RTS&T CODE STATUS

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Abstract

The paper describes the main features of the RTS&T2010 the modern version of the RTS&T (Radiation Transport Simulation and Isotopes Transmutation problem) code system [1]. The RTS&T code performs detailed Monte Carlo simulations of many type of particles transport in complex spatial geometries with composite materials in the energy range from thermal energy up to 100 TeV. The RTS&T code considers interaction of low-, intermediate-, and high-energy particles with condensed matter, including hadron-nucleus interactions inside the target, generation and transportation of secondary particles, deposition of energy and production of radionuclides in the target. Recently, the transfer of ions was added and tested. The modern version of the RTS&T code supports a researches in the fields of accelerator and reactor technologies, radiotherapy, space radiation, and in many other fields which are related to particle and ion transport phenomena.

INELASTIC HADRONIC AND PHOTONIC INTERACTIONS

Inelastic hadronic and photonic interactions are simulated within RTS&T code by several energy-dependent models based on the different microscopic and macroscopic approaches (Fig. 1) [2].

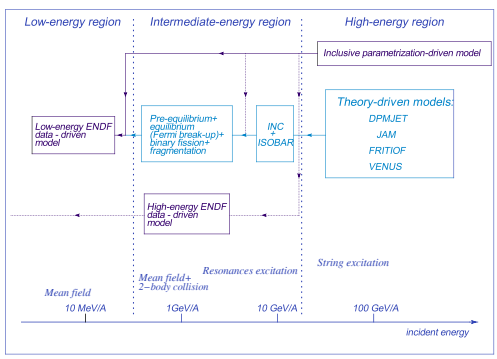

Figure 1: Inelastic hadronic and photonic interactions are simulated within RTS&T code by several energy-dependent models based on the different microscopic and macroscopic approaches.

High-Energy Region

To simulate of hadron(nucleus)-nucleus inelastic collisions at $E > 5$ GeV the modified versions of some micro-models (DPMJET-II/III, JAM, FRITIOF,VENUS, RQMD) or an inclusive parametrization-driven model can be used. These codes has been completed with a simulation of the nuclear destruction at fast stage of the interaction, with a calculation of the excitation energy of the nuclear residual nuclei and with a simulation of the nuclear relaxation stage in the framework of the statistical evaporation model to calculate the characteristics of the inelastic hadron-nucleus and nucleus-nucleus interactions at the energies higher 3-5 GeV per nucleon.

Intermediate-energy region

In the RTS&T calculations, the hadron-induced nuclear reaction process in the energy region about 20 MeV to 5 GeV is assumed to be a three-step process of spallation (intranuclear cascade stage), pre-equilibrium decay of residual nucleus and the compound nucleus decay process (evaporation/high-energy fission competition). To calculate the intranuclear cascade stage, the Dubna-version of intra-nuclear cascade model coupled with the Lindenbaum-Sternheimer isobar model for single- and double-pion production in nucleon-nucleon collisions and single-pion production in pion-nucleon collisions was provided. Recently, an addition of multiple-pion channels was included in code package to simulate up to 5 pions emission. The pre-equilibrium stage of nuclear reaction simulation is based on the exciton model. The initial exciton configuration for pre-equilibrium decay is calculated at the cascade stage of reaction or postulated in general input. The equilibrium stage of reaction (evaporation/fission processes competition) is performed according to the Weisskopf-Ewing statistical theory of particle emission and Bohr and Wheeler or Fong theories of fission. To calculate the quantities determining the total fission width, Atchison prescriptions are used.

Low-Energy Region

The RTS&T code uses continuous-energy nuclear and atomic evaluated data files to simulate of radiation transport and discrete interactions of the particles in the energy range from thermal energy up to 20/150/3000 MeV. In contrast with is a well-known and widely used Monte Carlo code MCNP [4, 5] for neutron, photon, and electron transport simulations, the ENDF-data driven model of the RTS&T code does access the evaluated data directly. In current model development, all data types provided by ENDF-6 format can be used in the coupled multy-particle radiation

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transport modeling. Universal data reading and preparation procedure allows us to use various data library written in the ENDF-6 format (ENDF/B VI/VII,JENDL, JENDL-HE, FENDL, CENDL, JEF, BROND, LA150, ENDF-HE/VI, IAEA Photonuclear Data Library etc.). ENDF data preprocessing (linearization, restoration of the resolved resonances, temperature dependent Doppler broadening of the cross sections and checking and correcting of angular distributions and Legendre coefficients for negative values are produced automatically with the Cullen's ENDF/B Preprocessing codes [3] LINEAR, RECENT, SIGMA1 and LEGEND rewritten in ANSI standard FORTRAN-90.

ISOTOPES TRANSMUTATION PART OF THE RTS&T CODE

The isotopes transmutation process is described by a system of balance ordinary differential equations. For the isotopes concentration N_i, where $i = 1, M$ (M is the total number of nuclides which to participate in connected transitions) the given system of equations is the following:

$$\frac{dN_i(t)}{dt} = -N_i \cdot \left(\lambda_i + \sum_k \int_0^{E_0^k} \sigma_i^k(E) \cdot \phi^k(E,t) dE \right) + \sum_{j \neq i} N_j \cdot \left(\lambda_{ji} + \sum_k \int_0^{E_0^k} \sigma_{ji}^k(E) \cdot \phi^k(E,t) dE \right) \quad (1)$$

$$N_i(0) = N_i^0,$$

where $\sigma_i^k(E)$ is summary cross section of reactions presenting the change of i-th nucleus structure, $\sigma_{ji}^k(E)$ is the partial cross sections of i-th isotopes formation reactions from j-th mother nucleuses under action of particles of grade k with the energy E, λ_i - disintegration constant of the i-th isotopes, λ_{ji} - disintegration constant of the j-th isotopes on the channels were presented to i-th nuclide formation; $\phi^k(E,t)$ is the particles of grade k with the energy E total flux, maximum significance of which is E_0^k. Breaking a period of exposition of a material on a number of temporary sessions with $\phi^k(E,t) \equiv \phi^k(E)$, we receive from (1) the independent system of equations with constant factors:

$$\begin{cases} \frac{dN_1}{dT} = C_{11}N_1 + C_{12}N_2 + ...C_{1n}N_n \\ \frac{dN_2}{dT} = C_{21}N_1 + C_{22}N_2 + ...C_{2n}N_n \\ \cdots \\ \frac{dN_n}{dT} = C_{n1}N_1 + C_{n2}N_2 + ...C_{nn}N_n \end{cases}$$

with

$$C_{ij} = \begin{cases} - \quad (\lambda_i + \sum_k \int_0^{E_0^k} \sigma_i^k(E) \cdot \phi^k(E) dE), i = j \\ \lambda_{ij} + \sum_k \int_0^{E_0^k} \sigma_{ij}^k(E) \cdot \phi^k(E) dE, i \neq j \end{cases}$$

Given system of equations can be recorded in a matrix kind:

$$\frac{dN}{dt} = CN, \quad N(0) = N_0. \quad (2)$$

Analytical decision (2) is

$$N(t) = \exp(Ct)N_0, \text{ where} \quad (3)$$

$$\exp(Ct) = \sum_{s=0}^{\infty} \frac{C^s t^s}{s!}, C^0 = E.$$

We shall note a number of the equation system (2) features:

1. Practically at any modes of exposition or endurance of any material the isotopes transmutation process contains both fast and slow making, and the distinction between them can reach 20 and more orders. Such spread of significance's of elements of a matrix results to its bad conditionally $[cond(C) >> 1]$ and allows to assume, that a system of equations (2) is "stiff". Correctly the definition of "stiffness" of the equation system requires the calculation of own significance's λ of matrix C, that reasonably is a difficult problem for large-size matrixes. Usually for these purposes a ODE system use the following criterion - the system is "stiff" if inequalities are executed:

$$||C||_1^{-1} << H \quad |Cp(C)|^{-1} << H \quad (4)$$

where H is the duration of exposition session or endurance, $||C||_1$ and $Sp(C)$ is the norm and trace of matrix C respectively: $\|C\|_1 = \max\limits_{1 \leq i \leq n} \sum\limits_{j=1}^{n} |c_{ij}|$, $Sp(C) = \sum\limits_{i=1}^{n} c_{ii} = \sum\limits_{i=1}^{n} \lambda_i$. Numerical integration of "stiff" systems any obvious discrete methods (Runge-Kutta, Adams and etc.) results in effect "error explosion" at the chosen step $h \geq \max(\|C\|_1^{-1}, |Sp(C)|^{-1})$. Given restriction from above on a integration step can result in unreal times of account when connected transitions (chains combined with nuclear reactions of radiation disintegration) contain nuclides with strongly distinguished life-times. Hence, application of standard methods of numerical integration non-stiff systems in an isotopes transmutation problem unacceptably.

2. The majority of specialized methods of numerical integration of "stiff" systems of equations are based on implicit discrete methods (Rosenbrok, Kollahan and etc.), which in case of a system with constant factors require calculations of a return matrix $(E + hC)^{-1}$, where h is the integration step, E - unit matrix. As the overwhelming majority of matrix C elements is considerably less than 1, reference (manipulation) of a given matrix is made with a large error, which grows with an increase of its size and with a reduction of

the integration step. Using of arithmetic with a floating point of double accuracy to isotopes transmutation problem solution does not remove this problem (for example, at radioactive disintegration of ^{235}U nuclei, $C_{ii} = 3 \cdot 10^{-17}$ and, in case of small h, even the operation of summation the diagonal elements of matrices E and hC already passes on limit of allowable accuracy by use of the 64 bits computers).

The marked specific of an isotopes transmutation problem limits the applicability discrete methods of numerical integration of ODE systems, that makes the their universal settlement circuit unsuitable for construction. Direct use of the analytical decision (3) at large times and bad conditionality of the matrix C results in unjustified quantity terms at calculation exhibitor and high error. For the decision of a system of equations (2) in RTS&T code the circuit of calculation $exp(Ct)$ was applied recurrent, which gives satisfactory results even in case of brightly expressed "stiffness" of a equations system (2) in a wide range of intervals of time h.

To construct recurrent of the calculation circuit $exp(CH)$, where H is the duration of the exposition session, the interval H is broken into a number of any uniform sections h. Then isotopes concentration in each discrete moment of time $tn = nh, n = 0, 1, ...$ are defined by the formula:

$$N_{n+1} = N_n \exp(Ch) \quad n = 0, 1... \tag{5}$$

To the exponential $exp(Ch)$ calculating the additional recurrent matrix equation construction is required. Such step $h^{'}$ is chosen, which satisfied to following conditions:

$$h^{'} = \frac{h}{2^K}, \qquad h^{'} \ll \min(\|C\|^{-1}, |Sp(C)|^{-1})$$

where K is any integer value. Having calculated on (3) $exp(Ch^{'})$, we can find $exp(Ch)$, applying consistently formulas:

$$\exp(2Ch^{'}) = \exp(Ch^{'}) \exp(Ch^{'}),$$

$$\ldots.$$

$$\exp(2^K Ch^{'}) = \exp(2^{K-1} Ch^{'}) \exp(2^{K-1} Ch^{'}).$$

We shall record these equations as the recurrent matrix equation:

$$\phi_{k+1} = \phi_k^2, \text{ where } \phi_k = \exp(2^k Ch^{'}), \quad k = 0, 1, ..., K; \tag{6}$$

Thus, it is possible to choose so small size $h^{'}$, that high accuracy of representation $exp(Ch^{'})$ by decomposition (3) with small number of the members (s) is provided no matter how. On the other hand, the use recurrent of equations (5) and (6) for the decision of a system (1) considerably reduces number of steps of integration for the given interval H:

$$\frac{H}{h} = 2^{-K} \frac{H}{h^{'}}.$$

That removes a "large times" problem in any isotopes mixes. Valuation of a relative error of the numerical circuit of the decision of an equation system (1) to be made according to the Runge rule: i.e. results received for the steps $h^{'}(K)$ and $h^{'}/2(K+1)$ are compared. As indicative isotopes transmutation process with brightly expressed "stiffness" of equation system the spontaneous disintegration of ^{235}U nuclei is chosen, where in connected transitionse both short-period with a half-life period $T_{1/2}$ about 1 sec (^{211}Po, ^{215}Po), and long-period (^{231}Pa, ^{235}U) isotopes participate. Besides the chain-length of U transitions makes more than 10 links, that can also demonstrate reliability of a settlement method at the "extreme stiff situation" (see Fig. 2).

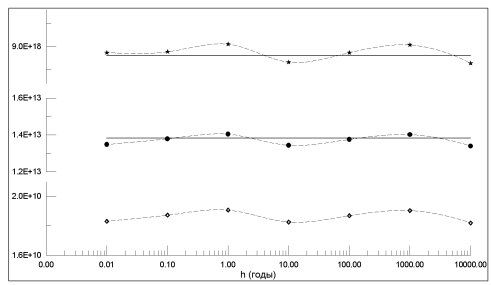

Figure 2: Dependence of settlement nuclear concentration of $^{211}Pb(\diamond)$, $^{227}Th(\bullet)$ and $^{231}Pa(\star)$ from a step of integration h at ^{235}U disintegration in current of 10000 years.

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