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A Code System for ADS Transmutation Studies

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Key words: ADS, codes, spent fuel

Introduction

An accelerator driven reactor physical system can be divided into two different subsystems. One is the neutron source the other is the subcritical reactor. Similarly, the modelling of such system is also split into two parts. The first step is the determination of the spatial distribution and angle-energy spectrum of neutron source in the target region; the second one is the calculation of neutron flux which is responsible for the transmutation process in the subcritical system. Accelerators can make neutrons from high energy protons by spallation or photoneutrons from accelerated electrons by bremstrahlung (e-n converter). The Monte Carlo approach is the only way of modelling such processes and it might be extended to the whole subcritical system as well. However, a subcritical reactor may be large, it may contain thermal regions and the lifetime of neutrons may be long. Therefore a comprehensive Monte Carlo modelling of such system is a very time consuming computational process. It is unprofitable as well when applied to system optimalization that requires a comparative study of large number of system variants. An appropriate method of deterministic transport calculation may adequately satisfy these requirements.

Thus, we have built up a coupled calculational model for ADS to be used for transmutation of nuclear waste which we refer further as M-c-T system. Flow chart is shown in Figure.

Components of the M-c-T system

Source calculation in the target region

Recently, the particle transport codes in the intermediate energy range (from 20 MeV to 3 GeV) are undergoing intensive development. The first code, the L(ahet) C(ode) S(ystem)[1], coupling the high energy transport code HETC with low energy (under 20 Mev) MCNP, was made available some years ago. Nowadays, it seems, that the MCNPX code[2] supersedes LCS by enabling the full tally capabilities of the

MCNP code[3] in the whole energy range of interest and in the same time it includes the newest nuclear reaction models.

Though both LCS and MCNPX are applicable to modelling of spallation neutron source, however, none of them has capability for bremstrahlung photoneutron production. This is planned to be included into a new release of MCNPX which in this moment is not available. Also, evaluated photonuclear data were appeared in a processable form only in the last year. Therefore, in order to investigate photonuclear process as a possible neutron source for ADS, the MCNP4B, MCNP4C and later the MCNPX were enhanced with photonuclear capability by our specially elaborated patches[4] and a peripherial program has been created for including the available photonuclear data into the MCNP photon table.

In our first version of M-c-T system the LCS and MCNP (enhanced with photonuclear capability) were used for spallation and e-n converter calculations, respectively. Both produce low energy neutron source file in RSSA format as defined in MCNP code. Now, they can be both succeded by MCNPX which is also enhanced with photonuclear capability in the above mentioned way.

In the course of system study one must investigate the actual boundary of target region. This is not by all means the boundary of target itself, rather the boundary across which the current of neutrons of energy over 20 MeV is negligible. In order to check the fulfilment of this condition the current of neutrons over 20 MeV through the boundary of the target region must be tallied. Therefore, special trying calculations should be performed in order to establish the boundaries of the source region.

Flux calculation in the whole system

The flux in the subcritical reactor induced by the spallation or photoneutrons is calculated by means of three-dimensional, S_N code TORT[5]. The main advantage of the discrete ordinates method over Monte Carlo approach is in shorter computing times when the system is large, change of flux in the whole system is more order of magnitude and the lifetime of neutrons is long. In particular, if there is a rotational symmetry the calculation will be yet faster.

Because the neutron spectrum in a subcritical system is strongly space-dependent the preparation of few-group constants for TORT needs special attention. Therefore, instead of using any prefabricated multigroup library, we set out from the evaluated nuclear data JEF2.2 which are to be processed with the NJOY[6] code. The GENDF output of NJOY is converted to MATXS format. The macroscopic constants (in GIP format) for TORT calculation are prepared from composition data and from MATXS file by means of the TRANSX code[7]. Isotope generation multigroup cross-section library (TMDEFI file) for calculation of composition changes is created by means of a TIBSO module.

Source for S_N code from Monte Carlo output

The accelerator generated neutrons form a volume source to be placed in TORT calculation process. The data for space, angular and energy distribution of this source are contained in the RSSA file produced by any of the above Monte Carlo codes. From these data a multigroup source strength distribution defined in TORT mesh points is to be created.

As a first step the RSSA file is processed by the interface program DISTRAO. It averages the continuous space energy distribution of neutrons obtained from the

Monte Carlo process over the mesh volumes and group energy intervals. The result of averaging is written to a file of FLXMOM format defined in the TORT package. However, the coordinate system and/or the computational platform of target region calculation may be different from those which will be used by TORT. Therefore, a second interface program, FLXDB, is needed in order to perform the required coordinate transformation and/or binary to ASCII and ASCII to binary conversion that may be required by platform change.

Once a source distribution for a target region is obtained (by a long term computing process), many variants for subcritical reactor combinations can be investigated in a relatively low computing cost.

Because the result of Monte Carlo calculation is used as a volume source rather than a surface current, there is no need to transport neutrons under 20 MeV inside the target region by Monte Carlo method. The transport of neutrons under 20 MeV is performed by TORT in the whole system.

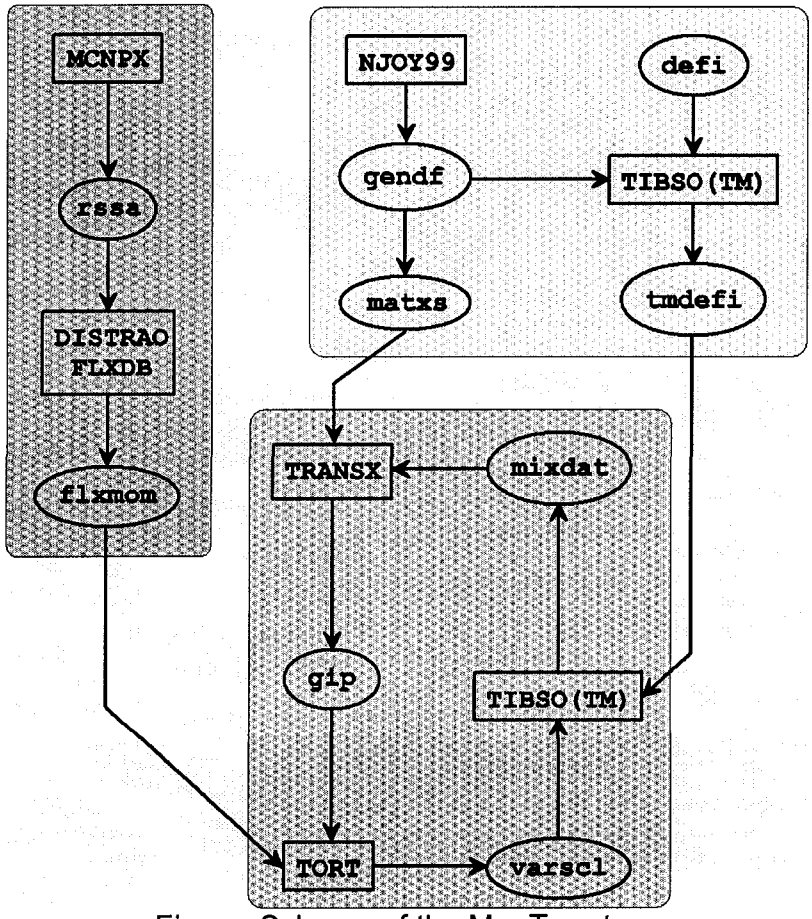

Figure. Scheme of the M-c-T system

Calculation of isotope composition

Reactor systems fueled with flowing mixtures of solved actinides will be an important issue of our investigations. In this case, it is assumed that the composition of mixture may be a subject of continuous control in the outside part of the loop. That is some of fission products may be continuously removed and new actinides may be added.

Such chemical intervention can hinder the build-up of the equilibrium decay chains so the usage of an ORIGEN type[8] code for calculation of isotope composition in

different parts of system is discouraged. Therefore, we intend to use the multinodal TIBSO code[9] for this purpose. The TIBSO code can continuously update its activation cross-section library according to the change of flux in different part of system.

Course of calculation

Source calculation, either spallation or e-n converter, is a time consuming procedure but it should be performed only once if the subcritical system is to be optimalized. The group constant preparation with NJOY from evaluated data is also made in the beginning.

The TRANSX ⇒ TORT ⇒ TIBSO... series (see Figure) is to be performed many times until an equilibrium composition is obtained. TORT calculation produces a flux in the subcritical system in a VARSCL file. Using this flux TIBSO calculates the new isotope compositions in the system (MIXDAT file). TIBSO also takes the manipulation on composition performed in the outside part of the loop into account. The new macroscopic constants, obtained from TRANSX are fed back to TORT.

Application of M-c-T system to concrete ADS is in progress.

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