

MONTE CARLO REACTOR PHYSICS CALCULATIONS FOR CRITICAL ASSEMBLIES AND LWR FULL CORE MODELS

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ABSTRACT

Monte Carlo criticality calculations with both point-wise and multigroup nuclear data are presented. The validation of methods and data by re-calculation of benchmark experiments is summarised. Then, results of applications to reactor physics calculations for large power reactors are given. Details of these calculations are analysed, like the convergence of power distributions, reaction rates, and neutron spectra in small spatial regions. For compact systems like benchmark experiments and research reactors the Monte Carlo method is well established. For full core power reactor design and safety related calculations the applicability must be still demonstrated and further experience should be obtained.

1. INTRODUCTION

The Monte Carlo method is a reference tool for criticality calculations since it enables the very detailed description of the problems in phase space. Especially the method with continuous description of energy dependent cross sections solves problems with complex configurations of resonance absorbers and moderators with a high degree of accuracy. The more regular configurations also can be treated by methods based on multigroup theory if a sufficient number of groups are used or the corresponding spectrum for condensation of few group constants describes the cell adequately. Here, in particular a detailed calculation of the spectrum in the resolved resonance range is required at least for a regular cell to take into account both self and mutual shielding effects due to all resonances of a mixture of resonance absorbers.

The successful application of the described methods is proven by a large number of re-calculations of carefully evaluated experiments, so called benchmarks. In the following section, our contribution to the validation of methods and corresponding basic nuclear data are summarised. Since from the present results it can be concluded that the Monte Carlo method and the corresponding nuclear data sets allow the treatment of a large variety of problems from first principles with a comparable small error due to the geometrical problem description and the nuclear data base, the method is also suitable for calculating configurations for which experiments are not yet performed, or for configurations ex-

pected after severe accidents for which experimental data do not exist. Furthermore, the method is suitable to prove and validate the design methods applied in reactor calculations.

It is obvious that there is the possibility to use the Monte Carlo method also for design and safety related calculations for large power reactors. Besides the high need for computer time, it has to be proven whether one can obtain sufficiently reliable results for such large systems partly with weakly coupled regions due to the size of the reactor. A further task is the treatment of complex material composition of power reactors due to the inhomogeneous burn-up distribution. Here, problems arise due to high computer time and memory requirements which necessitate effective storage concepts and parallel computing.

2. APPLICATION FOR SMALL CRITICAL SYSTEMS

For the validation of program systems and nuclear data bases, Monte Carlo methods, especially with continuous representation of the energy dependency of cross sections, as realised in the program MCNP, are established and serve generally as best estimate methods. This was demonstrated by the re-calculation of a large number of well defined and “clean” experiments (benchmarks), e.g. from the International Handbook of Evaluated Criticality Safety Benchmark Experiments [1], KRITZ-2 [2], ANS benchmarks [3], VENUS-2 [4], and others [5].

The nuclear point data libraries to be used with MCNP [6], as well as the data for the thermal range represented by $S(\alpha, \beta)$ scattering laws, were generated with NJOY [7]. A very extensive set was generated from the JEF-2.2 file, and data containing limited numbers of nuclides also from other evaluations (preliminary JEFF-3, ENDF/B-VI rel.5, and JENDL-3.2). The point data were generated with a uniform reconstruction accuracy of 0.1 %, with temperatures up to 3000 K on fixed grid points. For temperatures between the grid points, an interpolation procedure is applied.

The result of these calculations showed an overall good agreement with the corresponding experimental values, partly depending on the nuclear data sources which the calculations were based on.

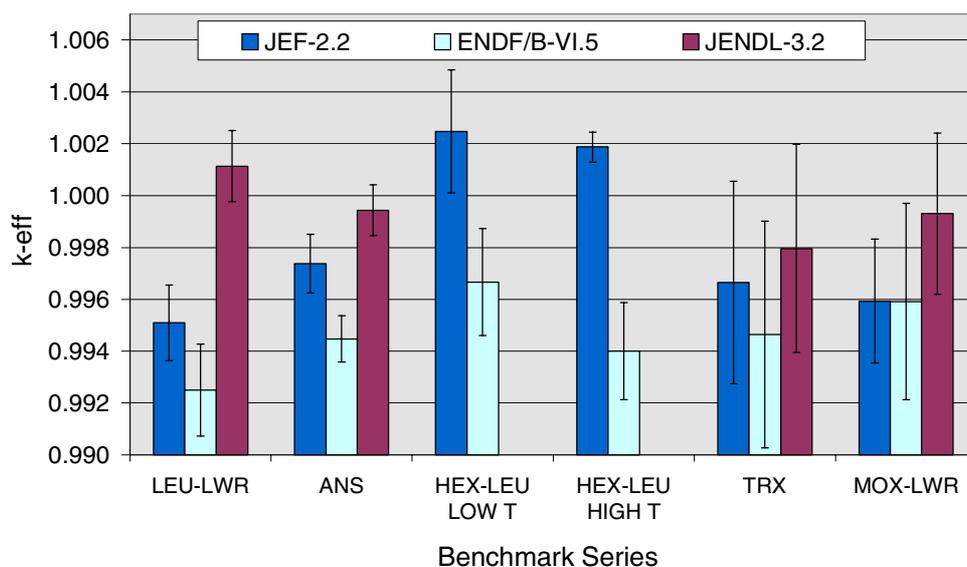


Figure 1. MCNP results for multiplication constants of heterogeneous systems with different nuclear data.

This is demonstrated in Fig. 1, where averages of MCNP results for the multiplication constants of heterogeneous LWR systems obtained with different nuclear data libraries are displayed. The multiplication constants derived from the experiments are all 1.0. Averages are given for square lattices with LEU and MOX fuel (LEU-LWR and MOX-LWR), hexagonal lattices with LEU fuel (HEX-LEU), as well as for a set of ANS LWR benchmarks and TRX experiments.

For most of the benchmarks considered, the experimental values are slightly underestimated by the JEF-2.2 results. For Uranium systems, this underestimation becomes more pronounced when ENDF/B-VI rel.5 data are used; the same trend is observed with JEFF-3 data (see also [5]). With the Japanese JENDL-3.2 library, the multiplication constants are calculated higher on the average, leading to the most satisfying overall agreement between calculations and measurements. The described problems of ENDF/B-VI rel.5 data for U-235 are subject of further investigation in corresponding evaluation groups and hopefully will be solved in near future to have a consistent and problem independent data base for criticality calculations.

To investigate the influences of the nuclear data in more detail, we present the results of our calculations for the KRITZ-2 experiments, which are currently subject of an international benchmark effort under the auspices of OECD/NEA. The KRITZ-2 assemblies are compact square lattices with LEU or MOX fuel, inside a vessel with light water. The detailed description of the configurations denoted as KRITZ-2:1, 2:13, and 2:19, which is publicly accessible, can be found in [2]. These are two Uranium cores and a MOX core, each in a cold and hot state with a temperature of ~ 240 °C. The array size is between 25 x 24 and 44 x 44 pin cells, and the moderated fuel height is between 65 and 110 cm. Criticality was obtained by varying the water level and the boron concentration in the moderator.

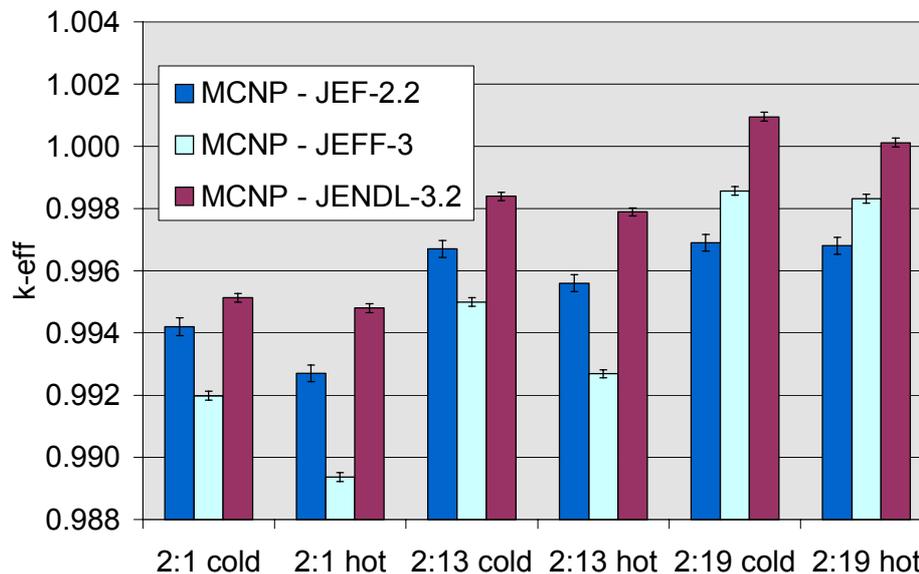


Figure 2. MCNP results for multiplication constants of the KRITZ-2 experiments with different nuclear data.

Figure 2 presents the multiplication constants for all KRITZ-2 assemblies obtained with MCNP and different nuclear data libraries. The k_{eff} from the experiments is 1.0 in all cases. No detailed information is available on the experimental uncertainties; according to [2], the 1σ value is supposed to be $\sim 80 \times 10^{-5}$, which had been presented in earlier work. The results with our standard JEF-2 library underestimate the experimental values for all assemblies, in particular for those with LEU. This is consistent with a general trend for heterogeneous systems displayed in Fig. 1. When using JEFF-3

data, the calculated multiplication constants for the LEU assemblies become even smaller, leading to discrepancies of about 1 % for the assembly 2:1. This is due to the increased U-235 capture cross section in JEFF-3; this nuclide is not relevant in the MOX assemblies, where the differences are small. Calculations with ENDF/B-VI rel.5 data, which are comparable to JEFF-3, give very similar results. With the JENDL-3.2 data, the situation is much improved for the LEU assemblies, although there remains a discrepancy between calculation and experiment of ~0.5 % for the assembly 2:1. For the MOX cases 2:19, the agreement with experiment is very good.

In addition to the Monte Carlo method with a point-wise representation of the nuclear data, we also applied Monte Carlo and deterministic codes with multigroup nuclear data. The calculation sequence with group data starts from a master library, generated with NJOY from the JEF-2.2 file, with an energy structure of 292 groups, with 127 thermal groups below 3 eV, covering the upscatter energy range. For the unresolved resonance region, Bondarenko factors are available and the module BONAMI of the SCALE package [8] is applied. For the resolved resonance region, the cross sections are stored on a hyperfine energy grid (up to 26 000 energy points) and by directly solving the transport equation by means of a 1D first collision probability method within the spectral code RESMOD [9], problem dependent weighted cross sections are generated for the assembly under consideration. If desired, these cross sections are finally homogenised over spatial regions and collapsed to a broad energy group structure. For the KRITZ-2 calculations, the cross sections were homogenised over the pin cell regions, with no special treatment for the fuel pins at the core surfaces, and collapsed to an 18 group structure with 6 thermal groups. Both homogenisation and condensation were performed with the SCALE module XSDRN-PM.

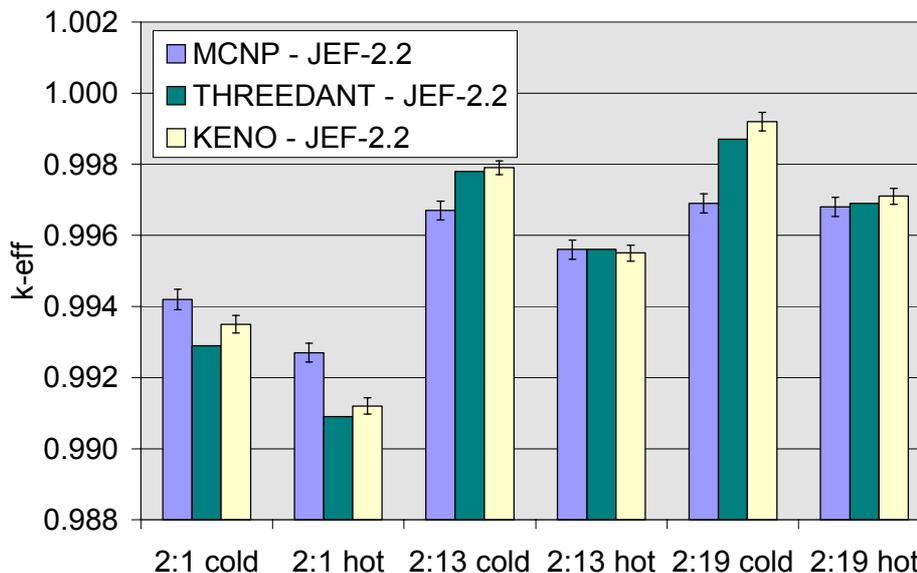


Figure 3. Results for multiplication constants of the KRITZ-2 experiments with different transport codes.

The final 3D calculations were performed with the multigroup Monte Carlo code KENO-Va [8] and the S_N code THREEDANT [10]. Figure 3 displays the multiplication constants obtained with the different codes. There is good agreement between the MCNP and the THREEDANT results for all cases, with maximal differences of less than 0.2 %. Here, one should keep in mind that the nuclear data representations for the two codes are very different (point data for MCNP vs. broad group data with additional steps in the generation process for THREEDANT). When comparing the THREEDANT and

KENO results, which both use the same JEF-2 based nuclear data, the agreement is excellent, with differences of 0.05 % and less.

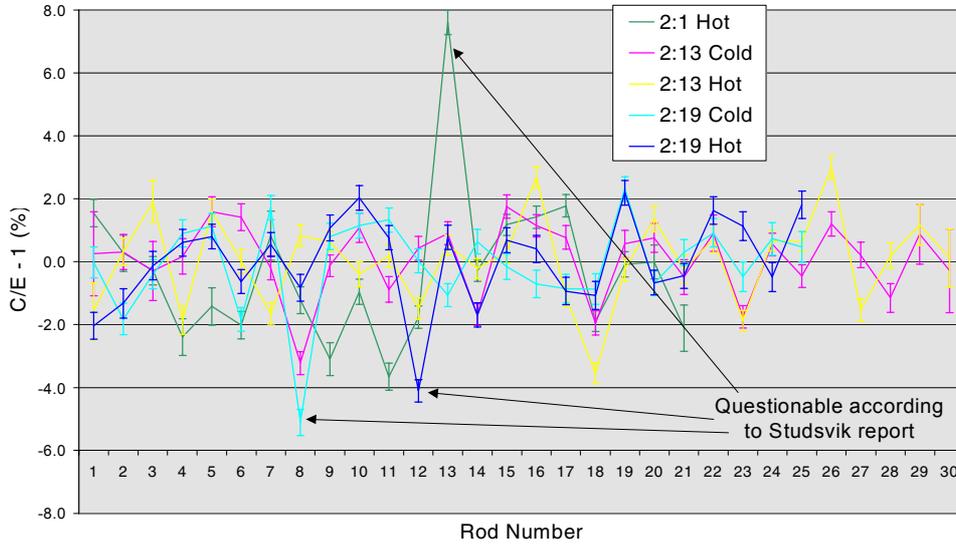


Figure 4. MCNP results for pin fission rates of the KRITZ-2 experiments compared with the measured values.

Our aim was to obtain information on the quality of the calculation results not only for integral quantities like k-eff, but also for local quantities like reaction rates and power distributions. For the KRITZ-2 assemblies, experimental information exists on fission rates at certain pin positions. The fission rates at these positions were also calculated with MCNP and THREEDANT. The agreement between measured values and MCNP results, displayed in Fig. 4, is generally satisfactory, with discrepancies $\leq 2\%$ for most of the pin positions; large differences show up for pin positions where the experimental values are doubtful according to [8].

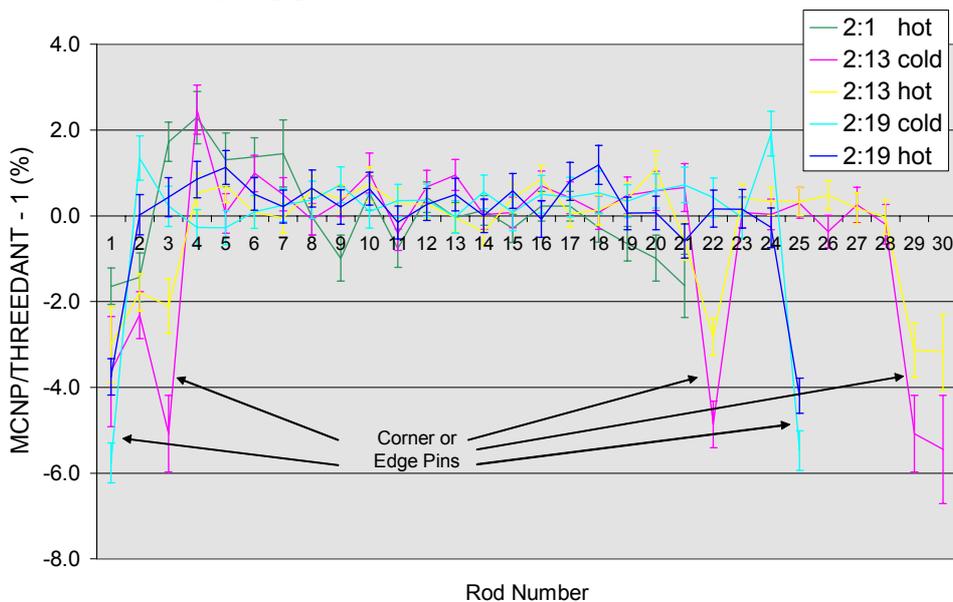


Figure 5. Comparison of THREEDANT and MCNP results for pin fission rates of the KRITZ-2 experiments.

In Fig. 5, fission rates for the KRITZ-2 assemblies calculated with the MCNP and THREEDANT codes are compared. One recognizes that the discrepancies lie within a 2 % band, with the exception of some positions with differences up to ~6 %; these are positions of corner or edge cells. The discrepancies partly originate from the one-dimensional cross section processing, which is performed in the same way for all pin cells, and does not correctly take into account the edge of the core, and partly from the rather coarse mesh in the S_N calculations (one mesh per pin cell in the fuel zone).

Another system studied in depth is the VENUS-2 experiment, also subject of an OECD/NEA benchmark activity; the 3D treatment is currently under way, results of 2D calculations are already published [4]. VENUS-2 is a heterogeneous quadratic cold LWR lattice consisting of 12 units (4 x 4 with missing corner units) with 15 x 15 pin cells each, with a hole of 10 x 10 pin cells in the centre. It contains Uranium of different enrichment in the inner part, and MOX in the outer zones. Table I shows the multiplication constants calculated with MCNP with various nuclear point data. Again we observe an underestimation of 1.0 with ENDF/B-VI rel.5.

Table I. MCNP results for multiplication constants of the VENUS-2 experiment with different nuclear data. Statistical uncertainties are ~ 0.0001 (1 σ).

	JEF-2.2	ENDF/B-VI rel.5	JENDL-3.2
k-eff	1.0028	0.9979	1.0037

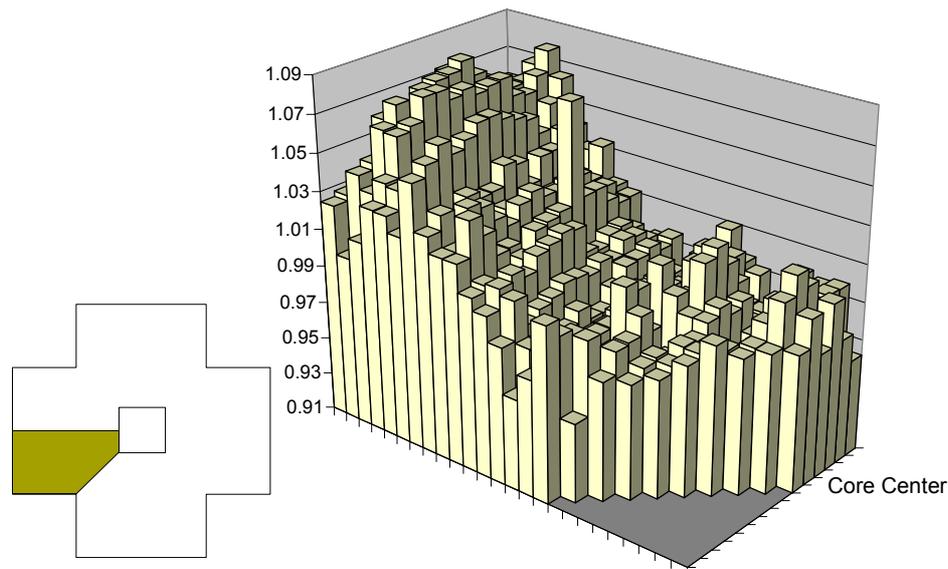


Figure 6. C/E from MCNP calculations for the fission rate distribution in the VENUS-2 benchmark (1/8 core). The shape of the whole core along with the displayed sector is sketched.

In Fig. 6, the deviations of the C/E ratio from 1 for the VENUS-2 fission rate distribution are displayed, calculated with MCNP. The agreement between calculations and measurements is satisfactory, with the exception of some regions in space. In particular, in a zone near the outer boundary (inside the MOX region), the discrepancies become unacceptably high. This trend was observed, however, also with all other submitted results of the 2D benchmark, whatever code and data were used [4], such that this issue should be investigated in more detail, also with respect to the experimental uncertainties. Within the 3D benchmark, also axial fission rate distributions for selected pins were calculated, but the experimental results are not yet released, and therefore, at the moment the quality of the results cannot be definitely assessed.

Additionally, for a system representing low enriched heterogeneous metallic Uranium fuel moderated by water, the TRX benchmarks [11] can be regarded. For these systems, the U-238 density is by a factor of two higher than in corresponding UOX fuel. Therefore, the self-shielding is higher and the resonance integral of U-238 is smaller. Furthermore, the unresolved resonance range becomes more important, so that the treatment of unresolved resonance range by means of probability table method as implemented into MCNP-4C seemed to be necessary. In fact, small differences between calculations with and without explicit treatment of unresolved resonance range could be found, but these differences were only about 0.1-0.15 % in the multiplication factor and may be negligible. This is valid also for all other benchmarks reported here. Detailed results, especially reaction rate ratios, are shown in [12]; they agree well with experimental values inside the evaluated experimental error bounds.

From these findings, it can be concluded that Monte Carlo calculations for compact and medium sized configurations, especially for LWR lattices with U or Pu as fissionable material or research reactors of various types, converge reliably with respect to integral values like k-eff, but also for detailed reaction rate ratios (TRX benchmark) or power distributions (KRITZ-2 and VENUS-2 benchmarks). Using a sufficient number of energy groups and detailed spectra for the basic cell of regular lattices, also multigroup methods based on S_N theory (e.g. the programs THREEDANT, TORT) or Monte Carlo (e.g. the programs KENO, MORSE) yield sufficient results, as a comparison of THREEDANT, KENO-Va, and MCNP for the KRITZ-2 experiment showed. Since the pre-condition of a regular lattice is not always given, especially for cases regarded in evaluation of criticality safety, re-criticality due to melting, displacement of fuel or control rod materials or de-boration etc., the Monte Carlo method with continuous representation of energy fits better the neutron interactions and resonance self-shielding for non-regular situations.

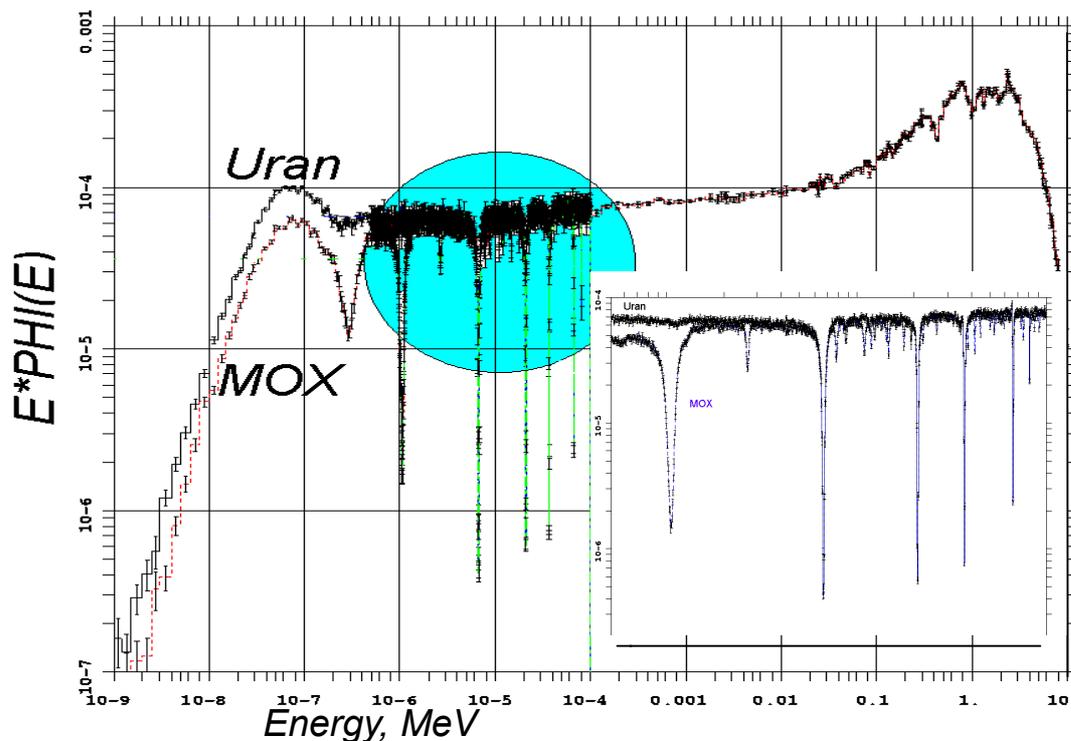


Figure 7. Detailed neutron spectra in neighbouring UOX and MOX pins calculated with MCNP

As an example, this can be demonstrated by detailed calculation of energy spectra and reaction rates in neighbouring MOX and UOX pins of a MOX assembly surrounded by UOX assemblies. Figure 7

shows spectra in MOX and UOX pins calculated by MCNP in a super fine energy resolution. The figure clearly shows the flux dips due to resonances in Pu and U-238. The corresponding (shielded) reaction rates and resonance integrals obviously converge sufficiently well so that the integral values like k-eff and power distribution can be determined for such lattices with sufficiently low statistical error. Comparisons of spectra in regular lattices calculated by means of a first collision method with 26 000 energy points in resolved energy range (RESMOD [9]) and MCNP show an excellent agreement in the frame of statistical errors of Monte Carlo calculations. This is one of the main reasons for good agreement of continuous energy Monte Carlo and multigroup transport calculations for regular lattices and a proof of the correct treatment of spatial and spectral interactions and shielding effects in MCNP.

3. APPLICATION FOR LWR FULL CORE MODELS

Important reactor design and safety parameters must be determined with a high degree of accuracy and reliability. Therefore, corresponding calculations must be performed by methods which are based on first principles and validated on experiments or operational data. Since the experiences with continuous Monte Carlo calculations based on the current evaluated nuclear data files are very promising for compact systems represented by a large number of benchmark experiments, one can conclude that this method is also applicable for large power reactors. Most design calculation methods for large power reactors use simplified methods for spectral and cell or assembly calculations and few group diffusion theory for 2D or 3D power calculations. These methods mainly are validated by comparisons with experimental data from operational conditions. An extension to ranges not covered by experiments or operational data may cause large uncertainties. For several problems in reactor safety and reactor design, an independent and validated method compared to design methods should be available for the verification of safety related parameters. Examples for such problems are severe accidents like reactivity accidents caused by control rods or by movement of fissionable or absorbing material in damaged cores, or changes of moderation conditions and de-boration of coolant as well. Furthermore, the proof and verification of fuel assembly designs with higher fissionable content and burn-up and the proof of reactivity coefficients is an important task of reactor safety.

Applications of MCNP-4C (continuous energy Monte Carlo) or KENO-Va (multigroup Monte Carlo) for 3D full core calculations are in principle possible, since the pure geometric description of core and reflector in detail is relatively easy due to the repeated structure options of these programs. These options enable a pin by pin description of all assemblies in the core together with a detailed description of control rods. For begin of life cores without burn-up and build-up of fission products, detailed 3D calculations even for large LWR can be performed.

As examples, full core calculations were performed for a typical large boiling water reactor (1300 MW_{el}) at begin of life. The core consists of 840 Uranium fuel assemblies of two different types of 8 x 8 arrays of fuel pins with different enrichments, with a central water pin, and 1 or 2 Gadolinium pins.

The core was calculated with MCNP-4C and KENO-Va. The model is very detailed, with explicit representations of each fuel pin, and each absorber pin for the controlled states. The MCNP calculations were performed with JEF-2.2 point data, and the KENO calculations with JEF-2.2 292 group data, generated with 1D RESMOD spectral calculations for the various fuel pin cells.

The results for the multiplication constants are summarised in Table II. For all calculated cases, the MCNP and KENO results are in excellent agreement, with relative differences not exceeding 0.3 %. This again indicates that the multigroup method may be successfully applied even for situations where

the pre-condition of regular lattices is not strictly fulfilled (perturbations by water gaps and absorber rods between the fuel assemblies), and that it is appropriate as an alternative to Monte Carlo calculations with point data, when independent calculation methods are desired.

Table II. MCNP and KENO results for multiplication constants of various states of a BWR core with JEF-2.2 nuclear data. Statistical uncertainties are ~ 0.0005 in MCNP and ~ 0.0003 in KENO (1σ).

	MCNP	KENO
Cold, uncontrolled	1.1327	1.1323
Cold, ~ 1 of 4 control rods withdrawn	1.0109	1.0091
Cold, controlled	0.9476	0.9457
Cold, controlled, 1 central control rod withdrawn	0.9767	0.9744
Cold, controlled, 5 central control rods withdrawn	1.0518	1.0510
Cold, controlled, 6 central control rods withdrawn by 53 cm	0.9983	0.9988
Hot, uncontrolled, 40 % void	1.0995	1.0960

The Monte Carlo calculations of effective multiplication constants for the different configurations listed in Table II converged in reasonable time and matched the usual statistical checks, provided that a reasonable neutron starting source is chosen. Not only the total reactivity worth of control rod banks, but also the reactivity as a function of bank position can be determined by Monte Carlo with sufficient statistical accuracy as shown in Fig. 8 for a 350 MW_{el} PWR at BOL.

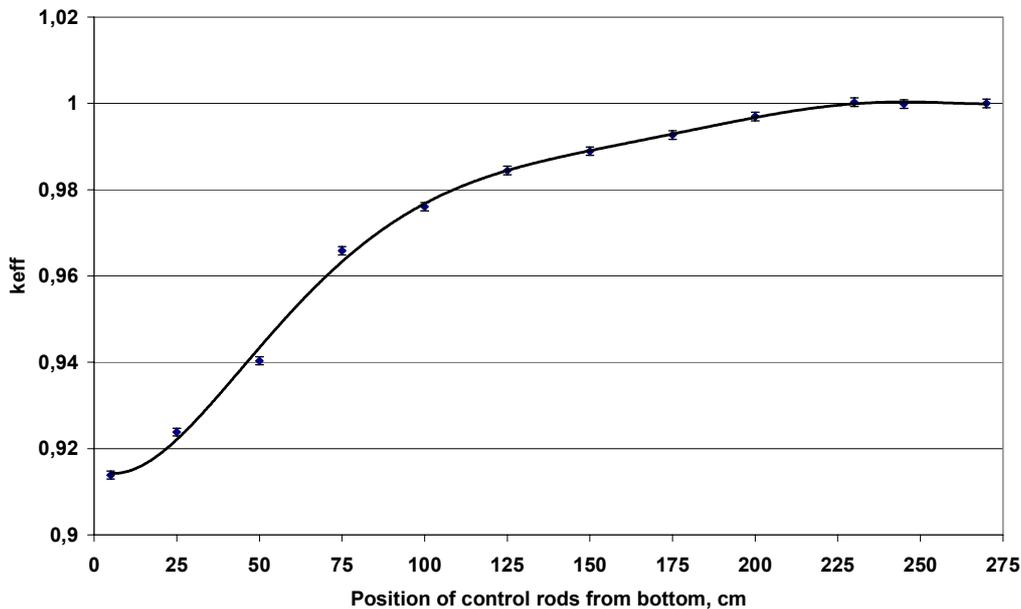


Figure 8. MCNP results for k-eff as a function of control rod position for a 350 MW_{el} PWR at BOL.

We found, however, some problems for the axial and azimuthal power distributions for large cores due to the weak coupling of core regions. Here, the power distributions converged very slowly with a different characteristic compared to the effective multiplication constant. This was the case for all Monte Carlo programs applied (MCNP, KENO-V and MORSE). An example is the axial power distribution from a full core calculation of the large BWR described above, in the cold state at BOL. This distribution did not converge according to the evaluated statistical errors given for axial intervals as shown in Fig. 9. The estimated relative statistical error after 1000 generations with 20000 neutrons

per generation was less than 0.12 % (one standard deviation), but the corresponding power rates in symmetric intervals differed by more than 4 % after about 500 generations and about 2 % after 1000 generations.

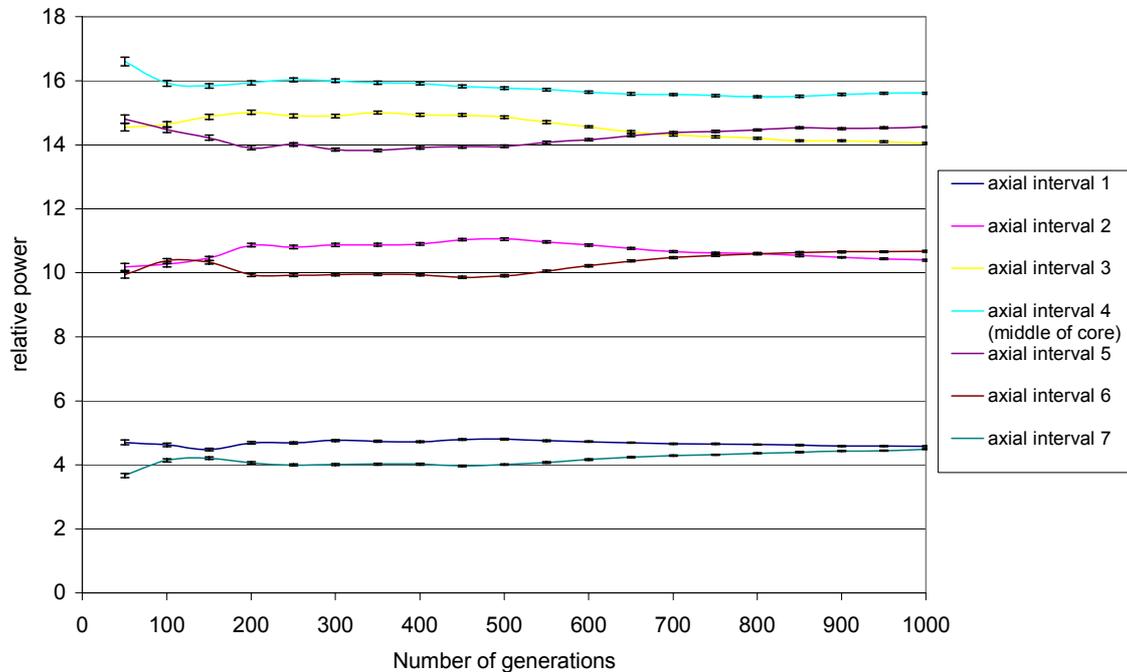


Figure 9. Relative power in 7 axial intervals for an MCNP full core BWR calculation at BOL (cold state) as a function of the number of generations with 20000 particles. Error bars: 3σ .

A similar situation was found for the power rates of the four quadrants which should be identical due to the core symmetry. In Fig. 10 the calculated power rates in the four quadrants are shown as a function of calculated generations. Here, too, after 1000 generations with 20000 neutrons deviations from symmetry of up to 4 % were found. To exclude a bias due to initial source distribution, the initial source distribution was chosen carefully and additionally, 200 generations with 20000 neutrons each were ignored for tallying the power distribution. Generally, we found that the estimated statistical errors of power rates were much lower than the deviations from the corresponding symmetrical position. It is interesting to note that the problem of convergence of axial power distribution was also found for a radial infinite lattice of fuel pins (KRITZ cell 300K) with a length of about 400 cm for the active fuel zone. Again there was a deviation from symmetry which was remarkable larger than described by the statistical error for power rates of corresponding axial segments. A two-dimensional deterministic calculation with TWODANT based on cross sections calculated by RESMOD showed correct symmetry and served as reference solution. Even after 1000 generations with 20000 neutrons deviations from reference solution of up to 3 % were found. The evaluated statistical error was remarkable lower. This is sketched in Fig. 11, where the MCNP power distribution after different numbers of generations along with the TWODANT reference distribution are given. If the axial importance was not kept constant, but taken as $1/\cos(Bz)$, the number of source neutrons per axial segment and consequently the statistical errors for axial segments with identical volumes could be kept approximately constant. This improved the convergence against the TWODANT reference solution if the axial symmetry was explicitly taken into account in the MCNP model. The deviation from the symmetric reference solution was reduced to about 0.2 %, and lay in about the range of the estimated error for axial power rates. If this symmetry was not assumed for the MCNP model, also the solution with modified importances showed similar deviations from symmetry like calculations with axially

constant importance. Here, more detailed investigations are necessary to find an improved procedure to obtain reliable reaction rate distributions for large systems.

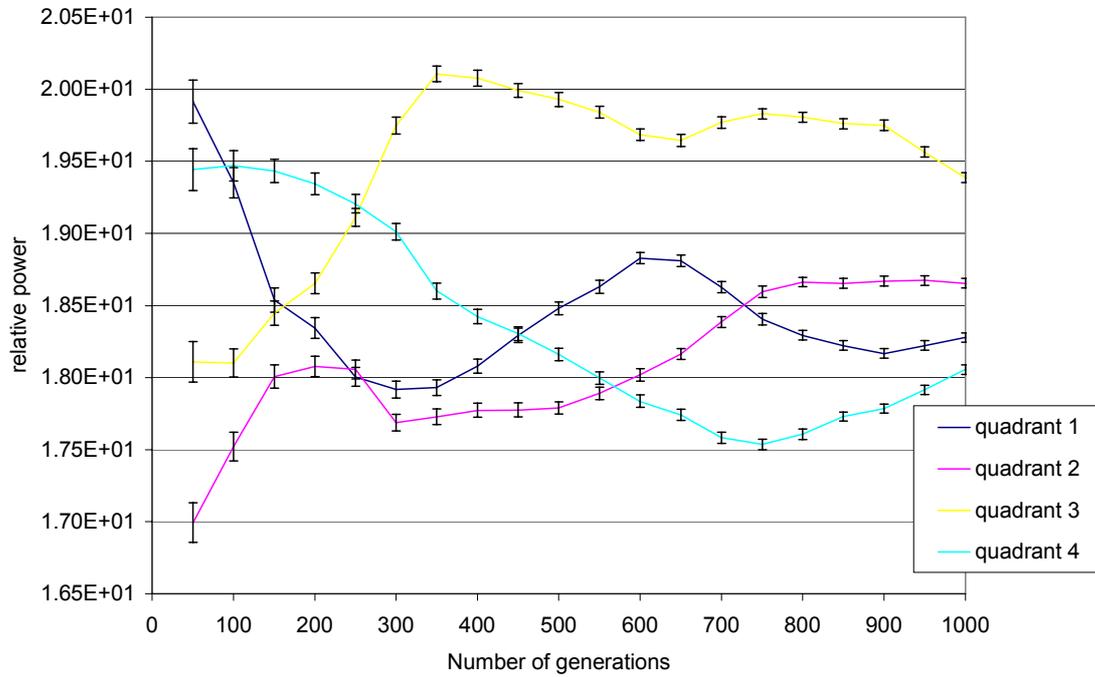


Figure 10. Relative power in the four quadrants of an MCNP full core BWR calculation at BOL (cold state) as a function of the number of generations with 20000 particles. Error bars: 3σ .

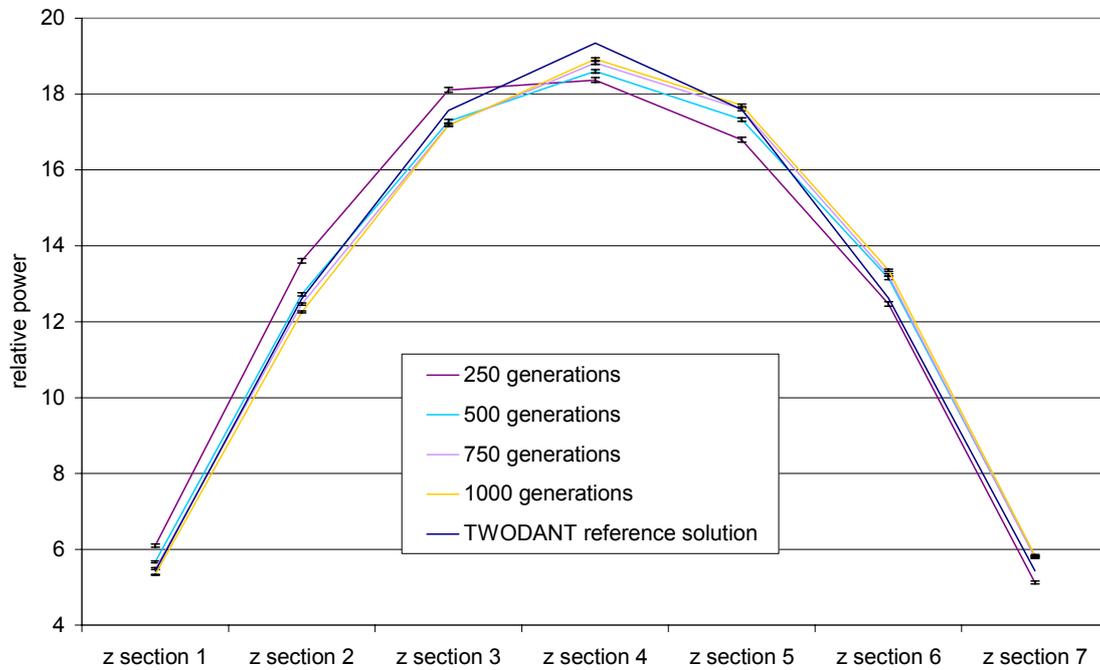


Figure 11. Relative power after different numbers of generations for a cold KRITZ pin cell as a function of the height; MCNP calculation with 20000 particles and TWODANT reference calculation. Error bars: 3σ .

The experience with the calculation of power distributions (and other reaction rate distributions) for large reactors showed that the calculated values have to be investigated carefully since the evaluated errors may be under-estimated. By means of optimisation of cell importances or other measures, the situation should be improved, especially the estimation of statistical errors. Of course, this may also require the simulation of much more neutron histories. The use of a massively parallel computer may be necessary to calculate such problems in reasonable time. Therefore, part of the MCNP calculations were performed on a CRAY T3E-512 using 64 or 128 nodes.

Further problems for full core calculations arise if the burn-up distribution has to be taken into account. The geometrical description is much more complicated since much more cells with different material description have to be identified. Even if the distribution of burn-up dependent number densities for the fuel materials are known (e.g. by design methods), the description of a large number of materials with many isotopes for actinides and fission products requires a very large memory, especially for MCNP-4C. The use of fission product cross sections with detailed pointwise representation of all resonances with a high reconstruction accuracy is practically impossible. Here, a compacted cross section set for minor fission products with about 300 energy points and only capture reaction reduces the memory requirement remarkably. An example of such a compact set compared to the full pointwise set is shown in Fig. 12. The compact cross section set is comparable to an infinite diluted multigroup cross section with 300 groups.

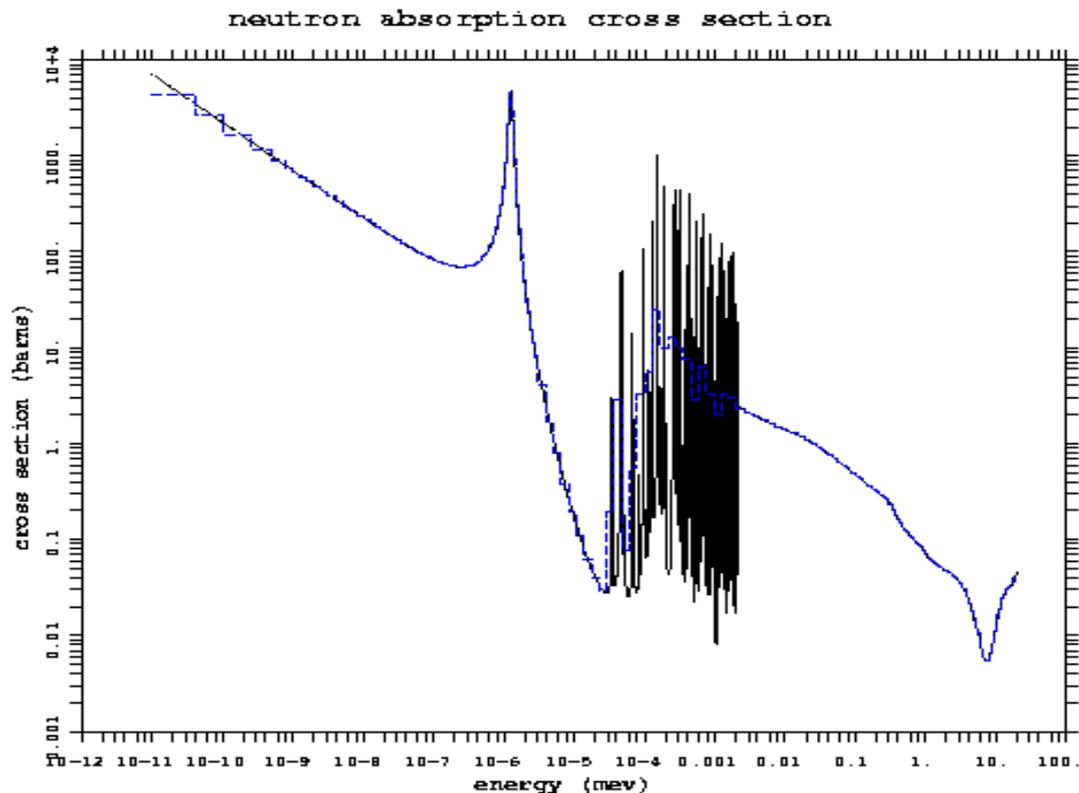


Figure 12. Neutron absorption cross section for Rh-103 in compact (blue) and pointwise (black) MCNP format.

Calculations with the explicit pointwise cross section sets for 85 fission products and 5 explicit and 80 compact fission products showed practically no difference in k_{∞} for a pin cell (see Fig. 13). This means that the compacted form of cross section sets is sufficient for most fission products. If, how-

ever, the compact fission products are neglected, huge differences between the calculated multiplication constants arise with increasing burn-up. Furthermore, the compact form of cross sections can also be used as macroscopic cross section since the elastic scattering can be neglected. This leads to a further reduction of memory requirements. The memory requirement for full core calculations with burn-up dependent cross section sets is a severe problem for parallel computers with distributed memory like CRAY-T3E with relatively small memory size per node.

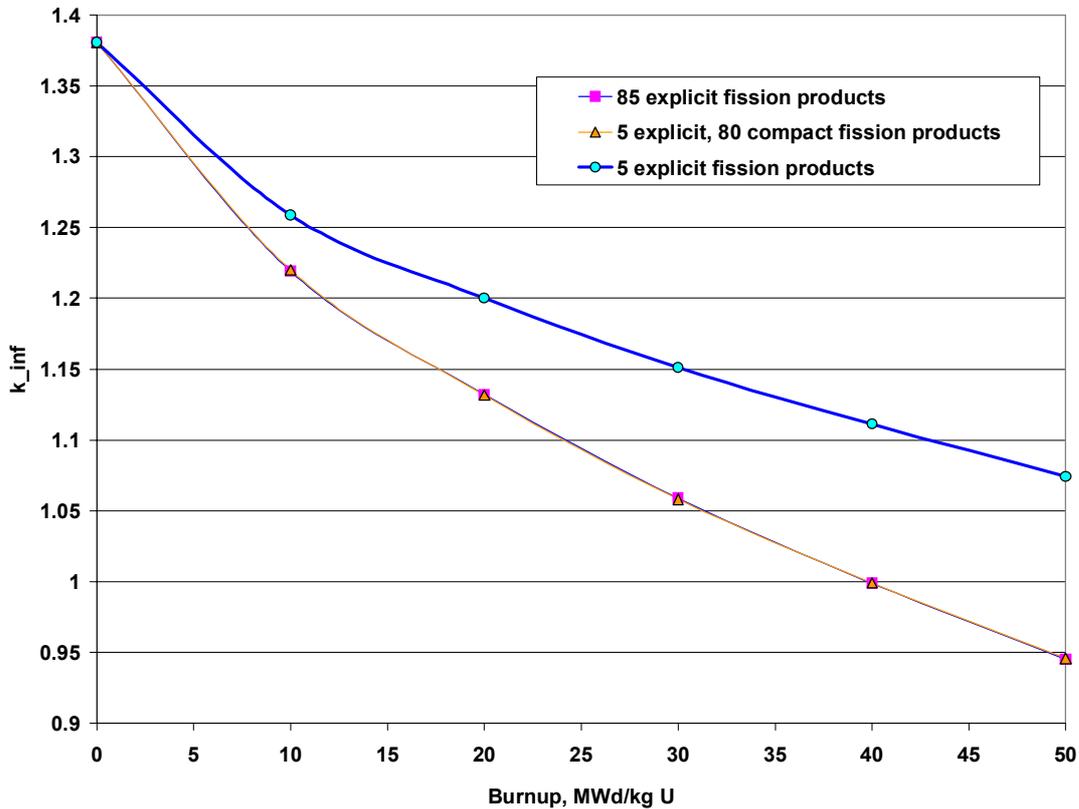


Figure 13. k_{∞} as a function of burn-up for a pin cell calculated by MCNP with 5 explicit fission product cross sections, and different representations for 80 additional fission products (explicit cross sections/compact cross sections/omission).

CONCLUSIONS

The Monte Carlo method with continuous representation of energy dependency of nuclear cross sections is a very important tool for reactor physics calculations. Due to the accurate and detailed description of geometry and nuclear reactions, the method serves as a reference method for a large variety of problems. The verification of the method together with corresponding nuclear data is performed internationally by a very large number of benchmark calculations and applications for compact systems. Benchmarks performed in this work validate the generated cross section sets. The results of calculations for different benchmarks and experiments are compiled and discussed for the nuclear data evaluations JEF-2.2/JEFF-3, ENDF/B-VI rel.5, and JENDL-3.2. For configurations with regular lattices, also methods based on multigroup deterministic (S_N) or multigroup Monte Carlo methods show comparable good results like MCNP if the nuclear data sets are based on the same evaluation and the calculation of weighting spectrum in the resonance range is based on the transport solution for the slowing down equation. The application of the Monte Carlo method for large scale LWR power

reactors is possible and gives reliable results for criticality values. Also for large LWR, the multigroup method can be applied with comparable accuracy to the continuous Monte Carlo method if the lattice is regular. The calculation of spatial distributions of reaction rates in large reactors needs a careful proof and choice of initial source distribution and the proof of convergence of spatial reaction rate or flux density distributions. For full core calculations with burn-up dependent material distribution, an effective memory management and compacting of nuclear cross section sets are necessary.

The good experience in MCNP applications for compact systems and the experience up to now for large LWR applications opens a further field of reactor physics calculations based on transport theory, e.g. for problems of reactivity accidents, and for problems of criticality safety regarding burn-up credit as well as for all kind of innovative fuel or core configurations.

ACKNOWLEDGEMENTS

This work was supported by the German Federal Ministry of Economics and Technology.

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