# Status and Development of Nuclear Design and Accident Simulation Methods

*A. Seubert, S. Langenbuch, W. Zwermann*

Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH
Forschungsinstitute, D-85748 Garching, Germany

**Abstract:**
An overview is given on nuclear design and accident simulation methods for light water reactors. The nuclear data libraries and computer codes which are presently used in GRS are described, as well as development activities which mainly aim at the application to full-scale reactor transport calculations. The methods cover the generation of nuclear data, fuel assembly calculations and stationary and transient calculations of reactor cores including the application of coupled codes for plant transients. In particular, a summary is given on the experience applying deterministic neutron transport methods to large critical experiments and reactor core benchmark problems.

## 1 INTRODUCTION

The simulation methods for nuclear design and accident analysis have reached a high level of accuracy and reliability. However, at the same time the fuel strategy for light water reactors (LWR) is continuously optimised, e.g. uranium fuel with higher enrichments and MOX fuel are introduced. For both fuel types, higher burn-up values should be reached. The use of new fuel is accompanied by optimised core loading procedures to improve economics of fuel and to reduce the fluence at the pressure vessel. The safety evaluation of such new conditions requires improved and validated analytical methods. In this paper, the status of available methods in GRS is described together with the further research and developments.
The nuclear calculations for LWRs are typically performed in a sequence of steps. These steps are:

- providing basic nuclear data libraries,
- fuel assembly calculations,
- steady state reactor calculations for operational conditions,
- transient 3-D reactor core calculations for accident conditions including the overall plant behaviour.

The general structure of this paper follows these steps.

## 2 NUCLEAR DATA LIBRARIES

### 2.1 Objective

The analysis of critical systems requires adequate nuclear cross sections as a pre-requisite for accurate neutronics calculations. For such calculations, all relevant nuclear reactions within the full energy range have to be taken into account. The data should be available for all relevant nuclides of the systems considered and should cover the relevant temperature range. Especially, the resonance structure of the cross sections and the spatial and spectral interactions and shielding effects have to be considered explicitly.

### 2.2 Nuclear Data Libraries in Use

Nuclear basis data are evaluated internationally. These evaluated data mostly are available in the public domain. Among them, the JEFF (Joint Evaluated Fission and Fusion File, Europe) [JEF-05], ENDF/B (Evaluated Nuclear Data File, USA) [OBL-04], and JENDL (Japanese Evaluated Nuclear Data Library) [JEN-02] files are commonly used. They are complete for practical applications concerning the number of nuclides and nuclear reactions, and validated by a large number of critical experiments.
These basis data have to be processed to generate either data for the reaction cross sections on a very fine energy grid (so-called point data), which can be used with Monte Carlo codes like MCNP [BRI-00], or data for energy intervals, supplemented by information on the resonances (so-called multi-group data), from which few-group data for deterministic transport codes can be produced. For the data processing, the programme system NJOY [MAC-94] is internationally applied.
At GRS, a nuclear point-data library mainly based on JEF-2.2 is used routinely for Monte Carlo calculations. This library was generated and validated in a common project with IKE Stuttgart [BER-01]. It contains data for the isotopes most relevant for nuclear criticality calculations (some 40 actinides, 180 fission products, and 70 structure and absorber materials) for several temperatures between room temperature and 3000 K. In addition to this point-data library, a multi-group library is used with 292 energy groups and a hyperfine representation in the resolved resonance region. It was generated also by IKE from JEF-2.2 basis data for the preparation of few-group data for Monte Carlo and deterministic transport calculations.

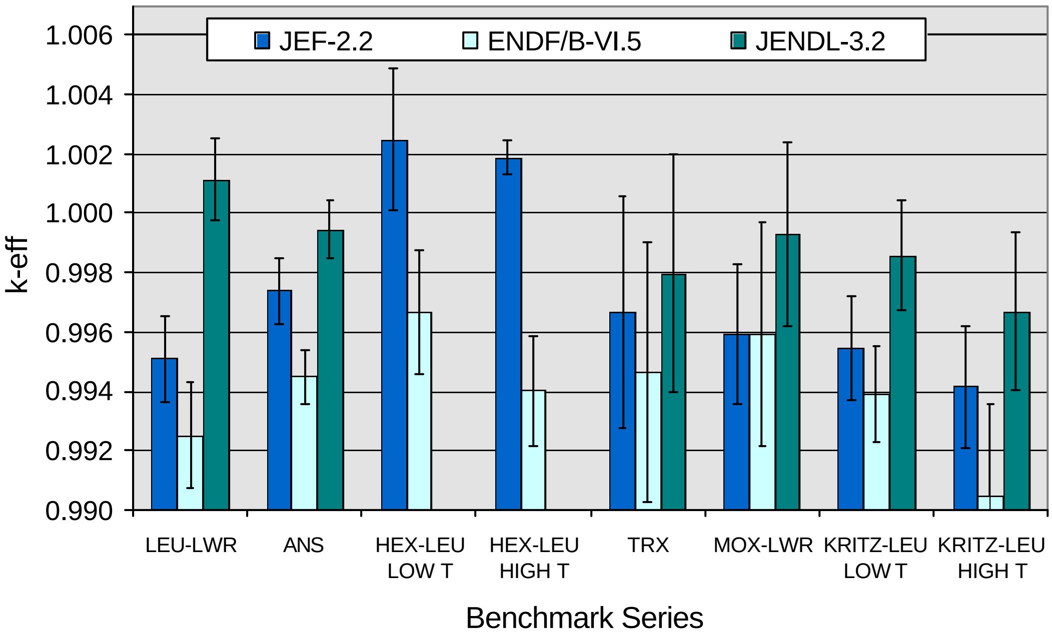


Figure 2.1: Comparison of multiplication factors calculated with MCNP and different nuclear point-data libraries for LWR-type lattice benchmarks.

For the validation of the point-data library, calculations for numerous experiments mainly described in the "International Handbook of Evaluated Criticality Safety Experiments (ICSBEP)" [NEA-95] were performed using the MCNP code. An example for arrangements of

regular LWR-type pin-cell lattices is presented in Fig. 2.1, where the average values of the calculated multiplication factors for groups of benchmark experiments are displayed. Calculations were performed with our standard JEF-2.2 library, and for comparison, with ENDF/B-VI.5 and JENDL-3.2 data. The results are quite satisfactory, with a slight trend of the JEF-2.2 calculations to underestimate the critical multiplication factor ($k_{eff}$ = 1.0) from the measurements. Several evaluations indicate that these deviations are due to the deficiencies in the U-238 capture cross section. This is presently being investigated.
For selected benchmark experiments, calculations were also performed with few-group data and compared with point-data Monte Carlo calculations. The results of such calculations for the KRITZ-2 and VENUS-2 benchmarks are discussed in Section 4.2.

### 2.3 Future Developments

Internationally, there are on-going activities to improve the data basis or release versions like JEFF-3.1 and ENDF/B-VII. The progress in this field will be observed to evaluate whether the updates are relevant for our applications.

## 3 FUEL ASSEMBLY CALCULATIONS

### 3.1 Objective

Within the scope of the LWR standard computation scheme, the determination of the reactivity and the nuclide inventory of fuel assemblies in terms of various burn-up states is fundamental for subsequent reactor core calculations. Based on the full nuclide inventory of a given burn-up state, fuel assembly calculations also serve as a means for providing few-group data, e.g. macroscopic cross sections, and for performing homogenisations over characteristic spatial regions, e.g. individual fuel assemblies or pin cells. Thus, fuel assembly calculations are the connecting link between nuclear point data and multi energy group libraries on one hand and core calculations on the other hand.

### 3.2 Methods in Use

Fuel assembly calculations at GRS are performed by applying external codes and also own developments. Codes as HELIOS [CAS-91] and the TRITON/NEWT sequence from the SCALE-5 code package [SCA-04] are routinely in use. HELIOS, developed and distributed by Studsvik Scandpower, is a 2-D cell and depletion code system based on the current-coupling collision probability method. Within each spatial element of a rectangular or circular cylindrical system, the 2-D integral transport equation is being solved by means of the collision probability method. Different spatial elements may be connected by appropriate coupling of interface currents. Due to this theoretical approach, HELIOS provides great flexibility in the geometrical modelling and so allows for the treatment of non-standard fuel assemblies, in particular research and advanced reactor concepts. Since HELIOS solves the integral transport equation in multi-energy group representation, the basic nuclear data is a 190 neutron and 48 gamma group library. It is mainly based on ENDF/B-VI. For faster calculations, a 47 neutron and 18 gamma energy group library is also available.
In the SCALE-5 release, the TRITON/NEWT burn-up system has been made available. It consists of a coupling of the 2-D Discrete Ordinates transport code NEWT for the reactivity and flux calculation and the code TRITON which solves the burn-up equations. Since the transport code solves the $S_N$ equations for non-orthogonal 2-D spatial meshing by applying the Extended Step Characteristic Approximation, NEWT provides a flexible geometric

modelling. The nuclear data may be based on SCALE multi-group libraries (with energy groups ranging from 238 to 44) which are derived from ENDF/B-V. At present, we are gaining experience with the application of the NEWT/TRITON sequence.
For being independent from external codes, the 3-D coupled reactivity and full inventory system KENOREST [HES-00] for PWR and BWR fuel assemblies has been developed at GRS. It consists of a coupling of the 3-D Monte Carlo code KENO V.a/VI and the 1-D burn-up code OREST [HES-88] which in turn is a combination of the 1-D spectrum code HAMMER and the 0-D full inventory depletion code ORIGEN. Whereas OREST provides the rod-by-rod full nuclide inventory, KENO performs 3-D reactivity and pin power distribution calculations for square and hexagonal fuel assemblies. The 83 energy group library used by KENO is derived from the 292 energy group library based on JEF-2.2. The ORIGEN neutronic data which are continuously being updated at GRS are based on ENDF/B-V/VI, JENDL-3.2 and EAF-97.

### 3.3 Recent and Future Developments

In recent developments of KENOREST, special attention has been drawn to an improved modelling of plutonium and actinide build-up or burnout for advanced heterogeneous fuel assembly designs. Therefore, in the new KENOREST release, a multi-region model of the pellet was implemented for a more detailed description of the radial burnout within the fuel rod. This multi-region model also allows for an improved treatment of burnable poisons, e.g. gadolinium. Updated ORIGEN neutronic libraries including additional neutronic reactions will be an improved basis for LWR inventory calculations.

## 4 STEADY STATE NUCLEAR CALCULATIONS

### 4.1 Objective

The prediction of stationary states of a reactor under various operating and accident conditions requires the determination of design and safety parameters with high accuracy. Apart from the determination of the reactivity for a given core loading, the main objectives of steady state reactor core calculations are the precise calculation of both the spatial neutron flux and power distribution, the detailed evaluation of the maximum fuel temperature and the determination of the fluence at the pressure vessel. Therefore, great effort is made for the development of neutronics models which are also coupled with thermal-hydraulics codes.

### 4.2 Methods in Use

At GRS, both external codes and own developments are routinely in use. The theoretical methods range from the application of the diffusion method in two energy groups to multi-group neutron transport and the Monte Carlo method.

#### *4.2.1 The 3-D Nodal Diffusion Code QUABOX/CUBBOX*

For 3-D reactor core calculations, nodal methods have been developed for efficient solutions. GRS uses the reactor core model QUABOX/CUBBOX [LAN-77a, LAN-77b], which has already been developed in the seventies. It solves the neutron diffusion equation with two energy groups by a neutron flux expansion method based on local polynomials. The set of equations is solved by a matrix decomposition method that can be efficiently applied for

static and transient calculations. The mesh corresponds in the radial plane to the fuel assembly size and in the axial direction also a coarse mesh can be chosen. The macroscopic nuclear cross-section data for two energy groups are calculated from data libraries using flexible representations e.g. multi-dimensional function tables or polynomial approximations. These nuclear data have to be precalculated by fuel assembly codes for the full range of parameters covering the core conditions that should be investigated.
Feedback effects may be calculated by a parallel coolant channel model as implemented in the programme HYCA which consists of a 1-D flow channel model and an average fuel rod for each channel. The mapping between fuel assemblies and thermal-hydraulic channels can be defined by input. Another option for determining the feedback parameters is available by the coupled code ATHLET-QUABOX/CUBBOX, which is discussed in section 5.2. The application of QUABOX/CUBBOX is restricted to square lattices and two prompt neutron energy groups. The reactor core model QUABOX/CUBBOX can be applied to steady state calculations and to reactor core transients with defined time-dependent core boundary conditions.

#### *4.2.2 The Monte Carlo Codes MCNP and KENO*

The capability to handle continuous energy nuclear data libraries in combination with the treatment of complex geometries in exact representation without discretisation make the Monte Carlo method a reference tool for nuclear applications. At GRS, the Monte Carlo codes MCNP and KENO are in routine use. MCNP is a general-purpose *Monte Carlo N-Particle code* that can be used for neutron, photon, electron or coupled neutron/photon/electron transport. The code treats an arbitrary three-dimensional configuration of materials in almost any geometry. Specific areas of application cover criticality safety, radiation protection and shielding as well as radiography, dosimetry and medical physics. Typically, point-wise cross-section data are used, although group-wise data can be used. For neutrons, all reactions given in a particular cross- section evaluation are accounted for.
KENO V.a is a three-dimensional Monte Carlo criticality transport program developed for use as a module of the SCALE code package or as a standalone program. It treats nuclear data in multi energy group representation with arbitrary scattering order where anisotropic scattering is treated by using discrete scattering angles. New features of the SCALE-5 release are the capability of KENO V.a to compute angular fluxes and flux moments and to treat also point-wise nuclear data.

#### *4.2.3 The Deterministic Discrete Ordinates Code Systems DANTSYS and DOORS*

DANTSYS and DOORS are two of the most popular code systems that solve the multi-group form of the stationary Boltzmann transport equation for neutral particles in discrete ordinates representation. Within the $S_N$ theory, angular fluxes of the discretised spatial problem region are calculated by solving the transport equation along specific angular directions called discrete ordinates. Starting in one corner of a mesh, at the highest energy, and with starting guesses for implicit sources, boundary conditions and recursion relationships are used to sweep into the mesh for each discrete direction. The calculation then proceeds to lower energy groups. Integral quantities such as scalar flux are obtained from weighted sums over the directional results. Both code systems contain separate modules that treat the transport problem in one, two and three spatial dimensions for both Cartesian and curvilinear geometries. In DANTSYS, the *Diffusion Accelerated Neutral-Particle Transport Code System,* developed by the Los Alamos National Laboratory (USA), the corresponding 1-D, 2-D and 3-D codes are named ONEDANT, TWODANT and THREEDANT, respectively. For space-angle discretisation, the diamond-difference and adaptive weighted diamond schemes are used.

Like DANTSYS, the *Discrete Ordinates Oak Ridge System* DOORS, developed by the Oak Ridge National Laboratory (USA), consists of independent codes for solving the $S_N$ equation in one (ANISN), two (DORT) and three (TORT) spatial dimensions. DOORS treats neutral particle transport problems for both Cartesian and curvilinear regular geometries (including a discontinuous spatial mesh capability) with various methods being applied to treat the spatial dependence, including nodal and characteristic procedures. Anisotropic scattering is treated using a variable order Legendre scattering cross section expansion.
Over the past few years, extensive experience has been made at GRS with the application of the above mentioned Monte Carlo and deterministic transport codes to numerous benchmark problems. With respect to the Monte Carlo codes, detailed studies using different data libraries have been made. The following examples of applications are presented: the KRITZ-2 and VENUS-2 critical experiments, the VVER-1000 full core benchmark, the C5G7 3-D extension MOX fuel assembly benchmark and the PWR MOX/$UO_2$ core transient benchmark.

## 4.3 Applications

### *4.3.1 The KRITZ-2 and VENUS-2 Benchmarks*

KRITZ-2 and VENUS-2 are critical experiments with square lattices of LWR conditions. In addition to the critical parameters, in these experiments fission rate distributions were measured. We calculated these assemblies not only to compare with the experimental results, but in particular to compare few-group deterministic calculations with reference Monte Carlo calculations based on nuclear point data. The few-group calculations were performed with homogenized cross sections for each pin cell. All data are based on the JEF-2.2 data file, which is routinely used at GRS for neutron transport calculations.
The KRITZ-2 assemblies [JOH-90] are square lattices with uranium (KRITZ-2:1, 2:13) or MOX fuel (KRITZ-2:19), inside a vessel with light water, each in cold state at ambient temperature, and a hot state with a temperature of about 240 °C. Criticality was obtained by adjusting the water level and the boron concentration in the moderator. The VENUS-2 core [NEA-04] consists of twelve 15x15 units of LWR pin cells, arranged in a cross shape. The inner part of the core consists of uranium pin cells with different enrichments, the outer parts consist of MOX pin cells. Forty pins in the central part of the core are replaced by pyrex absorber pins.

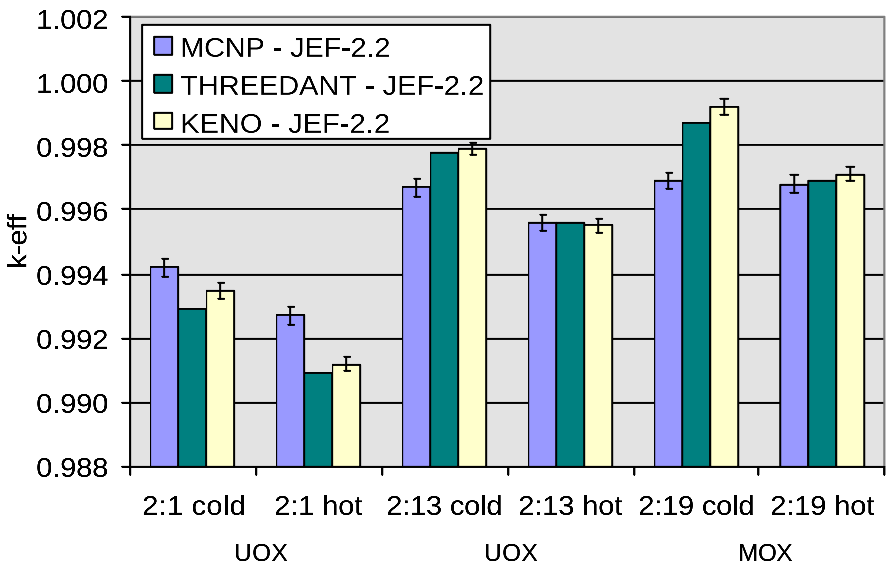


Figure 4.1: Multiplication Constants for the KRITZ-2 assemblies calculated with different neutron transport codes; the data libraries used are based on JEF-2.2.

Figure 4.1 displays the multiplication constants for the KRITZ-2 assemblies obtained with different transport codes, namely the Monte Carlo code MCNP with point data, as well as the deterministic $S_N$ code THREEDANT from the DANTSYS code system [ALC-95] and the Monte Carlo code KENO from the SCALE-4.4 code system, both with few-group data using 18 energy groups. There is very good agreement between the corresponding results for all cases; the differences are not exceeding 0.2 %. The generally observed low values calculated for the uranium assemblies need further investigations as already indicated in section 2.2.

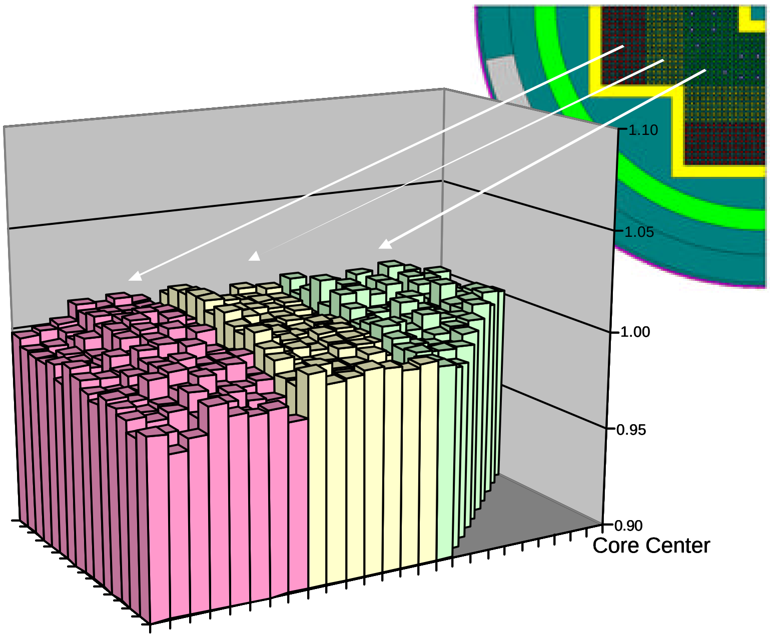


Figure 4.2: Ratios of the pin-wise fission rates for the VENUS-2 core, calculated with MCNP with nuclear point data and THREEDANT with 18-group data, based on JEF-2.2.

Figure 4.2 presents a comparison of the results for the VENUS-2 core from a calculation by MCNP with nuclear point data, and by THREEDANT with 18 energy group data, along with a sketch of the VENUS-2 geometry. The figure shows the ratios of the corresponding radial fission rate distributions. The results of MCNP and THREEDANT are in excellent agreement, with differences up to 2.5 % only at the core periphery and the interfaces between the different fuel zones. This confirms that for LWR fuel lattices, deterministic few-group calculations with energy groups in the order of 10 to 20 are well suited to generate results of a similar accuracy as the Monte Carlo method with nuclear point data.

*4.3.2 The VVER-1000 Full Core Benchmark*

To extend the application of MCNP to full-scale reactor core calculations, GRS has participated in the computational OECD/NEA VVER-1000 full core benchmark [ALY-02]. The reactor core, which is represented in two-dimensional geometry, is loaded with uranium and MOX fuel assemblies, each of them containing also gadolinium fuel pins. The fuel assemblies are in various burn-up states from the fresh state up to 40 MWd/kg HM; the corresponding nuclide compositions are provided with the benchmark specification, including actinides and important fission products.
The calculations were performed for five uncontrolled states and one controlled state: (1) operational state at full power, (2) hot zero power state at overall constant temperature, (3) cold state with high boron concentration, (4) operational state without boron, (5) hot zero

power state without boron, (6) hot zero power state with inserted control rods. For all these states, multiplication constants and fuel assembly wise fission rate distributions were determined. In addition, pin-wise fission rate distributions were calculated for three selected fuel assemblies in the operational state at full power.

| State | MCNP | σ | MCU | σ |
|---|---|---|---|---|
| 1 | 1.03770 | 0.00007 | 1.03341 | 0.00013 |
| 2 | 1.05132 | 0.00010 | 1.04719 | 0.00012 |
| 3 | 0.93416 | 0.00010 | 0.93237 | 0.00010 |
| 4 | 1.13871 | 0.00011 | 1.13390 | 0.00012 |
| 5 | 1.15400 | 0.00010 | 1.14932 | 0.00012 |
| 6 | 1.04729 | 0.00011 | 1.04267 | 0.00009 |

Table 4.1: Monte Carlo results for the multiplication factor of the VVER full core benchmark.

For the MCNP-4C calculations, nuclear point data mainly on the basis of JEF-2.2 were used. For all states, calculations were also performed with the Monte Carlo code MCU [GOM-99] with its accompanying MCUDAT-2.2 nuclear data library, and the results were compared. Table 4.1 gives the calculated multiplication constants with their corresponding statistical uncertainties. An acceptable agreement is observed in all cases, with slightly higher MCNP values and a maximum difference of ~ 500 pcm.

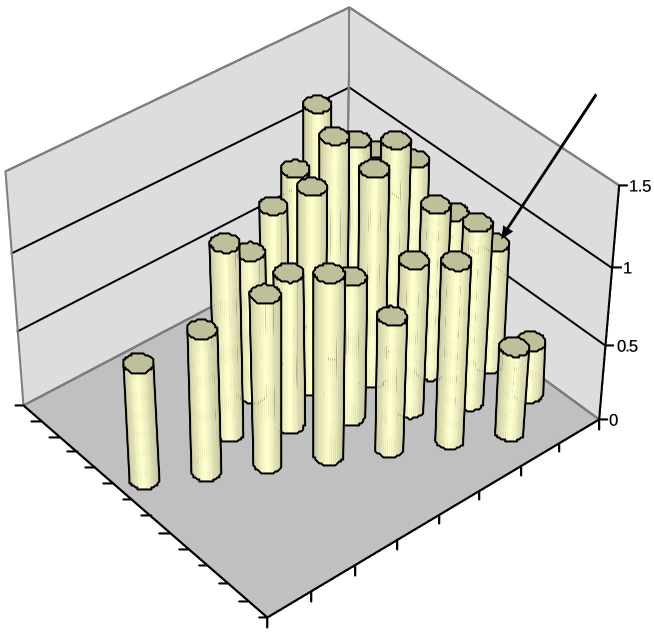


Figure 4.3: Fuel assembly fission rate distribution for the full power state of the VVER-1000 core benchmark, calculated with MCNP. The statistical uncertainties are σ ~ 0.05 – 0.2 %.

In Fig. 4.3, the fuel assembly fission rate distribution for the operational full power state is displayed. The distribution exhibits a typical shape with its maximum close to the core periphery and a local minimum in the core centre, due to the core loading with most of the fresh fuel assemblies placed in the outer region of the core. The distributions calculated with MCNP and MCU are in very good agreement for all six reactor states, with typical relative differences of 1 – 2 % and a maximum difference of 4 % in one case.

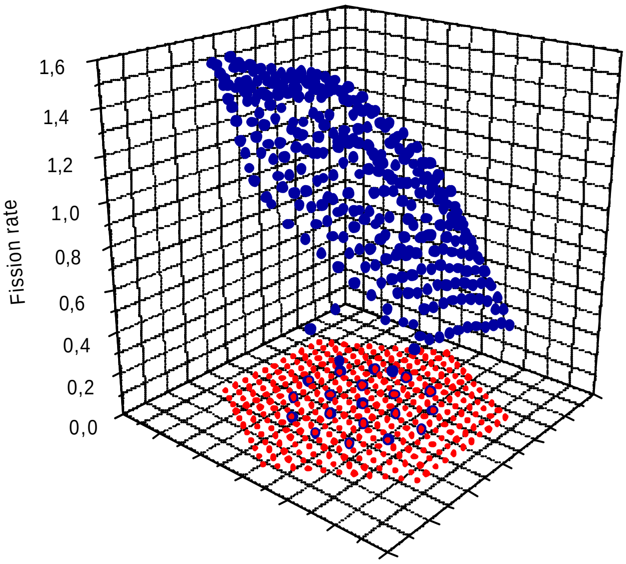


Figure 4.4: Pin-wise fission rate distribution in a peripheral fuel assembly (indicated by an arrow in Fig. 4.3) for the full power state of the VVER-1000 core benchmark, calculated with MCNP. The statistical uncertainties are $\sigma \sim 1$ %.

Figure 4.4 shows the pin-wise fission rate distribution for one selected fuel assembly calculated with MCNP. The tilt in the distribution is according to the position of the fuel assembly at the periphery of the reactor core. The statistical uncertainties for the pin-wise values are $\sigma \sim 1$ %. A very large number of neutron histories have to be tallied to make the statistical uncertainties satisfactorily small for such local quantities. A comparison of the pin-wise values calculated with MCNP and MCU, normalized to the same fuel assembly fission rates, yields excellent agreement for all three fuel assemblies under consideration. The relative differences exceed 2.5 % only for ~ 60 out of 936 fuel pin positions, with maximum values of 4 %. The relative statistical uncertainties of the MCU values are similar to those of MCNP.

*4.3.3 The C5G7 3-D Extension MOX Fuel Assembly Benchmark*

The C5G7 3-D extension MOX fuel assembly benchmark [SMI-03] is designed to test the capabilities of modern deterministic transport methods and codes to calculate whole core flux distributions sufficiently well without relying upon spatial homogenisation techniques. The configuration considered is a small three-dimensional PWR core with 90° symmetry containing two $UO_2$ and two MOX fuel assemblies in one quarter of the core. Each assembly consists of a 17×17 lattice of square pin cells as shown in Fig. 4.5 (middle) with the side length of each pin cell equal to 1.26 cm. Fuel pins, control rod guide tubes, control rods and fission chambers are of circular shape with a 0.54 cm radius. As indicated in Fig. 4.5 (right), all fuel pin cells are composed of two different materials corresponding to the fuel-clad mix and the surrounding moderator which has the same material composition as the water reflector. In contrast to the fuel pin cells, both the control rod guide tubes and the fission chambers are also present in the upper axial reflector. The overall dimensions of the problem are $64.26 \times 64.26 \times 64.26\ cm^3$ with the 2-D dimensions of each fuel assembly being $21.42 \times 21.42\ cm^2$. The benchmark is subdivided into three cases in which different control rod configurations have to be investigated: the *Unrodded* state and two *Rodded* states (*A* and *B*) in which the control rod clusters are partially inserted into the core at different depths. For all material compositions, a seven-group set of isotropic cross sections is provided and intended to be used for the transport calculation, including the Monte Carlo reference solution. Based on this cross section set, the multiplication constants and the pin-wise fission rates for three different axial slices have to be calculated for all three control rod cases.

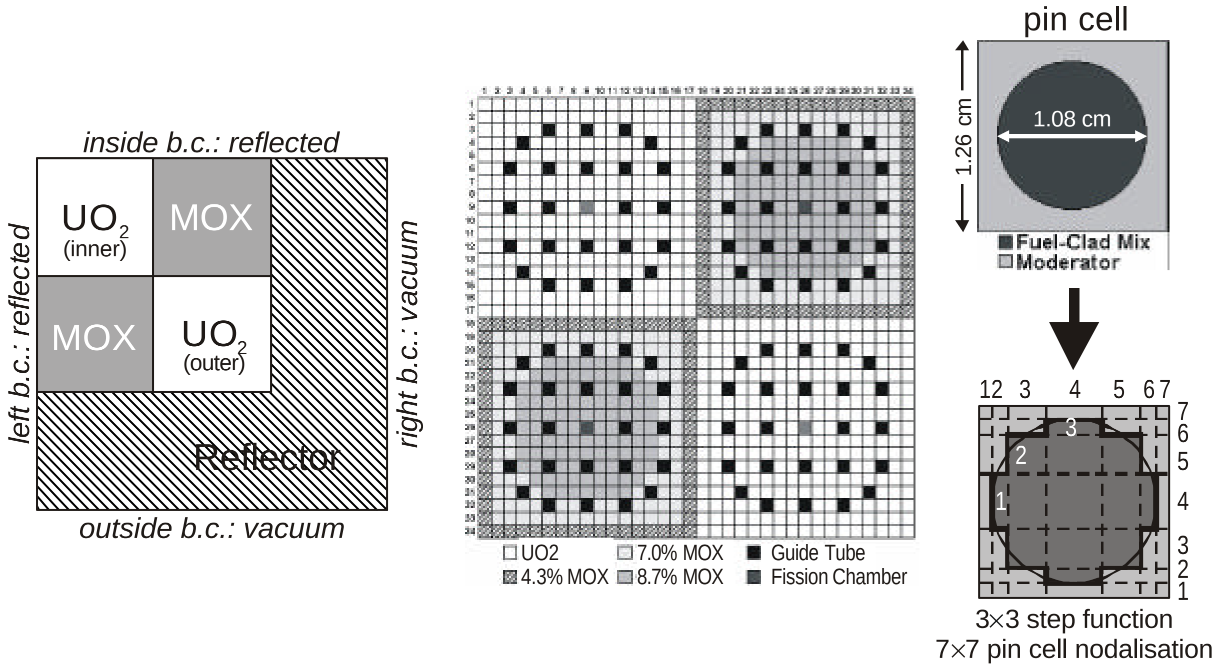


Figure 4.5: Left: Top view of C5G7-3D fuel assembly arrangement including the surrounding reflector. Centre: Pin cell layout of the fuel assemblies. Right: Approximation of the circular fuel rod boundary by a 3×3 step function.

The demand for no homogenisation at the level of pin cells requires an accurate representation of the circular fuel rod within the Cartesian geometry that was used for spatial discretisation. This is met by approximating the fuel rod boundary by an $n \times n$ step function such that, by strictly preserving the cross sectional area of the fuel rod, the area between the actual fuel rod boundary and the step function is minimised. This results in a $(2n + 1) \times (2n + 1)$ Cartesian nodalisation of each fuel pin cell. Concerning the axial discretisation, a basic mesh size of 3.56 cm is used. For a more accurate modelling of the neutron flux at interfaces between adjacent axial zones, if different material compositions are facing each other, the outermost mesh of both slices is halved to 1.785 cm. Consequently, close to an interface two nodes of this fine mesh size are used as indicated by thick lines in Fig. 4.6. Since for the *Unrodded*, *Rodded A* and *Rodded B* configuration there are one, two and three axial interfaces, respectively, the overall number of axial slices ranges from 20 for the *Unrodded* to 24 for the *Rodded B* case. Due to this detailed pin cell discretisation, the spatial discretisation of the whole core requires more than 1.6 millions of nodes for the most-elaborate discretisation with n = 3.

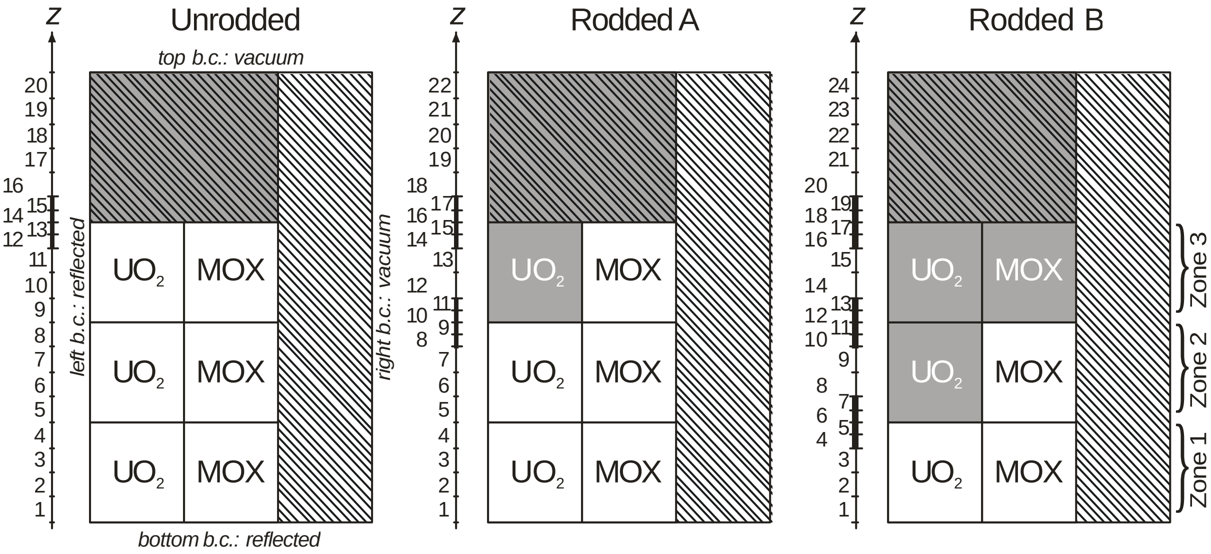


Figure 4.6: Side view of the C5G7 geometry including the details of the spatial discretisation along z-direction for the three control rod configurations with the numbers counting the axial meshes. The control rod positions are indicated by the shading whereas the hatched area denotes the reflector.

For the calculations, the $S_N$ order was also varied by using three different level-symmetric quadrature sets $S_4$, $S_8$ and $S_{16}$. The effective multiplication constant $k_{eff}$ and the relative deviation of the pin-wise fission rate from the Monte Carlo reference solution have been evaluated as a function of the order $n$ of the pin cell nodalisation. The calculations are repeated for the three different quadrature sets used. Concerning the multiplication constants, the results of our most-elaborate solution ($n$ = 3 and $S_{16}$) agree within about 0.3% with the reference solution. Obviously, there is a stronger dependence on the order of pin cell nodalisation than on the quadrature order. This qualitatively also applies to the deviation of the pin-wise fission rate from the reference solution with the deviation getting smaller as the order of the pin cell nodalisation or quadrature increases. Concerning the maximum percent error, the solution compares well to the results of the other international benchmark participants [SMI-05].

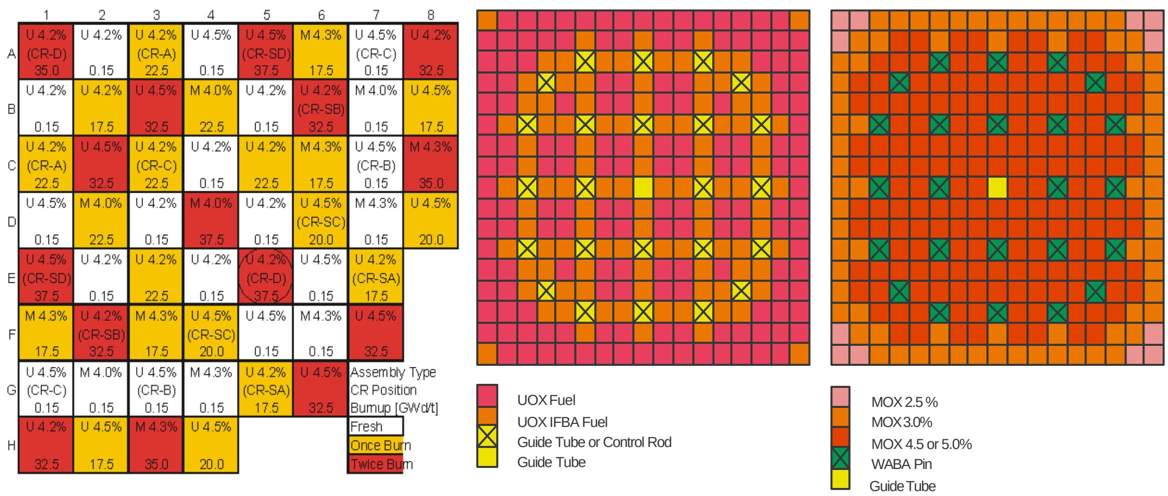


Figure 4.7. Core configuration (left) and fuel assembly layout for the $UO_2$ (centre) and MOX (right) assembly. In the core configuration, CR-A to CR-D denote four different control rod banks, and CR-SA to CR-SD refer to the four shutdown rod banks. The control rod ejection occurs in assembly E5.

*4.3.4 The PWR MOX/$UO_2$ Core Transient Benchmark*

Under the auspices of the OECD/NEA Working Party on the Physics of Plutonium Fuels and Innovative Fuel Cycles (WPPR) and the U.S. NRC, the PWR MOX/$UO_2$ Core Transient Benchmark [KOZ-03] is designed for assessing the ability of modern reactor kinetics codes to simulate a control rod ejection transient of a core partially loaded with MOX fuel. The localised perturbations of neutronic core parameters caused by the rod ejection may be enhanced by the presence of MOX fuel. In order to allow for a realistic simulation, the problem chosen for this benchmark represents a four-loop Westinghouse PWR core. The core contains 193 fuel assemblies and has 90° rotational symmetry. The fuel assembly arrangement of one quarter of the core is shown in the left of Fig. 4.7. It contains $UO_2$ and MOX fuel assemblies with different enrichments and at several burnup levels. The enrichments are 4.2% and 4.5% for $UO_2$, and for the MOX fuel, the $Pu_{fiss}$ content is 4.0% and 4.3%. Up to seven burnup states are taken into account, ranging from 0.15 GWd/tHM to 35.0 GWd/tHM. The core is surrounded by a single row of reflector assemblies of the same width as the fuel assembly containing a 2.52 cm thick baffle. The outer radial boundary condition is vacuum. In axial direction, the active fuel length amounts to 365.76 cm, a uniform fuel composition is assumed. Like in the radial direction, axial reflectors of the same height as the fuel assembly width are added to the top and bottom of the active core, and the axial boundary conditions are vacuum. Each assembly consists of a 17×17 square lattice as shown in Fig. 4.7 (centre and right). The pin cell pitch equals 1.26 cm according to the assembly width of 21.42 cm. For controlling the reactivity of the fresh fuel, 104 Integrated Fuel Burnable Absorbers (IFBA) pins are used in the $UO_2$ assemblies. A number of 24 Wet Annular Burnable Absorber (WABA) pins located at the guide tube locations have a similar purpose for the MOX assemblies. The benchmark consists of a stationary part and a transient part simulating the control rod ejection. We only considered the stationary part for which the effective multiplication constant ($k_{eff}$) and the assembly and pin power distribution for both the "All Rods Out" (ARO) and "All Rods In" (ARI) configuration at hot zero power state are to be calculated. The calculations were performed using the DORT as distributed by the OECD/NEA Data Bank.

For all materials, burnup levels and thermal-hydraulic reactor states, we performed fuel assembly calculations for all four $UO_2$ and MOX fuel assembly using HELIOS in order to generate pin cell homogenised cross sections in eight and sixteen energy groups and $P_1$ scattering order. Using these pin cell homogenised cross sections, the DORT calculation was performed for one quarter of the core in Cartesian geometry. Each pin cell is divided into 2×2 meshes which results in 289×289 meshes in x-y plane with the mesh size equal to half a pitch, i.e. 0.63 cm.

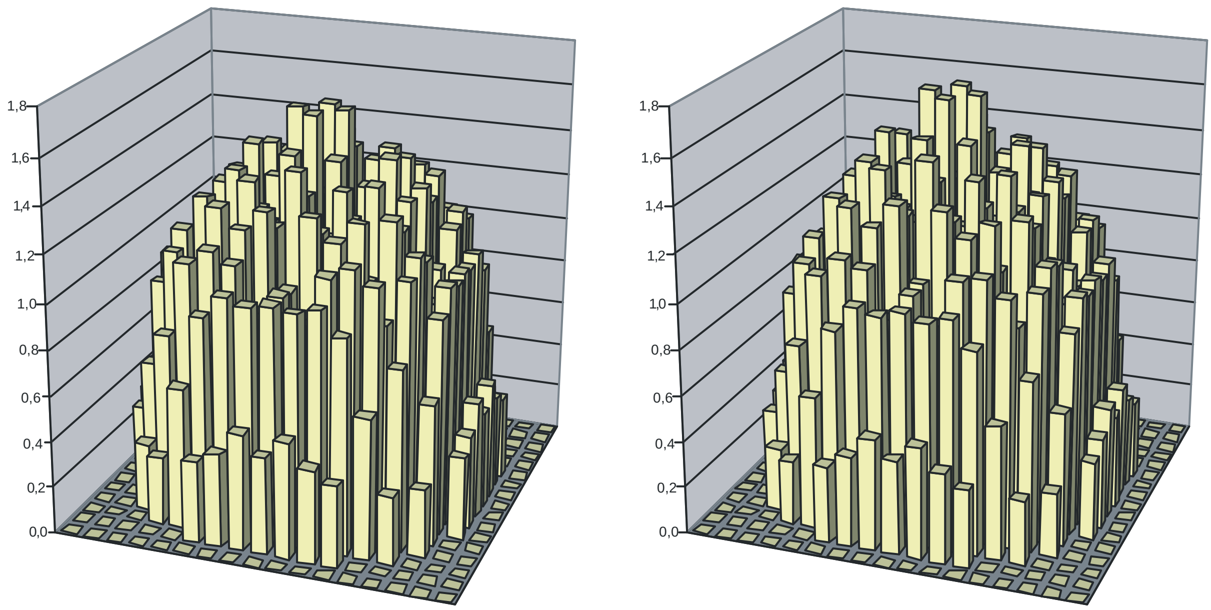


Figure 4.8: Whole core assembly power distribution of the ARO reactor state of the PWR MOX/$UO_2$ core benchmark. The DORT solution (left) using pin cell homogenised 8-group cross sections in $P_1$ scattering order is compared with the MCNP result (right) obtained with JEF-2.2 nuclear point data.

| DORT | MCNP | DeCART |
|---|---|---|
| 1.05877 | 1.06065 ± 0.00005 | 1.05852 |

Table 4.2: Effective multiplication constants of pin-by-pin calculations for the ARO reactor state of the PWR MOX/$UO_2$ benchmark: DORT with 8-group cross sections ($P_1$ scattering order), MCNP with JEF-2.2 nuclear point data and DeCART with 47-group cross sections (transport-corrected $P_0$ scattering order).

In addition to our DORT solution for the ARO reactor state, we also performed an MCNP calculation with nuclear data based on the JEF-2.2 library. In Table 4.2, the corresponding effective multiplication constants are listed together with the eigenvalue of a DeCART solution. The latter has been made available on the benchmark website and was prepared by the Nuclear Engineering Department of the Seoul National University, Korea, and the Korea Atomic Energy Research Institute using transport-corrected $P_0$ scattering order cross sections based on the HELIOS 47 energy group library without spatial homogenisation. Obviously, the eigenvalues compare very well with each other. Test calculations with $S_4$, $S_8$ and $S_{16}$ quadratures and 16 energy groups have shown that there is almost no dependence on the quadrature order and the number of energy groups used in DORT, i.e. even $S_4$ quadrature order and eight energy groups turn out to be sufficient, thereby significantly saving CPU time. This also applies to the assembly power distribution of the whole core which is shown in Fig. 4.8 for the DORT (left) and the MCNP (right) solution. However, there are still some discrepancies in the assembly power distribution of up to about 5% at the core boundary. So far, the origin of these differences has not yet been resolved entirely and needs some further systematic investigations.

## 4.4 Recent and Future Developments

At present, the majority of 3-D core models applied to LWR are based on the diffusion approximation of the neutron transport with homogenised fuel assemblies in two energy groups. This approach is essential for the development of efficient nodal solution methods,

but it limits the accuracy of local power values for single fuel rods. Stimulated by increasing computer power, current developments in the neutron kinetics field concentrate on the direct solution of the multi-group transport equation (deterministic approach) and also on Monte Carlo methods which enable first-principle calculations based on continuous energy dependence of nuclear data.
Demands for future developments may also arise from situations in which cores with mixed uranium and MOX fuel loadings are considered as well as when fresh fuel assemblies are beside high burn-up fuel. Common to these cases is the presence of different material-dependent (and thus spatial-dependent) neutron fission spectra. For such cases and other situations with, e.g., steep flux gradients close to control elements, the traditional LWR nuclear standard procedure – as far as it relies upon core calculations in diffusion approximation with two prompt neutron energy groups – may not be sufficient to correctly predict local reaction rates.

## 5 TRANSIENT REACTOR CORE AND PLANT CALCULATIONS

### 5.1 Objective

Reactor core transients determined by strong changes of the spatial power density distribution or by asymmetric conditions at the core inlet should be studied by 3-D reactor core models simulating spatial neutronics with thermal-fluiddynamic feedback. Typical core transients relevant for safety evaluation are the control rod withdrawal accidents during start-up and the very fast reactivity insertion accidents by a control rod ejection in a PWR or the control rod drop accident in a BWR.
For accident conditions which are determined by the strong coupling of the coolant flow in the primary loop and the neutronics in the reactor core, coupled codes should be applied. In these coupled codes the 3-D reactor core model is fully integrated into the thermal-hydraulic system code simulating the plant system.

### 5.2 Methods in Use

It was an international effort to develop and to validate coupled codes for applications in safety analysis. GRS has developed the coupled code system ATHLET-QUABOX/CUBBOX by coupling the thermal-hydraulic system code ATHLET [LER-98] with the reactor core model QUABOX/CUBBOX [LAN-96a, LAN-96b]. Within bilateral co-operations also other 3-D reactor core models have been coupled with ATHLET like BIPR8 from Kurchatov-Institute, DYN3D from FZ Rossendorf, KIKO3D from KFKI (AEKI) Budapest and SADCO from RDIPE. In the international framework all known system codes like CATHARE, TRAC or RELAP have been coupled with 3-D reactor core models. For the validation of these coupled codes several benchmarks have been performed within the OECD activities for LWR core transient benchmarks. A separate presentation is dedicated to this topic during this seminar [IVA-05]. Following benchmark cases have been studied for LWRs: a PWR main steam line break (MSLB) benchmark for TMI-1 [NEA-99, LAN-03], a BWR turbine trip (TT) benchmark in Peach Bottom-2 [NEA-01, LAN-04] for which experimental data were available. For both benchmark problems good results were obtained by the coupled code ATHLET-QUABOX/CUBBOX. For the PWR MSLB benchmark, the observed differences between different solutions have been sufficiently explained. For the BWR turbine trip transient very good agreement was achieved for measured data like pressure, reactor power and local power values from local power range monitors. The benchmark activity is continuing by an analysis of a VVER-1000 transient [NEA-02].

### 5.3 Recent and Future Developments

Important aspects for future developments arise from increased safety requirements which can only be met by improved calculation models. In particular, optimised fuel rod modelling including refinements of the fuel-cladding gap description or burnup-dependent fuel rod heat conduction may become more and more relevant. International activities therefore continuously focus on whole core calculations with pin-wise representation.
This also applies to transient core calculations. At GRS, therefore, considerable effort is being made to develop transport codes that directly solve the time-dependent $S_N$ transport equations in multi-energy group representation without further approximations. Stimulated by the good experiences gained with the application of the DOORS codes to numerous benchmarks and critical experiments, both the 2-D code DORT and the 3-D counterpart TORT have been extended for treating time-dependent problems (DORT-TD and TORT-TD), thereby preserving their original capabilities of solving the stationary $S_N$ transport equation. For the discretisation of the time derivative, the unconditionally stable fully-implicit time discretisation scheme has been applied. Since this procedure results in a (formal) stationary transport equation with a time-dependent external distributed source that is to be solved for the fluxes at each time step, stationary transport codes like DOORS are well suited for the solution of implicitly discretised time-dependent problems. Provision must be made for the delayed neutrons. Their spatial concentration must be accounted for by the solution of an additional balance equation which in DORT-TD and TORT-TD is also discretised implicitly with respect to the time variable.
In a first step, the 2-D code DORT-TD has also been coupled with the ATHLET thermal-hydraulic system code. Experiences have been gained with the application to the research reactor FRM II in Garching [PAU-03]. The most-recent development is the transient version TORT-TD which in principle allows for full 3-D transient core calculations. First test calculations based on the transient part of the PWR MOX/$UO_2$ control rod ejection transient benchmark (see section 4.1) are in progress. To this aim, a general capability for control rod element movements has been implemented. At present, we are working on the implementation of feedback models. As a part of these, a fuel rod heat conduction model is currently being included which allows for the calculation of the radial temperature profile of fuel rods composed of different material layers with varying temperature-dependent heat conduction coefficients. In combination with cross section libraries that are parametrised with respect to thermal-hydraulic quantities like temperature and moderator density, TORT-TD will be capable of performing 3-D time-dependent transport calculations including feedback with arbitrary numbers of prompt and delayed neutron energy groups and arbitrary scattering order.

## 6 CONCLUSION

This paper gives an overview on the methods and computer codes, which are developed and applied in GRS to nuclear design and accident simulations. All steps of nuclear calculations are covered either by computer codes which have been originally developed by GRS or by external codes for which GRS has achieved extended application experiences.
The main field of code development work in GRS was the field of static and transient reactor core calculations by the reactor core model QUABOX/CUBBOX and the field of thermal-hydraulic plant transient and accident analysis by the system code ATHLET.
In the past, the nuclear data for core calculations have been mainly provided by the standard fuel assembly burn-up codes CASMO or HELIOS within co-operations with other institutions for specific applications. For reference calculations and independent evaluations of fuel assembly designs a nuclear data library based on recent releases of JEF-2.2, ENDF/B-V and JENDL-3.2 was established to perform Monte Carlo calculations by MCNP using point data.
During the validation of nuclear data libraries by critical experiments, great experience was gained for MCNP calculations. It was demonstrated at the example of the VVER-1000

reactor core benchmark that full-scale core calculations with pin-wise resolution are feasible. The calculational scheme using the Monte Carlo code MCNP with point data is considered as a reference tool to study critical systems with complex geometry and material compositions.

An important aspect of fuel assembly calculations is the determination of the reactivity dependence on burn-up and the accurate determination of nuclide inventories. In this field GRS has developed the reactivity and nuclide inventory code KENOREST to have an independent method available for comparisons with other standard solution methods. This programme which uses updated and extended ORIGEN libraries, allows nuclide inventory calculations of high accuracy using a complete set of nuclides and corresponding reaction chains avoiding reductions and simplifications. The validation of KENOREST is on-going.

For best-estimate reactor core and plant transients, the coupled code ATHLET-QUABOX/CUBBOX was developed. In the framework of the international OECD benchmark activities for LWR core transients, it was extensively validated and compared with other available coupled code systems. Meanwhile, all internationally known system codes have the capability of integrated 3-D reactor core models. It is agreed that coupled codes are important to perform realistic plant transient analyses for all accident conditions with strong coupling between coolant flow and neutronics.

The application of the diffusion approximation for reactor core calculations may limit the accuracy for local pin-wise effects relevant for safety. Therefore, the further code improvements in the nuclear field tends to apply neutron transport methods for future reactor core calculations. In GRS the deterministic neutron transport codes from the DANTSYS and DOORS packages have been successfully applied for a series of stationary problems. In first prototypes the DORT/TORT codes of 2-D/3-D geometry have been extended for transient calculations and experience has been obtained by solving benchmark problems. The future application for reactor core calculations needs still more computer capacity and improvements in providing multi-group data including burn-up and thermal-hydraulic dependence. The positive experience gained in GRS is very promising for future developments.

## References


[ALC-95] R.E. Alcouffe, R.S. Baker, F.W. Brinkley, D.R. Marr, R.D. O'Dell, W.F. Walters, "DANTSYS: A Diffusion Accelerated Neutral Particle Transport Code System", LANL LA-12969-M (1995).

[ALY-02] S.S. Alyoshin et al., "Core Benchmarks for Verification of Production Neutronic Codes as Applied to VVER-1000 with MOX Fuel Plutonium from Surplus Russian Nuclear Weapons", PHYSOR, Seoul, Korea, Oct. 2002.

[BER-01] W. Bernnat, S. Langenbuch, M. Mattes, W. Zwermann, "Nachrechnung von LWR-Benchmarks mit dem Monte-Carlo-Programm MCNP auf Basis verschiedener Kerndatenevaluierungen", Jahrestagung Kerntechnik, May 2001

[BRI-00] J.F. Briesmeister, Editor, "MCNP – A General Monte Carlo N-Particle Transport Code – Version 4C", LANL Report LA-13709-M (2000)

[CAS-91] J.J. Casal, R.J.J. Stamm'ler, E.A. Villarino, A.A. Ferri, "HELIOS: Geometric Capabilities of a New Fuel-Assembly Program", Intl. Topical Meeting on Advances in Mathematics, Computations, and Reactor Physics, Pittsburgh, USA, April 1991

[GOM-99] E.A. Gomin, L.V. Maiorov, "The MCU Monte Carlo Code for 3-D Depletion Calculation", Proc. Of Intern. Conf. on Mathem. And Comput., Reac. Phys. And Envir. Analyses in Nuclear Applications, Madrid, Spain, Sep. 1999

[HES-00] U. Hesse, B. Gmal, T. Voggenberger, M. Baleanu, K. Hummelsheim, W. Heinicke, W. Zwermann, S. Langenbuch," KENOREST, A New Three Dimensional Fuel Assembly Code System Combining Keno-V.A and OREST for Reactivity and Inventory Calcula¬tions", ANS Interna¬tional Topical Meeting

PHYSOR 2000, Pittsburgh, Pennsylvania, USA, May 2000
[HES-88] U. Hesse, "OREST – The HAMMER-ORIGEN Burn-up Program System: Methods and Results", Nuclear Technology, Vol. 82, Aug.1988.
[IVA-05] K. Ivanov, E. Sartori, E. Royer, S. Langenbuch, K. Velkov Validation of coupled thermal-hydraulic and neutronics codes in international co-operation, EUROSAFE2005, Brüssel, November 7-8, 2005
[JEF-05] "JEFF-3.1 Joint Evaluated Fission and Fusion Data Library", May 2005, available from NEA Data Bank: http://www.nea.fr/html/dbdata/pubs/jeff31-cd.html
[JEN-02] K. Shibata et al., "Japanese Evaluated Nuclear Data Library Version 3 Revision-3: JENDL-3.3", J. Nucl. Sci. Technol. 39, 1125 (2002)
[JOH-90] E. Johansson, "Data and Results for KRITZ Experiments on Regular $H_2O$/Fuel Pin Lattices at Temperatures up to 245°C", STUDSVIK/NS-90/133 (1990)
[KOZ-03] T. Kozlowski, T. J. Downar, "OECD/NEA and U.S. NRC PWR MOX/$UO_2$ Core Transient Benchmark," Working Party of the Physics of Plutonium Fuels and Innovative Fuel Cycles, OECD/NEA Nuclear Science Committee (2003)
[LAN-03] Langenbuch, S., Schmidt, K-D., Velkov, K., Analysis of the Pressurized Water Reactor Main Steam Line Break Benchmark by the Coupled Code System ATHLET-QUABOX/CUBBOX, Nuclear Technology, Vol.142, Number 2, May 2003.
[LAN-04] Langenbuch, S., Schmidt, K-D., Velkov, K., Analysis of the OECD/NRC BWR Turbine Trip (TT) Benchmark by the Coupled Code System ATHLET-QUABOX/CUBBOX, Nuclear Science and Engineering, 148,270-280 (2004)
[LAN-77a] Langenbuch, S., Maurer, W., Werner, W., Coarse Mesh Flux Expansion Method for the Analysis of Space-Time Effects in Large LWR Cores, Nuclear Science and Engineering, 63, 437-456,(1977)
[LAN-77b] Langenbuch, S., Maurer, W., Werner, W., High-Order Schemes for Neutron Kinetics Calculation based on a Local Polynomial Approximation; Nuclear Science and Engineering 64, 508-516,(1977)
[LAN-96a] Langenbuch, S., Lizorkin, M., Rhode, U., Velkov, K., 3-D Neutronic Codes coupled with Thermal-Hydraulic System Codes for PWR, BWR and VVER Reactors. OECD/CSNI Workshop on Transient Thermal-Hydraulic and Neutronic Codes Requirements, Annapolis, Md., U.S.A., November 5-8, (1996)
[LAN-96b] Langenbuch, S., Austregesilo, H., Fomitchenko, P., Rhode, U., Velkov, K., Interface Requirements to Couple Thermal-Hydraulic Codes to 3-D Neutronic Codes. OECD/CSNI Workshop on Transient Thermal-Hydraulic and Neutronic Codes Requirements, Annapolis, Md., U.S.A., November 5-8, (1996)
[LER-98] Lerchl,G., Austregesilo, H., ATHLET Mod 1.2 Cycle A, User's Manual, March, GRS-P-1/Vol.1,Rev.1. (1998)
[MAC-94] R.E: MacFarlane, D.W. Muir, "The NJOY Nuclear Data Processing System, Version 91", LANL Report LA-12740-M (1994)
[NEA-01] Solis, J., Ivanov, K., Sarikaya, B., Olson, A., Hunt, K., Boiling Water Reactor Turbine Trip (TT) Benchmark, Volume 1: Final Specifications, NEA/NSC/DOC(2001) 1
[NEA-02] B. Ivanov, K. Ivanov et al., VVER-1000 Coolant Transient Benchmark, Vol. I: Main Coolant Pump (MCP) Switching On - Final Specifications, NEA/NSC/DOC(2002)6
[NEA-04] "Benchmark on the Three-dimensional VENUS-2 MOX Core Measurements", OECD/NEA Report NEA/NSC/DOC(2003)5, January 2004
[NEA-95] International Handbook of Evaluated Criticality Safety Benchmark Experiments NEA/NSC/DOC(95)03 (release Sept.2005), available from NEA Data Bank: http://www.nea.fr/abs/html/nea-1486.html
[NEA-99] NEA/NSC/DOC(99) 8, PWR Main Steam Line Break (MSLB) Benchmark, Volume 1: Final Specification.
[OBL-04] P. Oblozinsky, "The Status of the ENDF Project", WPEC Meeting, Aix-en-

Provence, France, May 2004
[PAU-03] A. Pautz, A. Birkhofer, “Coupling of Time-Dependent Neutron Transport Theory with Thermal Hydraulics Code ATHLET and Application to the Research Reactor FRM-II”, Nucl.Sci.Eng. 145, 320-341 (2003)
[SCA-04] “SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation”, NUREG/CR-0200, Rev. 7, ORNL/NUREG/CSD-2/R7, (2000)
[SMI-03] M. A. Smith, G. Palmiotti, T. A. Taiwo, E. E. Lewis, N. Tsoulfanidis, “Benchmark specification for deterministic MOX fuel assembly transport calculations without spatial homogenisation (3-D extension C5G7 MOX),” NEA/NSC/DOC, 6 (2003).
[SMI-05] M. A. Smith, E. E. Lewis, B.-C. Na, N. Tsoulfanidis, G. Palmiotti, T. A. Taiwo and R. N. Blomquist, Benchmark on deterministic transport calculations without spatial homogenisation, NEA/NSC/DOC(2005), *in preparation*