Monte Carlo Transport Codes for use in the Space Radiation Environment

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PHITS (Particle and Heavy Ion Transport code System)

(for availability see Reference 1)

PHITS (Particle and Heavy-Ion Transport code System) [1] is a general purpose particle and heavy-ion MC transport code which can transport neutrons from thermal energies up to 200 GeV. The 3-dimensional Monte-Carlo radiation transport code was developed with collaboration of several institutes including JAEA, RIST, KEK and Chalmers University of Technology. The same method as in the MCNP4C code [2] is employed for neutrons with energies between 1 meV and 20 MeV based on the Evaluated Nuclear Data such as the ENDF-B/VI [3], JENDL-3.3 [4,5]; and for p and n up to 3 GeV for the JENDL-HE [6,7] file.Above 20 MeV, the Bertini model with free p-p and n-n cross sections parameterized according to Niita et al. [8] is used up to 3 GeV, while the simulation model JAM (Jet AA Microscopic Transport Model) developed by Nara et al. [6] is used above 3 GeV for nucleons, above 2.5 GeV for pions, and for all energies for all other baryons. JAM is a hadronic cascade model, which explicitly treats all established hadronic states including resonances with explicit spin and isospin as well as their anti-particles. For protons and other hadrons, JAM is used above 1 MeV, but for charged particles below 1 MeV only the ionization process is considered until the particles are stopped. PHITS also uses Evaluated Nuclear Data for photon and electron transport below 1 GeV in the same manner as in the MCNP4C code based on the Ion Transport System (ITS) code, version 3.0 [9]. The energy range of electrons and photons is restricted to the energy region 1 keV - 1 GeV at the present, but the extension of the maximum energy of these particles is in progress. PHITS can also transport nuclei in any solid, gas or liquid material. Below 10 MeV/n, only the ionization process for the nucleus transport is taken into account, but above 10 MeV/n the nucleus-nucleus collisions up to 100 GeV/n is described by the simulation model JQMD (JAERI Quantum Molecular Dynamics) developed by Niita et al. [10]. In the QMD model, the nucleus is described as a self-binding system of nucleons, which are interacting with each other through the effective interactions in the framework of molecular dynamics. One can estimate the yields of emitted light particles, fragments and excited residual nuclei resulting from the heavy ion collision. The QMD simulation, as well as the JAM simulation, describes the dynamical stage of the reactions. At the end of the dynamical stage, excited nuclei are created and must be forced to decay in a statistical way to get the final observed state. In PHITS the GEM model [11] (Generalized Evaporation Model) is default employed for light particle evaporation and fission process of the excited residual nucleus.

When simulating the transport of charged particles and heavy ions, the knowledge of the magnetic field is sometimes necessary to estimate beam loss, heat deposition in the magnet, and beam spread. PHITS can provide arbitrary magnetic fields in any region of the setup geometry. PHITS can simulate not only the trajectory of the charged particles in the field, but also the collisions and the ionization process at the same time. For the ionization process of the charged particles and nuclei, the SPAR code [12] is default used for the average stopping power dE/dx, the first order of Molière model for the angle straggling, and the Gaussian, Landau and Vavilov theories for the energy straggling around the average energy loss according to the charge density and velocity. In addition to the SPAR code, the ATIMA package, developed at GSI [13, 14], has been implemented as an alternative code for the ionization process.

The total reaction cross section and the lifetime of the particle for decay, are essential quantities in the determination of the mean free path of the transported particle. According to the mean free path, PHITS chooses the next collision point using the MC method. To generate the secondary particles of the collision, we need the information of the final states of the collision. It is therefore very important that reliable data of total non-elastic and elastic cross sections is used for the particle and heavy ion transport. In PHITS, the Evaluated Nuclear Data is used for neutron-induced reactions below 20 MeV. For neutron-induced reactions above 20 MeV a parameterization is used. As for the elastic cross sections, the Evaluated Nuclear Data is also used for neutron-induced reactions below 20 MeV, and a parameterization is used above 20 MeV [8]. Parameterizations are also used for proton induced reactions for all energies, and for the double differential cross sections of elastic nucleon-nucleus reactions [8]. We have also adopted the NASA systematics developed by Tripathi et al., [15-17] for the total nucleus-nucleus reaction cross section, as an alternative to the Shen formula [18]. PHITS has been extensively used and benchmarked for many different application, including different space applications e.g. [19-29].

When estimating the biological damage of high energetic photons and charged particles, the contribution from the neutrons created both outside and inside the human must also be considered. It is therefore important to be able to calculate the kinetic energy distributions of the created secondary charged particles from photonuclear and neutron induced reactions. For low energetic neutrons, normally nuclear data is used. However, based on the one-body Bolzman equation, energy and momentum are not conserved in an event during the transport calculations. They are only conserved as an average over many randomly calculated events since the Bolzman equation only includes mean values of the one-body observables in the phase space and cannot give two-body and higher correlations. A feature has therefore been included in PHITS to treat low energy neutron collisions as "events" which means that the energy and momentum are conserved and make it possible to extract kinetic energy distribution of the residual nuclei, two particle correlations, etc. In PHITS, the transport algorithm has been changed for the low-energy neutrons from that on solving the Bolzmann equation to an algorithm based on an event generator. By using this event generator mode, energy and LET distributions for all charged particles, created by all charged particles and neutrons, can be calculated.

When estimating the direct biological effects of radiation, microdosimetric quantities, such as the lineal and specific energy, are better indexes for expressing the RBE of the primary and secondary particles in comparisons to the conventionally often used LET. Though, the use of microdosimetric quantities in macroscopic transport codes is limited because of the difficulty in calculating the provability distributions on macroscopic matter. Therefore mathematical functions, for calculating the microdosmetric probability densities in macroscopic material, have been incorporated in PHITS. This makes it possible to instantaneously calculate the probability densities of lineal and specific energies around the trajectories of high energetic primary and secondary charged particle tracks. A method for estimating the biological dose, the product of physical dose and RBE, for charged particles has also been established by using the improved PHITS coupled to a microdosimetric kinetic model [30-32]. Since the energy distributions of the secondary charged particles from neutron induced reactions can be estimated by using the "event generator" in PHITS, an estimation of the RBE of the neutrons can also be made. The accuracy of this will be evaluated in the near future.

References

[1] Niita K, Matsuda N, Iwamoto Y, Iwase H, Sato T, Nakashima H, Sakamoto Y, Sihver L 2010, PHITS: Particle and Heavy Ion Transport code System, Version 2.23, JAEA-Data/Code 2010-022.

Iwamoto Y, Niita K, Sakamoto Y, Sato T, Matsuda N 2007, Validation of the event generator mode in the PHITS code and its application, International Conference on Nuclear Data for Science and Technology 2007,

[2] J. F. Briesmeister, et al., MCNP General Monte Carlo N-Particle Transport Code, Los Alamos National Laboratory report; LA-12625-M (1997).

[3] V. McLane, et al., ENDF/B-VI Summary Documentation, BNL-NCS-17541 (1996).

[4] K. Shibata, et al., Japanese Evaluated Nuclear Data Library Version 3 Revision-3: JENDLE-3.3, J. Nucl. Sci. Technol. 39, 1125 (2002).

[5] Watanabe, Y. et al. Nuclear data evaluations for JENDL high-energy file. Proceedings of International Conference on Nuclear Data for Science and Technology, Santa Fe, USA, Sep.26-Oct.1, 2004; AIP CP769, p326-331, 2005.

[6] Nara, Y. et al. Relativistic nuclear collisions at 10A GeV energies from p+Be to Au+Au with the hadronic cascade model. Phys. Rev. C61:024901, 1999.

[7] T. Fukahori, et al., JENDL High Energy File. J. Nucl. Sci. Technol., Suppl. **2**, 25-30 (2002).

[8] K. Niita, H. Takada, S. Meigo, Y. Ikeda, High-energy particle transport code NMTC/JAM, Nucl. Instrum. Methods, B184, 406 (2001).

[9] J. A. Halbleib, et al., ITS Version 3.0: The Integrated TIGER Series of Coupled Electron/Photon Monte Carlo Transport Codes, SAND91-1634 (1992).

[10] K. Niita, et al., Analysis of the (N,xN') reactions by quantum molecular dynamics plus statistical decay model, Phys. Rev. C52, 2620 (1995).

[11] S. Furihata, Statistical analysis of light fragment production from medium energy proton-induced reactions, Nucl. Instr. and Meth. B171, 251 (2000).

[12] T. W. Armstrong, and K. C. Chandler, A Fortran program for computing stopping powers and ranges for muons, charged pions, protons, and heavy ions, ORNL-4869, Oak Ridge National Laboratory, (1973).

[13] H. Geissel, C. Scheidenberger, Slowing down of relativistic heavy ions and new applications, Nucl. Instr. Meth. B136-138, 114-124 (1998).

[14] C. Scheidenberger, H. Geissel, Penetration of relativistic heavy ions through matter, Nucl. Instr. Meth. B136-138, 114-124 (1998).

[15] R. K. Tripathi, F. A. Cucinotta, J. W. Wilson, Accurate universal parameterization of absorption cross sections, Nucl. Instr. and Meth. B117, 347 (1996).

[16] R. K. Tripathi, J. W. Wilson F. A. Cucinotta, Accurate universal parameterization of absorption cross sections II – neutron absorption cross sections, Nucl. Instr. and Meth. B129, 11 (1997).

[17] R. K. Tripathi, F. A. Cucinotta, J. W. Wilson, Accurate universal parameterization of absorption cross sections III – light systems, Nucl. Instr. and Meth. B155, 349 (1999).

[18] W. Shen, et al., Total reaction cross section for heavy-ion collisions and its relation to the neutron excess degree of freedom, Nucl. Phys. A 491 (1) 130-146 (1989).

[19] Sato T, Niita K, Iwase H, Nakashima H, Yamaguchi Y, Sihver L 2006, Applicability of Particle and Heavy Ion Transport Code PHITS to the Shielding Design of Spacecrafts, Radiat. Meas. 41, 1142-1146

[20] L. Sihver, D. Mancusi, K. Niita, T. Sato, L. Townsend, C. Farmer, L. Pinsky and I. Gomes, Benchmarking of calculated projectile fragmentation cross sections using the 3-D, MC codes PHITS, FLUKA, HETC-HEDS, and MCNPX", Acta Astronautica 63, 865-877 (2008).

[21] T. Sato, L. Sihver, K. Gustafsson, D. Mancusi and K. Niita, Shielding Design of Spacecrafts Using PHITS, American Nuclear Society Transactions, 99, 592 (2008).

[22] L. Sihver, T. Sato, K. Gustafsson, V.A. Shurshakov, and G. Reitz, Simulations of the

a. MTR-R and MTR Experiments at ISS, and Shielding Properties Using PHITS,
b. IEEEAC paper 1015 (2009).

[23] L. Sihver, et al., An update about recent developments of the PHITS code, Adv. Space Res. 45, 892-899 (2010).

[24] Sihver L, Sato T, Puchalska M, Reitz G 2010, Simulation of the MATROSHKA experiment at the international space station using PHITS, Radiat. Environ. Biophys. 49:3 351-357

[25] K. Gustafsson, L. Sihver, D. Mancusi, T. Sato, PHITS simulations of the Matroshka experiment", Adv. Space Res.46, 1266–1272 (2010).

[26] L. Sihver, M. Puchalska, T. Sato, T. Berger and G. Reitz, Monte Carlo simulations of MATROSHKA experiment outside ISS, IEEEAC paper 1585, ISSN: 978-142447350-2 (2011).

[27] T. Sato, et al., "Evaluation of Dose Rate Reduction in a Spacecraft Compartment due to Additional Water Shield", ISSN 0010_9525, Cosmic Research, Vol. 49, No. 4, pp. 319–324. © Pleiades Publishing Ltd. (2011).

[28] L. Sihver et al., Simulations of absorbed dose on the phantom surface of MATROSHKA-R experiment at the ISS, Adv. Space Res. 49, 230-236 (2011).

[29] M. Puchalska, L. Sihver, T. Sato, T. Berger, and G. Reitz, Simulations of MATROSHKA experiments at ISS using PHITS, Adv. Space Res. (accepted).

[30] Sato T, Endo A, Sihver L, Niita K 2011, Dose estimation for astronauts using dose conversion coefficients calculated with the PHITS code and the ICRP/ICRU adult reference computational phantoms, Radiat. Environ. Biophys. 50:1 115-123.

[31] T. Sato, Y. Kase, R. Watanabe, K. Niita, and L. Sihver, Biological Dose Estimation for Charged-Particle Therapy Using an Improved PHITS Code Coupled with a Microdosimetric Kinetic Model", Rad. Res. 171, 107-117 (2009).

[32] T. Sato et al., Analysis of Cell-Survival Fractions for Heavy-Ion Irradiations Based on Microdosimetric kinetic Model Implemented in the Particle and Heavy Ion Transport code System, Rad. Prot. Dos., 1-6, 2010.