DEVELOPMENT AND VALIDATION OF CALCULATION PROCEDURES FOR THE NEUTRON PHYSICS INVESTIGATION OF ACCELERATOR DRIVEN SUB-CRITICAL SYSTEMS

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1. INTRODUCTION

Neutron physics investigations for accelerator driven sub-critical systems are in progress at the Forschungszentrum Karlsruhe (FZK) since the early nineties. The first step of these efforts was the implementation and qualification of suitable calculation methods and codes, especially for the description of the spallation processes and for the coupling of the external neutron source with the transport calculations for the sub-critical reactor system. For the qualification of the calculation tools participation to several international benchmark investigations was very helpful. The applied high-energy codes could be validated by the participation to the NEA international code comparison of intermediate energy nuclear data [Filg95]. For the validation of the calculation of sub-critical reactor systems with strong external neutron sources, the IAEA ADS neutronic benchmark for lead cooled thorium/U^{233} fuel was a successful undertaking [Sles97, Gudo01]. The potential of nuclear waste incineration by the transmutation of long-lived minor actinides and fission products was already studied in an early stage [Sege94b,Broe96]. In this contribution only some application investigations related to an IAEA Coordinated Research Program for ADS are presented.

2. DEVELOPMENT OF CODES AND LIBRARIES

For the analysis of accelerator driven systems (ADS) the whole energy spectrum from several GeV down to thermal energies has to be covered. The traditional calculation tools for fission reactors only describe the energy range up to about 10 MeV for 26- and 69-group libraries at FZK [Broe92]. Other multi-group libraries and also the special libraries for Monte Carlo calculations (e.g. MCNP) apply energies in the range of the evaluated data libraries like ENDF/B, usually being 20 MeV. For the higher energies special methods, data and codes had to be adapted from other research areas, e.g. from high-energy accelerator investigations. In figure 1 the basic flowchart for our ADS investigations is shown. Three main components may be identified:

- Calculation of the neutron source with high energy transport codes
- Calculation of the steady state reactor with deterministic or Monte Carlo transport codes
- Burn-up or depletion calculations

In the following sections these components will be discussed in some detail.

[1] The view-charts presented at the meeting, together with some explanations, may be found at http://inrwww.fzk.de

2.1 PREPARATION OF CODES

In connection with the ADS investigations, a number of developments have been accomplished for the different calculation stages.

2.1.1 HIGH ENERGY SPALLATION CALCULATIONS

The investigations started with the implementation and qualification of the HETC and MORSE modules from the HERMES code system from the Jülich research center[Clot88]. The MORSE module was soon replaced by the more modern MCNP code [Brie97]. Later on, the LAHET code system LCS [Hugh98] from Los Alamos, being an improved coupling of LAHET and MCNP4B was adopted and applied. Moreover, FZK is beta-tester of the new MCNPX [Wate99] code system, in development at Los Alamos for ADS applications. In the meantime most calculations are performed with MCNPX. All codes mentioned before are based on Monte Carlo simulations, both in the energy region for spallation and in the lower energy region for neutron transport.

2.1.2 TRANSPORT CALCULATIONS

At FZK a strong effort was devoted to the qualification of the discrete ordinate code TWODANT [Alco90] for the transport calculations below a cutoff energy of 10 to 50 MeV, in order to save significant amounts of computing times for simplified geometrical models. In figure 2 a comparison of TWODANT and MCNP results is shown for the radial power density distributions in two axial positions of the IAEA ADS benchmark (see section 4). The TWODANT results were obtained on an IBM RS6000 workstation in about two hours of computing time, whereas the MCNP code needed several days on the same workstation. The very good agreement shows that for simplified geometrical models it is advantageous to apply deterministic codes.

2.1.3 DEPLETION CALCULATIONS

After the development of the PROSDOR system, a first semi-automated coupling of the codes HERMES, MCNP and KORIGEN [Sege94a], a fully automated coupling of the depletion calculations with the KAPROS/KARBUS [Broe92] code system, developed for critical fast, epithermal and thermal reactors, with the codes HETC/LAHET and MCNP/ TWODANT was implemented and validated. The KAPROS [Bach75] code system has been developed at FZK since many years. It is a very flexible fully modular system consisting of a controller program and a large number of independent application modules. Important features are the very flexible data-management on different storage levels (fast memory, hard-disc and tapes), the standardized interfaces (e.g. for cross sections, spectra, etc.) and the very powerful archiving and restart options. The system has been developed on an IBM mainframe computer and the first versions utilized the specific features of the mainframe computer environment at FZK with as a consequence, that transferring to other computer environments was very problematic. In the past 10 years a portable version for workstations with UNIX operating systems has been redesigned and realized. The first KAPROS applications were related to fast breeder reactors. In connection with investigations for tight light water reactors the treatment of up-scatter in the thermal energy region and of the resonance absorption in the epithermal region has been significantly improved. For fuel cycle studies a special module KARBUS was developed. The main tasks of KARBUS are [Broe92]:

- Preparation of multi-group cross section data, using the most adequate methods for the problem under investigation from options for fast, thermal and epithermal spectrum solutions. FZK has developed own formats for the storage of multi-group cross section data on direct access files. The data structures are optimized for application in all types of reactor spectra and combine characteristics of typical applications for thermal and fast reactors, e.g. up-scatter matrices, isotope-dependent fission spectrum matrices, separate treatment of elastic, inelastic, (n,2n), (n,3n) processes.

- Preparation and performing of multi-group reactor calculations. A number of alternative flux calculation codes may be selected with one- to three dimensions for the geometry and finite differences and nodal solutions for the transport or diffusion approximation of the Boltzman equation. Some of the earlier codes developed at FZK have a strong coupling with KAPROS; others are only loosely coupled by common interface files.
- Best estimate preparation of zone-dependent one-group cross sections for use in the depletion module BURNUP. The module BURNUP is a KAPROS implementation of the program KORIGEN [Fisc83], the well-known FZK depletion program developed from the ORIGEN code [Bell73]. As in ORIGEN, BURNUP treats all isotopes for which data is stored on the code-own libraries for one-group depletion calculations (in the meantime for up to about 3000 isotopes). If data for isotopes is available on the applied multi-group library the required one-group cross sections are provided by KARBUS, using selectable best-estimate weighting formalisms.

2.1.4 COUPLING OF THE CALCULATION STEPS

Figure 3 shows a more detailed overview of an actual KAPROS procedure, as applied for the solution of the IAEA ADS benchmark [Sles97, Gudo01]. However, it should be mentioned that the new MCNPX code combines LAHET and MCNP in one code. The application of MCNPX also may lead to some simplifications in the calculation scheme of figure 3. In general the code system KAPROS in conjunction with the powerful script languages of the UNIX operating systems are very flexible tools for the coupling of advanced computer codes.

2.2 DEVELOPMENT OF LIBRARIES

For the ADS investigations at FZK usually 69 group cross section libraries with the well-known WIMS [Aske66] energy group structure are applied. The upper energy boundary of these libraries is 10 MeV. As a consequence the ADS investigations utilize the formalisms of the high-energy codes above 10 MeV. These formalisms are not well qualified in the energy range up to about 300 MeV. In order to be able to study the influences of these approximations with multi-group calculations, an extended library with energies up to 50 MeV and 6 additional groups above 10 MeV of the WIMS structure has been established. First comparisons for the IAEA ADS benchmark show good agreement for the results of 69- and 75-group calculations, see e.g. [Broe98, Gudo00].

3. VALIDATION INVESTIGATIONS

The validation of calculation tools for accelerator driven sub-critical systems is a challenging task because no real experience is available 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.

3.1 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[Chig99], 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 (see section 4). The first experimental results for the sub-critical core show good agreement with MCNP calculations for a detailed core-model [Gudo01].

- In the MUSE program[Lebr99] 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 project within the 5-th framework program of the European Community. 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 [Rimp00]. First calculations at FZK showed large discrepancies 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 a number of isotopes of structural materials were recalculated for the 69-group library. In table 1 some of the FZK results are summarized.

Multi-group library / comments	K_{eff} S_8 transport 69 groups
G69P1UX3 Old standard library	1.0796
G69P1UD2 Extended library, minor corrections	1.0854
G69P1UD2 + Fe and Cr from JEF2.2	1.0470
G69P1UD3 JEF2.2 for nearly all materials	1.0159
G69P1UD3 + Alternative shielding approximation	1.0193
MCNP4C FZK solution (ENDF/B-VI)	1.0184

Table 1: FZK results for MUSE simplified benchmark 2

We may observe a strong overestimation of K_{eff} for the old standard library for this simplified model of an experimental reactor system. Updating with new JEF2.2 [NEA00] based group cross sections leads to comparable results of 69-group calculations and of MCNP4C and is in accordance with results of other participants to the MUSE project [Rimp00]. More detailed investigations showed that nearly all newly calculated isotopes contributed to a reactivity change into the same decreasing direction. It may be concluded that the participation of the MUSE project already has improved the 69-group constant library significantly.

3.2 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 must be 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, plans to construct a lead-bismuth eutectic (PBE) target as replacement in the existing SINQ accelerator at Villigen, Switzerland [Salv00]. The proton beam at the SINQ target amounts about 575 MeV at 1.74 mA (≈1 MW). 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) [Poit01]. 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. Preparatory investigations are presented in [Broe00]. First comparisons of the preliminary results show that our solutions usually are in satisfactory agreement with those of the other benchmark participants.

3.3 COUPLING OF A SPALLATION TARGET AND A SUB-CRITICAL REACTOR

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_{eff}≈0.95 leading to a system-power around 25 W. FZK supports this proposal and has recommended the realization as an ISTC project. 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 [Rogo00]. In table 2 a summary of the specification of the Russian critical assemblies is given.

Exp.	Critical Core radius cm)	Core Critical mass (gram)	Internal void radius (cm)	Thickness Lead reflector (cm)	External Assembly Radius (cm)	K_{eff}
B1	6.668	18773	-	-	-	1.000±0.0025
B2	6.000	13739	1.00	3.04	9.04	1.000±0.0040
B3	5.350	9722	1.00	28.45	33.80	1.000±0.0040

Fuel composition:Pu^{239} 95.30%, Pu^{240} 1.75%, Ni 1.28%, Ga 1.67%

Table 2: Specification of the Russian critical assembly data for lead benchmark

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. Table 3 shows the results with 2 libraries discussed in table 1. We may observe, that for the old library G69P1UX3 the results with Pb isotopes are completely wrong. The updated library G69P1UD3 gives satisfactory results. If we compare multi-group and MCNP4C results, we may observe the same trends: increasing K_{eff} values with increasing Pb-reflector. However, the MCNP4C results are somewhat higher.

Exp.	Case	G69P1UX3	G69P1UD3	MCNP4C
B1	M1	0.9892	0.9935	0.9960
	M2	0.9898	0.9880	
B2	M1 M4	0.9094	0.9921	1.0121
	M1 M5	1.0001	1.0017	
	M2 M4	0.9094	0.9877	
	M2 M5	1.0000	0.9973	
B3	M1 M4	0.8179	1.0007	1.0284
	M1 M5	1.0195	1.0185	
	M2 M4	0.8179	0.9975	
	M2 M5	1.0195	1.0153	

Experimental values: K_{eff}=1.000
M1: Ni isotopes in calculation
M2: Ni element in calculation
M4: Pb isotopes in calculation
M5: Pb element in calculation

Table 3: Results for Russian Criticality Benchmarks

4 SELECTED APPLICATIONS

A number of application investigations have been performed, e.g. preliminary analysis for Pu-incineration in ADS [Broe96, Broe00] and power flattening with multiple-beam designs for large ADS. [Broe00, Daga00, Gudo00]. In the next sections some investigations related to the international IAEA Coordinated Research Program (CRP) “Use of Th-based fuel cycle in accelerator-driven systems (ADS) to incinerate Pu and reduce long-term waste toxicities” are discussed.

4.1 IAEA ADS BENCHMARK FOR A TH-U^{233} BASED ENERGY AMPLIFIER

In 1996 the IAEA initiated in the framework of an IAEA CRP an international ADS benchmark based on a proposal of Rubbia et.al. [Rubb95] for an energy amplifier with a power of 1500 MW_{th} and based on Th-U^{233} fuel and lead coolant. For three values of the “beam shut-off” criticality (0.94, 0.96 and 0.98) the U^{233}-enrichment had to be determined and a number of parameters had to be calculated. For the FZK contribution [Broe97] the calculations of the neutron-flux density spectra and of reaction rates (total fission reaction rate, fission reaction rates for individual isotopes) have been carried out with the transport code TWODANT in S_4/P_1 approximation, using the actual 69-group constant library. The neutron source provided with the benchmark data has been transformed to our energy group structure in such a way that the number of neutrons per eV was conserved for each energy group.

4.2 BURNUP BEHAVIOUR

An important objective of the IAEA ADS benchmark was the determination of the time-dependence of the reactivity of the sub-critical reactor system. In the benchmark specifications the power-level and the time-steps are specified in detail. The cylindrical geometry model-specification contains 5 zones: lead, inner core, outer core, radial reflector and axial reflector. For our burn-up calculations each fuel zone was subdivided into 3 radial and 3 axial sub-zones, leading to a TWODANT (R-Z)-model with 22 zones. During the analysis of the results it pointed out that some other benchmark solutions were based on burn-up calculations without sub-division of the fuel zones. For that reason a comparison calculation without sub-division was carried out, leading to a TWODANT (R-Z)-model with 7 zones. In figure 4 FZK results for the time-dependence of the reactivity is shown. These results are in satisfactory agreement with solutions of other participants. We may observe that for the case K_{eff}=0.96 the influence of the sub-division of the fuel zones is remarkable.

4.3 POWER DISTRIBUTIONS

The technical feasibility of ADS is strongly influenced by the power density distribution in the system. So, another important issue of the IAEA ADS benchmark investigation was the comparison of the radial power distributions for the different sub-criticality levels. In general the agreement between the solutions of the participants was good. In figure 5 our radial power density distribution in the mid-plane of the reactor system is shown. Also the radial form-factors, defined as maximum-to-mean power density ratio, are given. We may observe that the form-factor strongly increases with decreasing reactivity of the system. Such values are not acceptable in large power systems. As a consequence of these observations at FZK a considerable effort was devoted to improve the power-density distribution, see e.g. [Daga00,Gudo00].

4.4 IAEA ADS BENCHMARK STAGE 3.1

In the course of the IAEA CRP a number of cases were defined in order to study specific problems related to ADS with thorium fuel. In stage 3.1 of the CRP the characteristics of plutonium incineration in ADS with thorium-based fuel was investigated. For this purpose, FZK has prepared the detailed input data for the fuel. The other benchmark specifications were unchanged. In figure 6 first preliminary results for K_{eff} are shown of solutions from five participants: IPPE Obninsk, Russia, NRG Petten, Netherlands, CIEMAT Madrid, Spain and FZK. We may observe very large discrepancies between these solutions. The burn-up results of Monte Carlo calculations of CIEMAT and NRG are 4-5% higher than the results of the deterministic codes from IPPE and FZK. Moreover, the strong influence of the lead cross sections may be observed for the FZK solutions. In figure 7 some influences of the applied cross section data on FZK-solutions is given. Generally, a strong increase of K_{eff} may be observed during burn-up, mainly caused by the build-up of U^{233} and the good conversion ratio in the Pu. The discrepancies of figure 6 are not yet clarified and there is a strong need for a third type of solution, e.g. with alternative Monte Carlo burn-up programs.

5 SUMMARY

Development and validation of calculation procedures for the neutron physics investigation of accelerator driven sub-critical systems (ADS) at FZK are discussed in some detail. For the three steps in such investigations, determination of the neutron source from the spallation processes, of the steady state neutron transport in the reactor system and of the long-term burn-up and depletion, adequate tools have been made available and coupled. For this coupling the modular code system KAPROS/KARBUS, developed at FZK, plays an important role. Extensive validation work has been performed. Some of the recent improvements of the applied multi-group libraries are explained in more detail. Selected applications, related to the IAEA CRP on the use of thorium fuel in ADS are presented. Large discrepancies in the results for ADS with Th/Pu fuel and lead coolant still have to be clarified.

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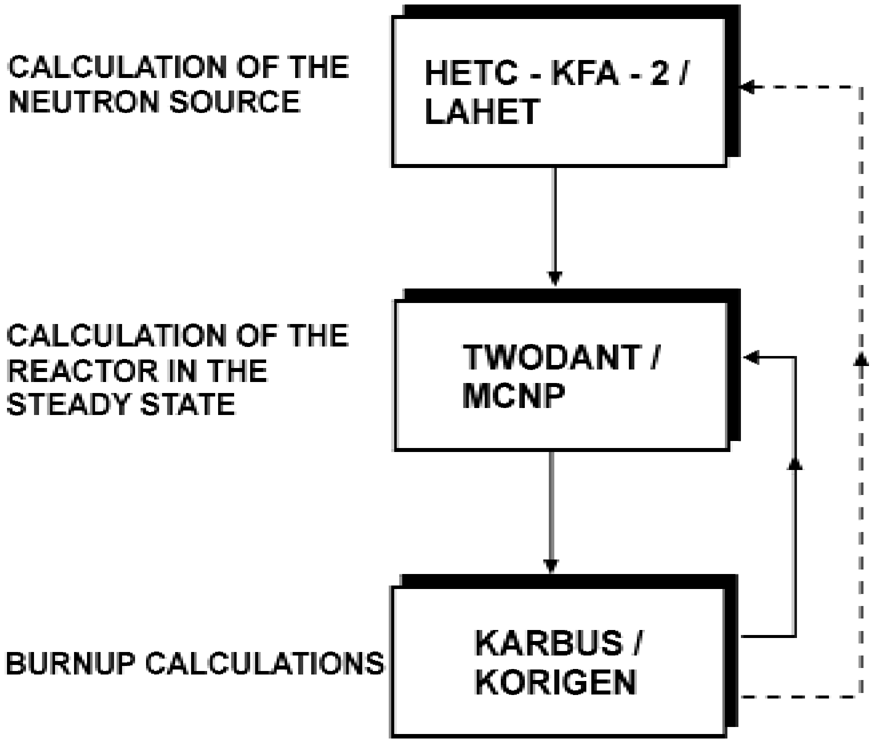

Figure 1: Simplified flowchart for a complete ADS calculation

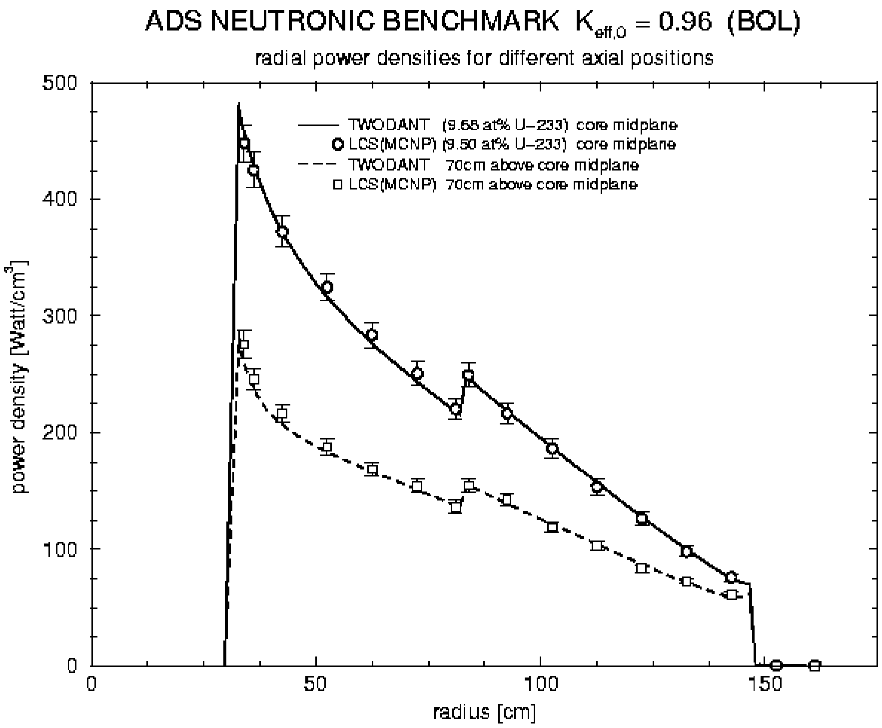

Figure 2: Comparison of radial power density distributions for the IAEA benchmark from TWODANT and MCNP calculations

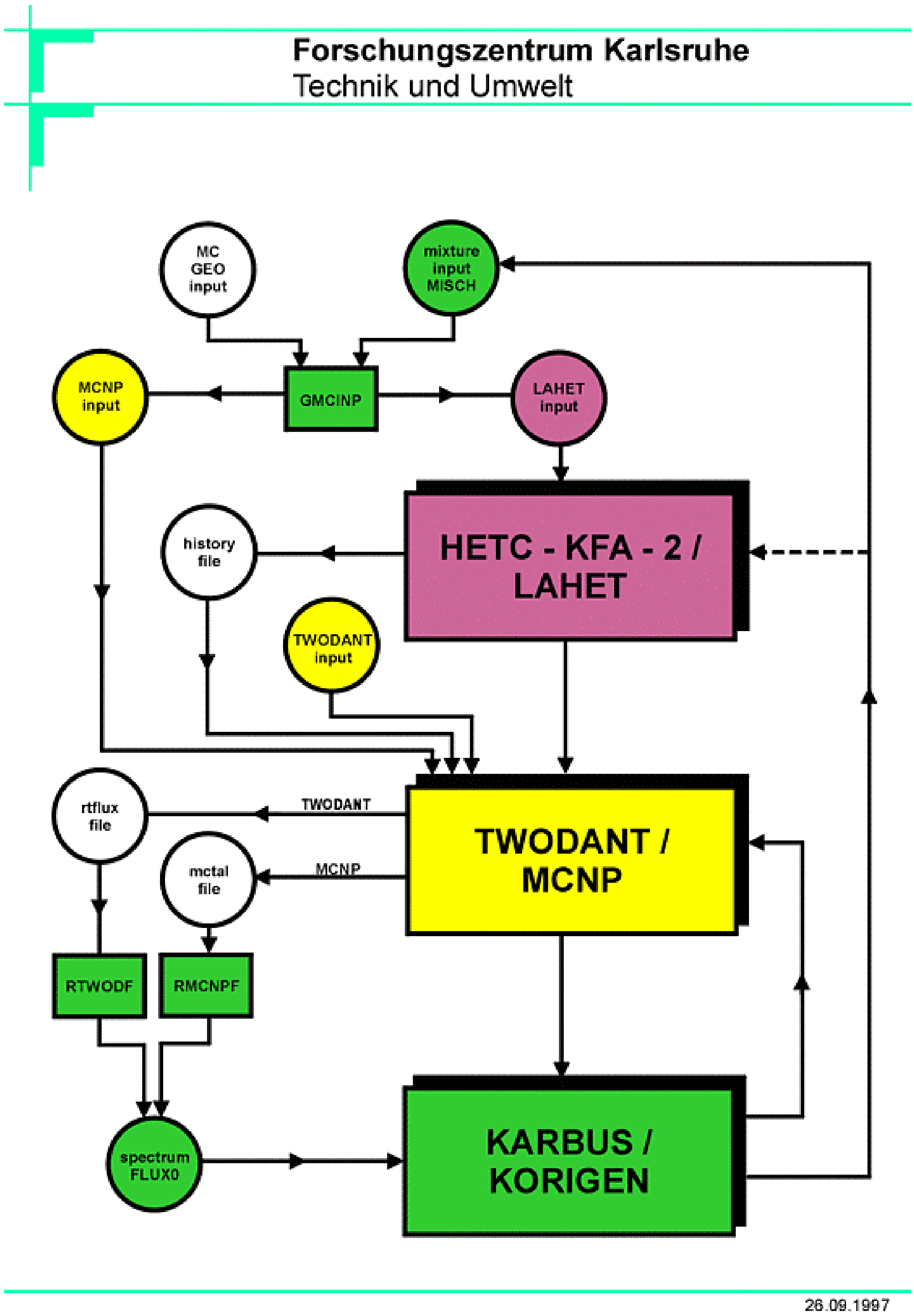

Figure 3: Detailed flowchart for a complete ADS calculation at FZK

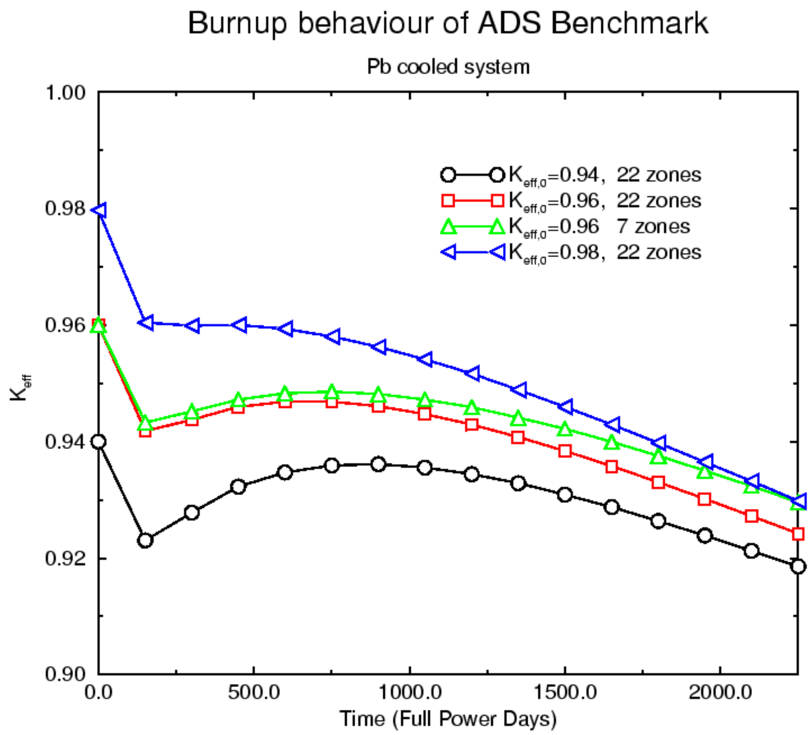

Figure 4: Reactivity of the IAEA ADS benchmark as a function of full power days

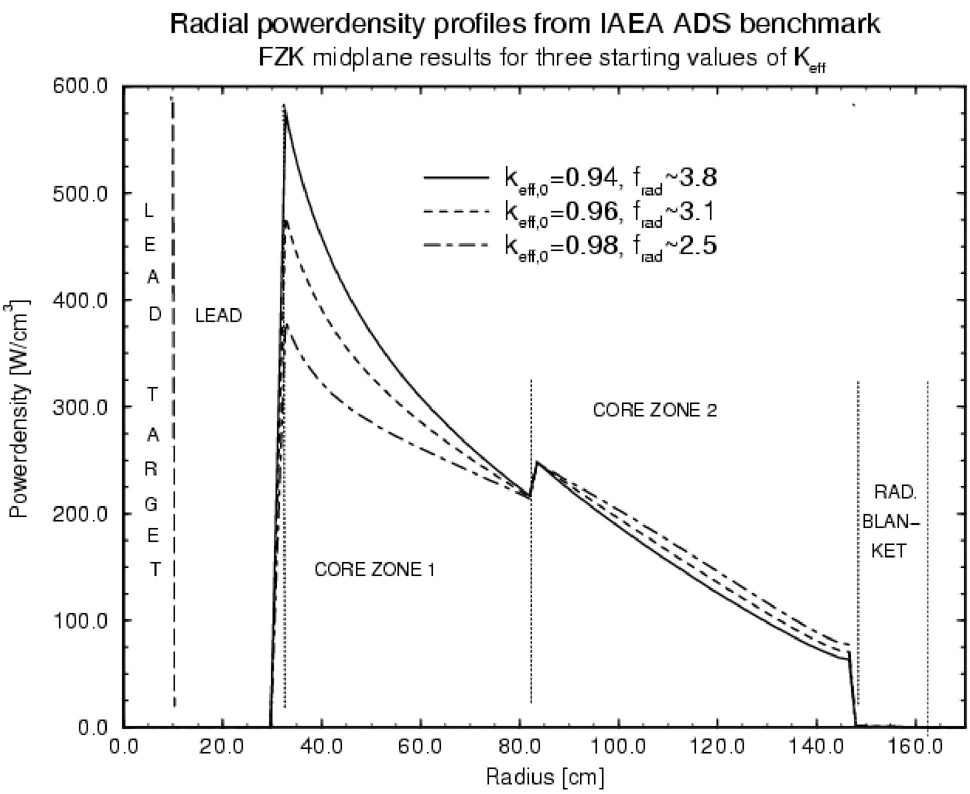

Figure 5: Radial power-density profiles for different levels of K_{eff} in ADS

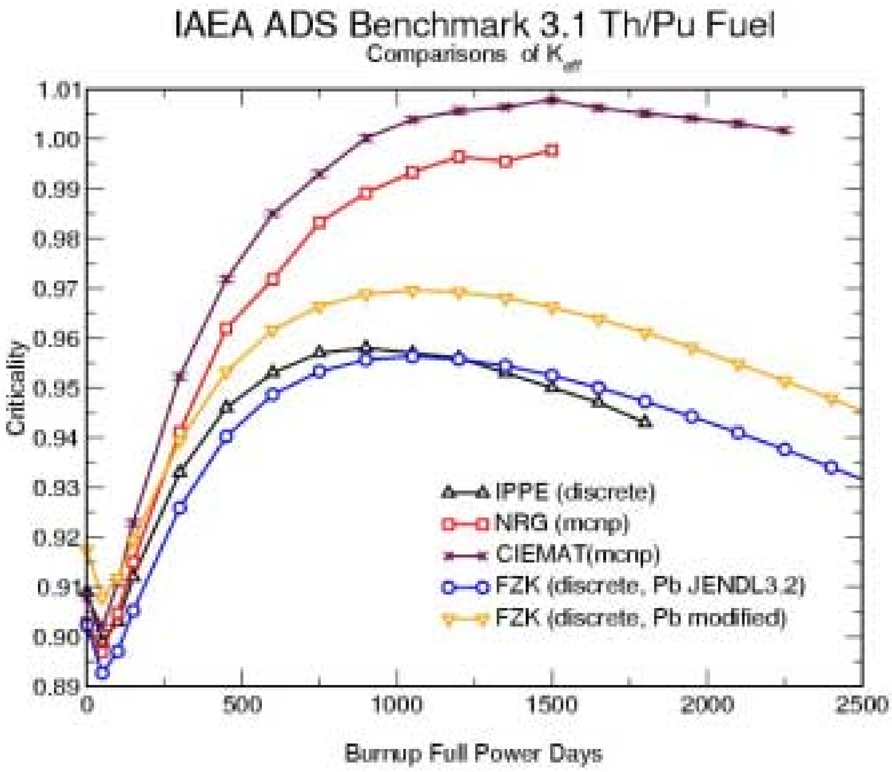

Figure 6: K_{eff} as a function of burn-up for IAEA ADS benchmark stage 3.1 (Th/Pu) fuel

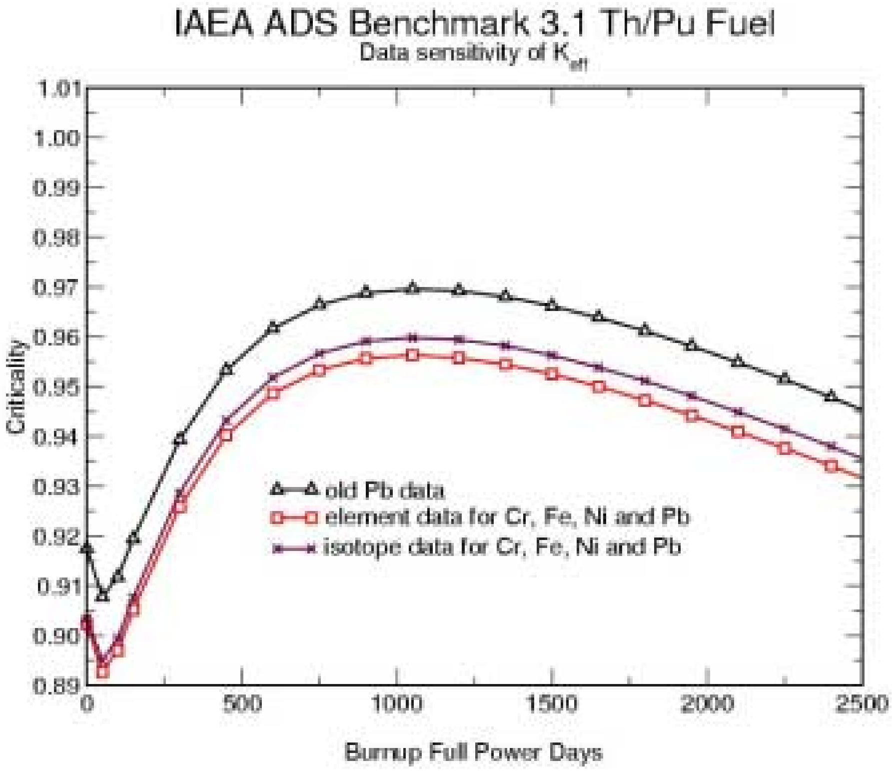

Figure 7 K_{eff} as a function of burn-up for IAEA ADS benchmark stage 3.1 (Th/Pu) fuel