Implementation of the CEM-Code into the MCNPX-Code

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Abstract

In the development stage of improving the physics abilities of MCNPX, the CEM code has been implemented into MCNPX as the nuclear reaction model for nuclei and pion induced reactions up to 5 GeV of kinetic energy.

The CEM code includes all the reaction stages of intra-nuclear cascade, preequilibrium and equilibrium and is an alternative for the existing MCNPX models.

The preliminary implementation fixes the uncompleted fission model of CEM by applying the RAL fission fragmentation model and provides a parameterized formula for the CEM input parameter a_f/a_n, the ratio of level density parameters at the fission saddle point shape and the compound shape of the excited nucleus. All the deficiencies are addressed in an improved CEM code that will replace the existing implementation when finished.

Thick target calculations employing lead and tungsten targets have been performed to validate the implementation and test the CEM models against the old MCNPX models.

1 Introduction

In an effort to develop a multi-particle transport code for high-energy physics applications with the functionality of the MCNP4B[1] code, the LAHET Code System (LCS)[2] has been merged with the MCNP4B code to create the MCNPX code.[3]

The MCNPX code is structured into two parts. In the low energy range, neutrons, photons, and electrons are transported mainly based on tabulated cross-section data, that have been used, tested, and improved over a long period of time. To transport high-energy particles, i.e. nucleons, anti-nucleons, mesons, and light ions, the code relies on

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the physics models of the LAHET code that are much less accurate than the tabulated data sets.

The enormous increase in interest in accelerator driven systems in the past few years has launched several international code comparisons[4,5] with the goal of pointing out the reliability of the codes and to make recommendations for improvements. In these code comparisons, the CEM[6] code has proven to be one of the best available tools to calculate nucleon and π-meson induced reaction cross sections and all types of production cross sections for incident particle energies up to 5 GeV. Furthermore the CEM code is presently in a phase of extensive testing[7] and improvement[8] with the use of newly available experimental data.

For these reasons, CEM has the potential to become the next generation nuclear reaction model in the MCNPX code, and has been implemented during the second stage of the code development dedicated to the improvement of the physics capabilities.

2 The MCNPX Nuclear Reaction Treatment

The MCNPX code uses various nuclear reaction models for different incident particle types and energies, all of the LCS. The models can be separated into an intra-nuclear cascade stage, a preequilibrium stage, and an equilibrium stage. In each stage secondary particles are created.

In the intra-nuclear cascade stage MCNPX uses the FLUKA89[9] model for kaons and antiparticles of any energy, and for nucleons and π-mesons above intermediate kinetic energies (about 3 GeV for nucleons and 2 GeV for mesons). The ISABEL model[10] handles light ions and is optionally used for nucleons and π-mesons in the intermediate energy range. The main model for nucleons and mesons in the intermediate energy range is the Bertini model.[11]

The residual compound nucleus resulting from the intra-nuclear cascade stage undergoes a preequilibrium stage[12] before it enters the equilibrium stage. In the equilibrium stage three deexitation channels compete: First, fragmentation of light excited nuclei described by the the Fermi breakup model,[13] second, evaporation of particles described by the EVAP[14] model, and third, fission reactions described by the RAL-fission model[15] or the optional ORNL fission model.[16]

The residual nuclei that result after a multiple loop of equilibrium deexitation undergo a final stage of gamma-deexitation with the PHT model.[2]

3 The CEM Nuclear Reaction Treatment

As in the LCS models of MCNPX, the nuclear reactions are modeled using an intra-nuclear cascade, preequilibrium and equilibrium stage.

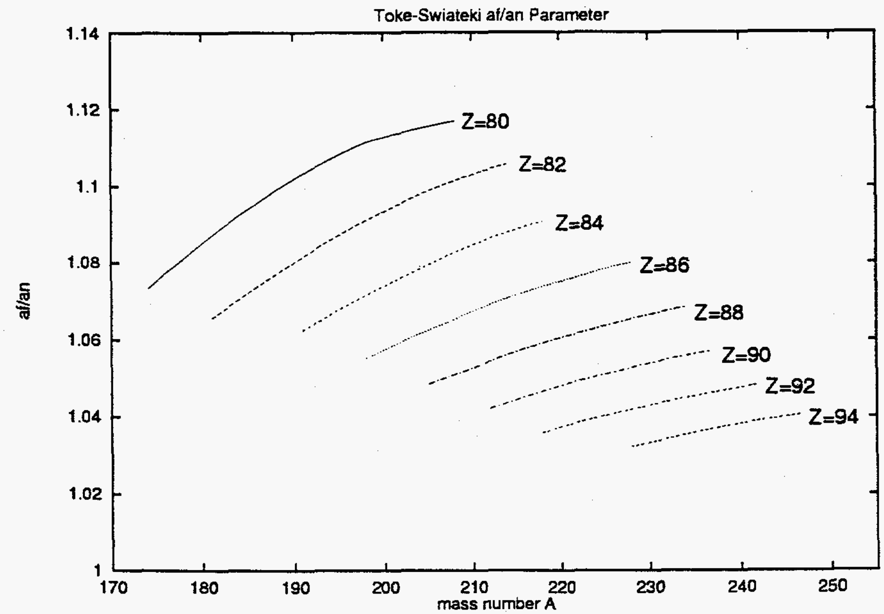

Figure 1: The a_f/a_n-parameter as a function of nucleus mass number A and proton number Z as calculated with the formulas given by Toke and Swiateki.[22]

The CEM code employs the standard Dubna ICM-model[17] as the intra-nuclear cascade model, and a modified exiton model for the preequilibrium stage and the evaporation channel of the equilibrium stage.[6] It is optimized for incident nucleon and pion particles with kinetic energies up to 5 GeV and for target materials consisting of carbon and heavier elements.

The implementation into MCNPX is based on a preliminary version of the CEM code, which includes many recent improvements to the standard CEM95 version.[18] These improvements are described in two contributions[8,19] presented in the SARE4-meeting.

This preliminary CEM version has a fission channel model that initiates the fission events, but lacks the fragmentation. In order to have an implementation, applicable to all kinds of target materials, the fission channel was completed by the RAL fission fragmentation using an existing MCNPX module. The fission fragments are feed back to allow further deexitation by particle evaporation. Furthermore, the CEM code requires the ratio of the level density parameters a_f/a_n of the nuclei at the deformed fission saddle point shape and the compound shape for calculating the fission channel width[20] to be user supplied. The ratio of level density parameters is material dependent, and has values in the range of 1.0 to 1.2. Although the range of possible values is restricted, the fission cross section has been found to be very sensitive to a_f/a_n.[21] To eliminate this parameter from the input list, a surface-layer corrected level density formula[22] was introduced into CEM using tabulated values of the integrated surface area and curvature of the deformed nuclei.[23] The implemented formula gives values of a_f/a_n versus the mass number A and proton number Z as shown in Fig. 1.

In the original CEM code, a_f/a_n is provided for the target nucleus at the start of the reaction and kept constant throughout the reaction. In the new modified version a_f/a_n is recalculated for each compound nucleus at the beginning of each step of equilibrium deexitation. In this way the a_f/a_n parameter fits the model much better.

Test calculations of reaction cross sections σ_{in} and fission cross sections σ_f for incident neutrons and protons with kinetic energies of 100 and 200 MeV for different target nuclei were performed to investigate the two options of the Iljinov's third level density formula[24] and the new Sierk approach.[8] The results in Table 1 show that the reaction cross sections calculated with the two level density options agree well, but the fission cross sections do not. Better values of fission cross sections for non-actinide nuclei are obtained using Iljinov's third level density formula, whereas better values for the actinide nuclei are obtained using the new Sierk formula.

4 Implementation of CEM into MCNPX

To obtain the best results, the CEM code was implemented into MCNPX with the parameterized a_f/a_n-formula, using Iljinov's third level density formula to calculate reaction channel widths for non-actinide target materials, and the new Sierk level density formula for actinide materials. The fission channel was completed by allowing fragmentation using the RAL modules. A final gamma deexitation stage is then performed for each residual nuclei exiting the equilibrium stage using the MCNPX-PHT model. To be able to easily exchange the present version of CEM with any improved new versions, the code was implemented as a closed module with defined interfaces to the MCNPX code.

The user interface of MCNPX has undergone only a minor change by adding a switch that allows to choose the CEM model as the nuclear reaction model for nucleons and pions. In terms of performance, a number of test calculations for different types of thin targets revealed that MCNPX using CEM consumes up to a factor of 8 more computing resources especially for heavy target materials.

5 Thick Target Test Calculation

Thick target test calculations have been performed with MCNPX comparing the new CEM nuclear reaction models against the old LAHET models.

The test problems simulated a 800 MeV proton pencil beam impinging on the base surface of a 60 cm long cylinder with 20 cm diameter. Natural lead and natural tungsten were chosen as target materials.

The calculated quantity of interest was the neutron leakage from the sides of the cylindrical targets comparing leakage spectra and the leakage profile along the cylinder axis. In both cases the new neutron cross-section tables[25] with an upper limit of 150 MeV were employed.

Table 1: Reaction cross sections σ_{in} and fission cross sections σ_f for incident neutrons(N) and protons(P) with kinetic energies of 100 and 200 MeV calculated with the completed CEM code comparing the two options of Iljinov's third[24] level density formula and the new Sierk approach with experimental values.

target	projectile	energy (MeV)	CEM-Iljinov's third σ_{in} (mbarn)	CEM-Iljinov's third σ_f (mbarn)	CEM-Sierk σ_{in} (mbarn)	CEM-Sierk σ_f (mbarn)	experimental σ_f (mbarn)	experimental energy (MeV)
U-238	N	100.	1679.	722.	1671.	1342.	1140.	120
		200.	1582.	553.	1621.	1268.	1180.	160
U-238	P	100.	1793.	1001.	1775.	1456.	1714.	100
		200.	1659.	711.	1708.	1364.	1615.	200
U-235	N	100.	1630.	487.	1657.	1351.	1500.	120
		200.	1634.	384.	1606.	1272.	1240.	380
U-235	P	100.	1757.	729.	1773.	1485.	1280.	23
		200.	1666.	559.	1629.	1313.	1443.	1000
Th-232	N	100.	1610.	32.	1663.	1217.	1030.	36
		200.	1605.	67.	1611.	1113.	900.	380
Th-232	P	100.	1759.	82.	1780.	1389.	1550.	80
		200.	1634.	130.	1637.	1187.	–	
Bi-209	N	100.	1524.	10.8	1530.	0.7	36	120
		200.	1471.	32.6	1529.	3.3	51	160
Bi-209	P	100.	1647.	63.5	1603.	2.8	103.4	100
		200.	1547.	98.6	1539.	6.6	158.9	200
Pb-208	N	100.	1544.	2.7	1522.	0.18	8	96
		200.	1512.	14.0	1508.	1.79	21	162
Pb-208	P	100.	1607.	21.3	1626.	1.1	36.6	100
		200.	1496.	37.4	1536.	4.3	75.5	200

The results are given in Fig. 2. The neutron spectra calculated with the old LAHET models seem almost indistinguishable from the calculations with the CEM models. However, the plot of the ratios of the spectra obtained with the CEM models and the spectra obtained with the LAHET models for the lead and tungsten targets reveals that CEM produces up to 20% more neutrons in the energy range of 10 to 100 MeV, and about 20 to 30% less neutrons in the energy range 1 to 10 MeV than LAHET. The plots of the neutron leakage profile show that the leakage calculated with CEM is generally somewhat lower in the first third of the cylinder compared to the calculation with the LAHET models, and is slightly higher over the remainder of the cylinder. The nuclear reaction cross sections of the CEM model seem to be lower than those of the LAHET models.

6 Conclusion and Outlook

The test calculations prove CEM working within the framework of MCNPX. The 20 to 30% differences in the leakage spectra when comparing with the original LCS reaction models of MCNPX of are in the range of what one expects.

Some improvements have to be made to speed up the CEM reaction models to make them competitive with the present MCNPX reaction models.

An improved CEM code is presently in development at LANL to address the deficiencies of the preliminary CEM version. This improved version will replace the presently implemented version as soon as it is finished.

Finally, it should be noted that CEM has the capabilities of calculating photo-nuclear reactions. This would be a beneficial extension of the MCNPX physics abilities in the future.

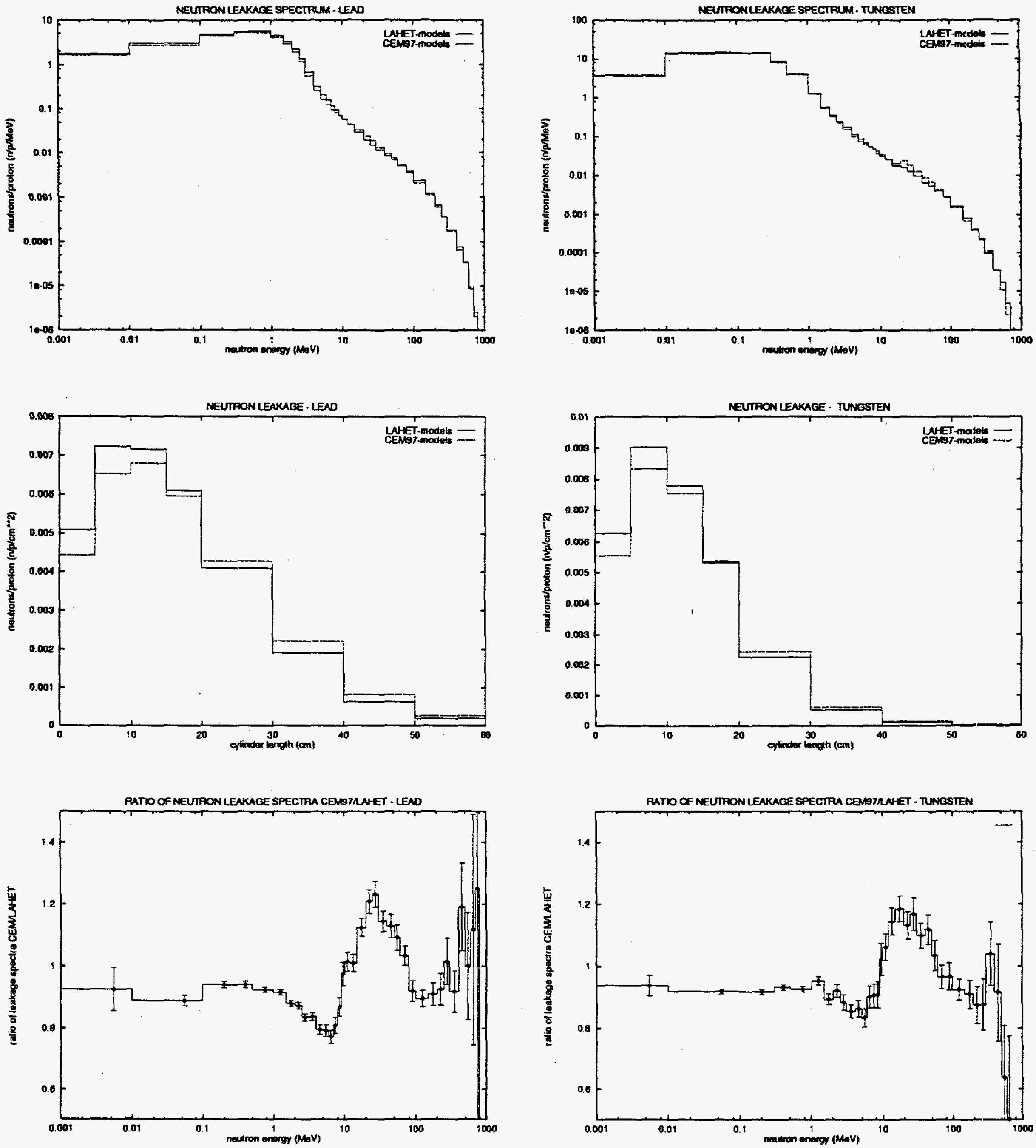

Figure 2: The neutron leakage spectra from the side surface of a target cylinder calculated with MCNPX using the CEM-models and the LAHET-models, respectively; the ratio of the CEM-spectrum and the LAHET-spectrum; and the neutron leakage of the side surface versus the cylinder length. Data are provided for the two target materials lead and tungsten.

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