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Physics Investigations for Innovative Nuclear Reactor Systems

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Abstract

In this contribution the actual status at FZK for the physics investigation of proposals for the design of innovative reactor systems is presented. At present two such systems are under investigation: the High Performance Light Water Reactor (HPLWR) and accelerator driven sub-critical systems (ADS). Available calculation tools, ongoing validation efforts and improvement of the dynamic simulation of ADS are discussed in some detail.

Zusammenfassung

In diesem Beitrag wird der aktuelle Status der Arbeiten im FZK für die physikalische Untersuchung von Entwürfe für innovative Reaktorsysteme beschrieben. Z.Zt. werden zwei solcher Systeme betrachtet: der „High Performance Light Water Reactor“ (HPLWR) und beschleuniger getriebene unterkritische Anordnungen (ADS). Die eingesetzten Rechenprozeduren, die laufenden Validierungsuntersuchungen und Verbesserungen für die dynamische Simulation von ADS werden eingehend diskutiert.

1. Introduction

An important issue of the R&D program NUKLEAR at FZK is to maintain the capability to analyse the physical characteristics of proposals for innovative nuclear reactor systems. For this purpose adequate state-of-the-art calculation tools have to be kept operable and must be validated as well as possible for the intended applications. At present two quite different innovative nuclear reactor systems are under investigation:

- High Performance Light Water Reactor (HPLWR) with main objective to improve the efficiency factor of modern light water reactors (LWR) by the use of supercritical water as coolant, a solution already applied in conventional steam generating power plants.
- Accelerator-driven sub-critical reactor systems (ADS) for use for the incineration of nuclear wastes. ADS may play an important role in the future for closing the back-end of the nuclear fuel cycle.

In section 2 a more general overview of the main calculation tools for reactor physics investigations is presented. In section 3 validation work in progress is discussed. Improvements for the dynamic simulation of ADS are discussed in section 4. Section 5 gives a summary and an outlook for future work.

2. Calculation tools for reactor physics investigations

FZK has a long tradition with own developments of multi-group calculation tools for fast reactor research. The investigation for a high converter LWR with MOX fuel (APWR) in the eighties complemented these procedures with specific solutions for epithermal and thermal reactor systems. For fuel irradiation and depletion calculations the programs KORIGEN [1] and BURNUP [2], based on the well-known one-group code ORIGEN [3] from Oak Ridge, USA, have been developed and extensively validated. All these computer codes and libraries are accumulated in the FZK/INR development of the fully modular code system KAPROS [4] and its sub-system KARBUS [2]. After a long period of strong coupling of these codes with FZK-specific hardware and software resources, which made them practically non-transferable, recently a portable version for UNIX workstations was completed. Actually, KAPROS/KARBUS is running now on IBM RS6000 machines with AIX OS and on INTEL based PC with LINUX OS.

Alternatively to the multi-group procedures, the Monte Carlo methods become of increasing interest due to their ability to describe complex geometries and to utilize continuous energy resolution. The former drawback of Monte Carlo codes to be very computing time consuming is of decreasing importance because of the strongly increasing speed of modern computers. FZK relies since many years on international available Monte Carlo programs, especially on the MCNP code, continuously in development at Los Alamos National Laboratory, USA. At present two lines of MCNP are in use at FZK:

- Version MCNP4C [5] for fission and fusion reactor applications.
- Version MCNPX-2.1.5 [6] for ADS applications. MCNPX combines most of the features of MCNP4C with the Monte Carlo techniques to describe the physics of the spallation processes in the energy regions of interest for ADS. Moreover, FZK participates to beta-testing of MCNPX (actual version MCNPX-2.3.3).

An essential aspect of the use of calculation tools for innovative reactor concepts is their validation for these applications. This can be performed both by comparisons with

alternative computation routes and with experimental data. However, confirmation of calculation procedures by relevant experimental results is indispensable. For this reason a number of actual tasks for the development of reactor physics codes is devoted to experimental validation. For this experimental qualification a number of projects in the framework of international cooperation are in progress, mainly within the 5. framework program (FP) of the European Community (EC) and in collaboration with the International Science and Technology Center (ISTC) in Moscow. The ISTC aims to coordinate the work of eastern nuclear weapon specialists in civilian projects, being partly funded by western partners.

3. Validation work in progress

3.1 HPLWR.

From the neutron physics point of view, the relevant consequence of supercritical water as coolant in a LWR is the strong axial variation of the coolant density. Although counter-measures like isolated water-moderator or solid-moderator rods are considered, these axial and radial variations lead to the need for careful validation of the applied calculation tools. At the present stage no experimental data for such fuel assembly configurations are available and validation work is restricted to code comparisons. At FZK it is planned to utilize multi-group procedures for the HPLWR design investigations, including reactivity coefficients and burn-up behaviour. As a first step benchmark investigations for different axial zones of the fuel assembly are in progress in cooperation with partners from CEA, France, VTT, Finland and KFKI, Hungary within the 5. EC FP [7]. At FZK Monte Carlo calculations with MCNP4C have been started for the complex full layout of a fuel assembly. Comparison with simplified MCNP4C models from VTT show good agreement if the same cross section database is applied. As next steps cross section data influences will be investigated and a simplified model for multi-group calculations has to be defined.

An additional complication for HPLWR design investigations is the strong feedback between the thermo hydraulic and the neutron physics design. For this reason automatic coupling of thermo hydraulic codes like RELAP5 [8], COBRA-IV [9] or other, more simplified models [10], with neutron physics codes is in progress. This will be realized by a loose coupling of the stand-alone thermo hydraulic codes with the modular KAPROS/KARBUS system.

3.2 ADS.

The validation of calculation tools for accelerator driven sub-critical systems is a challenging task because no real experience is available so far with such systems where the proton beam of a powerful accelerator has to be guided into a high power spallation target within a sub-critical reactor system. Several aspects have to be verified:

- Impact of a strong neutron source in a sub-critical reactor system.
- Characteristics of the spallation target.
- Coupling of the spallation target and the sub-critical reactor system.

At present projects related to these three aspects are in progress.

3.2.1 Impact of a strong neutron source in a sub-critical system

Two complementary experiments for the investigation of the effects of a neutron source in a sub-critical system are in progress:

- In the ISTC project B70, performed in Minsk/Sosny, Belarus, a powerful neutron generator with 14 MeV neutrons is coupled with a low-power sub-critical thermal reactor system with the objective to study the behaviour of the sub-critical system and to perform integral cross section measurements for important isotopes of the back-end of the nuclear fuel cycle. FZK is collaborator in this project. Furthermore, the IAEA has included this project in its on-going ADS Coordinated Research Program. The first experimental results for the sub-critical core show good agreement with MCNP calculations for a detailed core-model [11]. This experiment is complementary to the MUSE project in the next section.
- In the MUSE program the effects of neutron sources with increasing strength in different positions of the experimental low-power fast reactor MASURCA at CEA, Cadarache, France, are investigated. FZK is participating in the MUSE program within the 5. EC FP. One of the first steps in this project was the definition of benchmark models for the MASURCA reactor. Actually, this experimental reactor has some features not yet intensively investigated with KAPROS/KARBUS. The composition of the large reflectors leads to very strong self-shielding effects in structural materials, especially in iron. To investigate these effects, a very strongly simplified benchmark model was proposed by CEA [12]. First calculations at FZK showed large discrepancies up to 8% between the K_{eff} results of continuous energy MCNP calculations and of KAPROS/KARBUS multi-

group calculations with 26- and 69-group constant libraries. After this observation the isotopes of the benchmarks were recalculated for the 69-group library with the actual version of the standard program for group constant calculations NJOY [13], using the JEF2.2 [14] nuclear database. This updating with new JEF2.2 based group cross sections leads to similar results of 69-group calculations and of MCNP4C and is in accordance with results of other participants to the MUSE project [12]. More detailed investigations showed that nearly all new calculated isotopes contribute to the reactivity into the same decreasing direction. It may be concluded that the participation in the MUSE project already has improved the 69-group constant library. After a number of MUSE experiments with neutron sources with relatively small strength, in the presently running experiment MUSE-5 a strong new constructed neutron generator GENEPI with 14 MeV neutrons is utilized.

3.2.2 Investigations for a high power spallation target

Typical ADS design proposals for energy production or spent fuel incineration apply proton beams with energies around 1 GeV and currents larger than 1 mA, sometimes even larger than 100 mA. For the target materials usually heavy metals like tungsten, lead, bismuth are selected. The construction of such a high power device is a challenging task and several aspects like material behaviour, window cooling, and impact of spallation products have to be considered carefully. Most of the input data for these investigations are provided by the physics calculations. As a step towards the construction of a spallation target for ADS, the MEGAPIE initiative of FZK, CEA and PSI, Switzerland, intended to construct a lead-bismuth eutectic (PBE) target as replacement in the existing SINQ accelerator at Villigen, Switzerland [15]. The proton beam at the SINQ target amounts about 575 MeV at 1.74 mA (≈ 1 MW). In the meantime this project is supported by the EC in its 5. FP. In order to gain confidence in the results of the physics calculations for such a target, a MEGAPIE benchmark investigation was initiated with participation of CEA, PSI, FZK, CNRS (France) and ENEA (Italy) [16]. Parameters to be investigated are: heat deposition in structural materials, decay heat and activation, neutron flux distribution, spallation product yields, damages in structural materials and neutron leakage. After the preparatory investigations in [17], FZK has provided a nearly complete solution for this benchmark [18], mainly using the MCNPX-2.1.5 code with own database and auxiliary programs. First comparisons show that our results usually are in good agreement with the solutions of the other participants. For the analysis of the

spallation products a coupling with KAPROS/KAPROS/KORIGEN is in development, using standard output files of MCNPX.

3.2.3 Coupling of a spallation target and a sub-critical reactor system

A real irradiation of a slightly sub-critical system with a proton beam in order to investigate the generic problems with such a coupling is planned at JINR, Dubna, Russia. The proton beam of an existing accelerator with 600MeV, few μA , will be guided into a small sub-critical fast spectrum reactor core with MOX fuel, surrounded by a thick lead reflector. The sub-criticality level will be about $K_{\text{eff}} \approx 0.95$ leading to a system-power around 25 W. FZK supports this proposal and has the realization as an ISTC project recommended. The FZK cooperation within this project also resulted in an improvement of the multi-group data libraries of the KAPROS/KARBUS system. The Russian colleagues proposed to utilize Russian critical experiments with fast spectrum fuel with lead reflectors of increasing thickness as a benchmark investigation [19]. During the evaluation of these critical experiments an error on the standard 69-group library was detected: the group constants for the Pb-isotopes were not complete, but contained only data for depletion calculations. After updating as described above the improved library gives satisfactory results.

3.2.4 Enhancements of the nuclear databases

A traditional physics activity of nuclear science is the improvement of the databases. At FZK only minor activities are left in this area, mainly within the programs FUSION and NUKLEAR. The program NUKLEAR supports some activities within the 5. EC FP and collaborates with a number of ISTC projects. Measurements of cross section data for minor actinides and long-lived fission products is supported to improve the database for solving the problems of the backend of the nuclear fuel cycle. For ADS applications neutron and proton cross section measurements for important isotopes in the energy range up to several hundreds of MeV are in progress.

4. Improvements for the dynamic simulation of ADS

The dynamic simulation of ADS is an important application area to gain sufficient knowledge about the system control under normal and perturbed conditions. In ADS a number of characteristics deviate significantly in comparison with critical reactor systems. Moreover, the existence of a high power spallation source in the system is an additional

complication. An important observation is shown in figure 1 for the behaviour of the radial power-density profile in ADS with one proton beam in the centre of the core. We may observe a strong increase of the radial peaking factor if the value of K_{eff} decreases. This means that the basic assumption for the dynamic simulation of critical reactors, namely that during a reactivity change the space-dependent power-shape of the reactor does not change significantly and that the time-space dependent power distribution may be synthesised by the product of a time-dependent and a space-dependent component. Moreover it can be shown that first order perturbation theory, customarily used for the dynamic simulation of critical reactors, cannot be applied to ADS. For these reasons efforts have been started to provide more adequate computation tools for the dynamic simulation of ADS. The program SAS4A [20] was chosen as the basis for these developments because this code is well established for fast critical reactors and the actual ADS proposals mostly are based on fast spectrum systems.

4.1 Extension of the SAS4A code

The usual application of SAS4A assumes that during a dynamic simulation the space-dependent power-distribution (shape function) does not change and the time-evolution of the neutron-flux is based on the point kinetics model. Reactivity feedback effects, mainly caused by temperature and density changes in the core, are determined on the basis of pre-calculated tables, usually prepared by first order perturbation calculations. For ADS applications the following extensions of the SAS4A procedures are envisaged and to a large extent realized [21]:

- Treatment of the strong external source, including incorporation of source shut-off.
- Preparation of feedback reactivity tables based on ΔK_{eff} calculations. The present application is based on the CITATION [22] diffusion code. If required, the flexible coupling formalisms would enable the application of other flux calculation codes like the nodal transport code VARIANT [23] with moderate efforts..
- Recalculation of the power-distribution and the criticality during the simulation, using the restart options of the SAS4A code. This recalculation requires the feedback of the relevant temperature, composition and possibly geometry changes to the cross section code KARBUS and to the flux calculation code CITATION and has been realized with new KAPROS modules CTFILE and SASADS.

- Time-step selection will be flexible, but frequent power-distribution recalculation should be feasible. For this reason also optimal strategies for cross section calculations must be made available.

The KAPROS/KARBUS system usually utilizes 69-group libraries with the energy group structure of the well-known program WIMS [24]. This structure has been chosen because it is well suited for thermal, epithermal and fast reactor calculations. However, the computing times may become quite large and the use for SAS4A coupling is problematic if many recalculations are required. In such cases a speed-up of the cross section calculations may become mandatory. Several solutions may be considered for this purpose, e.g. the introduction of cross section libraries with a small number of groups or the use of pre-calculated tables with shielded microscopic cross sections. Few group constant cross section libraries are sensitive to the weighting spectrum applied in the group constant generation codes like NJOY [13]. This means that complete multi-group libraries have to be prepared for all systems with significant spectral variations. Preparation and validation of such libraries is a straightforward but tedious procedure. Generation of pre-calculated tables of shielded cross section also have severe drawbacks, e.g. for the calculation of Doppler effect if compositions significantly change. For the coupling of SAS4A with KAPROS/KARBUS a new formalism is under investigation: the creation of collapsed libraries, starting from a 69-group “master-library” and using system-specific weighting spectra. First tests with this new KAPROS module COLLIB show promising results. Systematic investigations with respect to the number of collapsed groups and to the selection of the group boundaries are in progress. The improved SAS4A procedures enable more accurate simulations of ADS but they still incorporate the point-kinetics treatment for the time dependent neutron flux amplitude. The use of small time-steps between succeeding flux and criticality calculations will result in long computing times. The next section describes shortly improved accurate fast calculation methods for the dynamic simulation of ADS.

4.2 Development of fast accurate calculation methods for dynamic ADS simulation

The space-time behaviour of nuclear reactor systems can be described by coupled differential equations for the balance of the neutron population and of the precursors of the delayed neutrons [21]. A commonly used solution method for critical reactors is the separation of a time-dependent amplitude function and a space-dependent shape function, leading to the point-kinetics formulation. The introduction of a weak time-

dependency of the shape function by recalculation during the simulation may improve this technique. However, as indicated in figure 1, this synthesis is not well suited for ADS and we have to look for other solutions. Our current research aims at examining alternative methods for the efficient calculation of dynamic parameters for point kinetics and, subsequently, multi-dimensional kinetics simulation of ADS. In particular, we examine the applicability of variational methods, (as described e.g. in [25]), as well as sensitivity theory for non-linear and non-homogeneous equations as originally developed in [26].

An important point for the dynamic simulation of nuclear systems is the efficiency of the formalisms to reduce the required computation time for acceptable solutions. The characteristics of the space-time behaviour of ADS show parameters varying over wide ranges. For example, as in critical reactors, the time-behaviour is determined by the prompt and delayed neutrons, having strongly different lifetimes. Further the space-dependent variations of the neutron fluxes are in large ADS much faster in the vicinity of the spallation sources than at large distances. In order to utilize such characteristics the application of multi-scale solutions is under investigation. First results for the time-dependent zero-dimensional equations are encouraging.

5. Summary and outlook

The present status of the main activities at FZK for the physics investigation of designs for innovative nuclear reactor systems has been presented. After a short overview of the available calculation tools, ongoing validation work is discussed. For HPLWR investigations coupling of thermo hydraulic and neutron physics codes is in development. Especially for the ADS investigations additional experimental data is needed. Benchmark investigations for simplified critical reactor models lead to significant improvements of the available 69-group cross section libraries. An important milestone for the development of ADS is the MEGAPIE initiative, started by FZK, CEA and PSI; the design, construction and utilization of a 1MW spallation device with PBE target and coolant for use in the SINQ neutron source at PSI. A neutronic MEGAPIE benchmark investigation showed good agreement of FZK results with those of other participants. Available methods for the dynamic simulation of ADS have been analysed. Utilization of formalisms developed for critical reactors is doubtful and should be qualified by adequate methods. Modification of the SAS4A code is in progress to enable more accurate dynamic ADS simulation. Proposals for alternative solution techniques are discussed.

6. References

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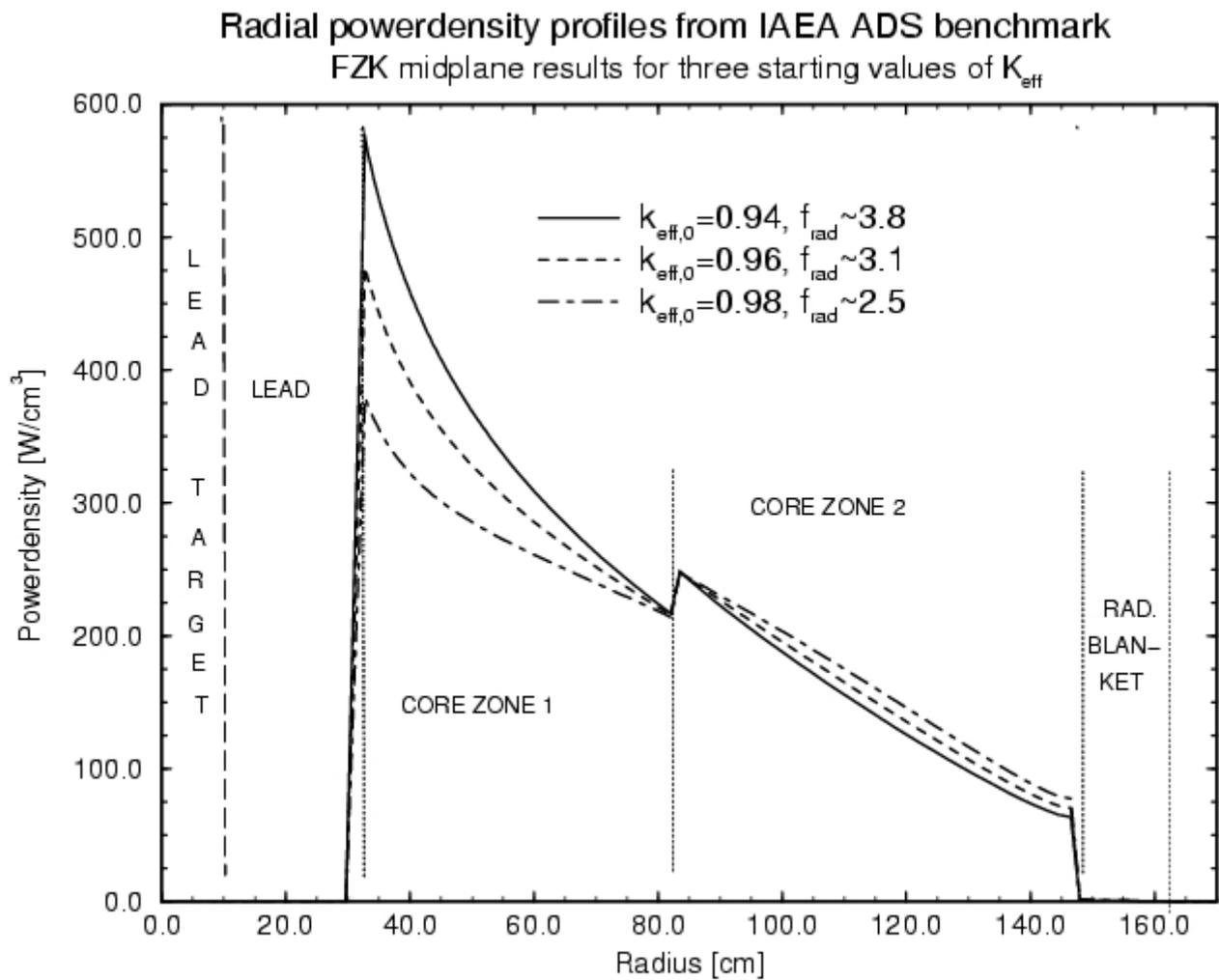


Figure 1: Radial power-density profiles for different levels of K_{eff} in ADS