-time processes in sub critical systems with external sources. A version of the SHERHAN code for the system with external sources is under development.

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