Validation of deterministic methods for XADS by MCNP code

A. Travleev, C.H.M. Broeders, R. Dagan

Forschungszentrum Karlsruhe
Institut für Reaktorsicherheit

Postfach 3640
D76021 Karlsruhe

travleev@irs.fzk.de

1. Introduction

The neutron physics analysis of modern reactor concepts such an ADS requires new methods of calculations. The MCNP code [1], based on the "natural" Monte-Carlo method for modeling neutron transport inherits from this method a possibility to represent complicated geometry, including vacuum, which is still a critical issue for deterministic methods. Moreover, common Monte-Carlo method does not make use of adjoint flux, which is very important for modeling of source driven sub-critical systems, such as ADS. In contrary to these advantages, MCNP cannot be used for transient calculations, since it requires usually much more CPU time than deterministic codes. Nevertheless, this code is very well suited for validation of deterministic models and methods.

This paper describes the evaluation of MCNP capabilities applied to a Lead Bismuth Eutectic (LBE) cooled experimental ADS (XADS) concept proposed by ANSALDO [2] in the project PDS-XADS of the 5. European Community Framework Program, and the validation of models suitable for deterministic methods.

2. LBE cooled XADS model proposed by ANSALDO

The MCNP model that describes the XADS concept [2] was developed by ANSALDO and represents the reactor very detailed (pin-wise structure, temperature distributions). Not all this information is necessary for neutron physics analysis of the core. Moreover, this model cannot be directly transferred into a form suitable for deterministic codes, e.g. required for transient calculations. Therefore some simplifications are necessary; as for instance fuel assembly (FA) homogenization, simplification of material compositions. The validity of such simplifications is investigated by direct comparison of MCNP results for initial (complicated) and simplified models.

2.1. Temperature effects

The initial model represents the "hot" stage of the XADS: the fuel has a temperature of 900 K, while the coolant and the structure temperature lies in the interval 570 – 780 K. Applying equal temperatures to all materials will simplify the model significantly. Here the impact of this simplification on K_{eff} is estimated.

The temperature of a material is defined in MCNP separately for different aspects of neutron transport:

- Temperature dependant data libraries are supplied for the resonance Doppler broadening
- For the free-gas approach of elastic scattering, other temperatures than in the data library can be specified (this value is supplied in MCNP input deck by "TMP" card), which defines the target nucleus velocity with which a neutron interacts.

- As density of materials depends also on temperature, we consider K_{eff} dependence on coolant and construction material density as part of temperature dependence.

Calculations show that the most important aspect that cannot be neglected is the Doppler broadening for fuel isotopes, which leads to change K_{eff} to 0.0059. Other aspects – temperature for free-gas approach and density of coolant and structure are of less importance and the change of K_{eff} due to these aspects are of order of magnitude less than that caused by Doppler broadening.

2.2. Homogenization effects

In order to turn to a homogeneous XADS model a set of modifications are performed for the detailed pin-wise model.

- Modifications on FA level:

1. Homogenization of the FA's interior except the FA wrapper. In this step 90 fuel pins and the central support pin are mixed with coolant inside the FA's wrapper.
2. Homogenization of the FA's wrapper. In this step it is mixed with the interior mixture, obtained in the previous step.
3. Homogenization of the coolant, adjacent to the FA's wrapper. After this step the whole homogenized FA is represented by one material.

After these modifications the core consists of homogeneous assemblies: 120 fuel assemblies, 162 empty assemblies and 12 absorber assemblies.

- The last modification is made on the core level:

4. Transition from hexagonal core structure to a cylindrical one. External radii of fuel zone, empty assemblies zone and absorber zone are chosen in the way that sectional areas of each material are preserved.

The calculations have shown that the biggest bias to K_{eff} is introduced by the first step – about 0.007. The difference in K_{eff} for pin-wise and homogeneous cylinder model, i.e. effect of all homogenization steps is 0.0071 (see table 1).

2.3. Vacuum modeling

The numerical scheme of a variety of deterministic codes may become unstable when void (vacuum) zones are introduced. Therefore the impact of the beam pipe vacuum tube to the criticality is estimated by MCNP. The difference in K_{eff} for models with vacuum and without (i.e. the beam pipe was filled up with LBE) is 0.00146.

3. Assessment of dynamics characteristics

The definition of dynamics parameters of the reactor, such as reactivity, delayed neutron fraction, neutron generation time is well established for critical systems in using the adjoint flux in deterministic methods. Since this approach is not valid for sub-critical systems [3], new solutions should be found for these calculations. Here the possibility to use the MCNP code for the assessment of the dynamics parameters is discussed.

3.1. Taking into account the external source

A MCNP calculation of the K_{eff} value for a multiplying system ("kcode" run) is valid only for critical systems. To represent a real sub-critical system with nonzero power level, one should take into account an external neutron source. Therefore, MCNP predictions for sub-critical systems when "kcode" option is used are valid only in the case of external source spatial and energy distribution equal to the fission source distribution of a critical system. Nevertheless, it is possible to estimate the multiplica-

tion factor of a sub-critical system with arbitrary external source, using “fixed source” mode of MCNP. Performed calculations show that the “fixed source” mode predicts the same K_{eff} value as the “criticality mode” if the form of the external source is equal to the distribution of fission neutrons from “criticality mode”. Two approaches for calculation of K_{eff} in terms of tallied values were considered [4]. However, the question of uncertainty of K_{eff} values obtained by these approaches is still open.

3.2. Delayed neutron fraction

For reasons discussed previously, the use of the common adjoint based method is not recommended for the calculation of the delayed neutron fraction in ADS. It is preferable to use another method, which shifts the accuracy of the calculation to the definition of the neutron yield per fission, commonly symbolized by v. The neutron yield is specified on the basic cross section data library for prompt neutrons as well as for the delayed ones. An improved treatment of delayed neutrons in the last version of MCNP [5] allows using this code for beta effective calculation. This means that one can perform a criticality calculation using the prompt neutron yield v_p and then successively repeat the calculation with a total neutron yield v_t. The difference between the two K_{eff} values introduces the value of β. Although this method could be too time-consuming for dynamic simulations, it is a good procedure to validate faster deterministic codes. Actually, a comparison of MCNP results with the results of deterministic solutions in KARBUS-E [6] is in progress after the implementation of these features in this code system. However, this method itself requires still careful theoretical and experimental validation.

3.3. Neutron generation time

In the following the value of the generation time obtained by deterministic codes is compared for source free cases to the one calculated in MCNP. This procedure is very important for source driven systems since it can evaluate the accuracy of the approximated generation time value suggested below for deterministic codes, based on MCNP “adjoint” free evaluations. Yet one has to check carefully what is the exact physical meaning of the suggested method in MCNP for “generation time” estimation due to the fact that it is a stochastic method. It should be mentioned that MCNP calculates different estimations of prompt neutron lifetime. Also, average times of neutron escape, capture, fission (so called “lifespans”) are estimated. It was observed, that lifespan of fission, calculated for the homogeneous XADS model is very close to the results of deterministic procedures (table 1), while other estimations (average time to escape and capture) are of the order of magnitude bigger, since in more extent affected by large reflector.

4. Summary

The validation of deterministic models of XADS performed by MCNP calculations shows acceptability of homogeneous representation of XADS for the current step of investigations. Calculations with different temperature modeling revealed a big importance of proper Doppler effect, while other aspects of temperature representation can be neglected. On the base of presented results in section 2, other XADS configurations have been investigated in FZK/IRS.

The assessment of dynamics parameters using MCNP is promising for sub-critical reactors but requires additional investigations.

ACKNOWLEDGEMENTS

Part of the presented work was funded in the 5. Framework Program of the European Community, contract number FIKI-CT-2001-0017.

5. References

[1] J.F. Briesmeister, Editor, "MCNP – A General Monte Carlo N–Particle Transport Code, Version 4C", LA-13709-M, Manual

[2] XADS Experimental Accelerator Driven System, ADS 1 SIFX 0500 – Rev. 0 June 2001, ANSALDO NUCLEARE Division of Ansaldo Energia SpA.

[3] R. Dagan, D.G. Cacuci, C.H.M. Broeders, "On the Use of Perturbation Theory for Dynamic Simulation of Accelerator Driven Systems", 17th ICTT, July 08-14 2001, London.

[4] R. Dagan, A. Travleev, C.H.M. Broeders, "Neutronic analysis of an XADS using Stochastic and Deterministic Numerical Methods", Internal IRS report.

[5] C.J. Werner, "Simulation of Delayed Neutrons Using MCNP", Progress in Nuclear Energy, Vol. 41, No. 1-4, pp. 385-389, 2002.

[6] C.H.M. Broeders, R. Dagan, V. Sanchez, A. Travleev, "KAPROS -E: a modular program system for reactor analysis, status and results for selected applications", submitted to Jahrestagung Kerntechnik May 2003 Berlin.

Table 1. Difference in K_{eff}, caused by homogenization. Last column shows the standard deviation of the difference.

step, i	description	K_i-K_{i-1}	σ
1	Homogenization of fuel pins and coolant inside FA wrapper	$-6{,}96\ 10^{-3}$	$5{,}9\ 10^{-4}$
2	Homogenization includes FA's wrapper	$-1{,}67\ 10^{-3}$	$5{,}9\ 10^{-4}$
3	Homogenization includes coolant between assemblies	$-5{,}79\ 10^{-4}$	$6{,}0\ 10^{-4}$
4	Cylindrical core	$2{,}10\ 10^{-3}$	$5{,}9\ 10^{-4}$
	total effect K_4-K_0	$-7{,}11\ 10^{-3}$	$5{,}9\ 10^{-4}$

Table 2. Mean generation time obtained by deterministic procedures, compared with mean time of fission from MCNP run.

method	mean generation time, $*10^{-6}$ sec., calculated for different fuel temperatures.	
	300 K	*900 K*
Transport based fluxes (TWODANT)	2.106	2.021
Diffusion based flux (CITATION)	2.105	2.024
"lifespan" parameter (MCNP)	2.123	2.047