

**CALCULATIONAL MODELING OF FUEL ASSEMBLIES OF VVER1000 TYPE  
WITH THE USE OF BURNABLE ABSORBER GADOLINIUM; COMPARATIVE  
ANALYSIS**

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**ABSTRACT**

In connection with the beginning of the use of fuel assemblies with burnable absorbers by integration of Gadolinium into the nuclear fuel at Ukrainian NPP the task of testing the code systems and the pertinent neutron cross section libraries for the new fuel arose. Taking into account the long term experience of German experts with calculations and evaluation of nuclear fuel containing Gadolinium it was decided to carry out a series of test calculations for fuel assembly lattices of PWR, VVER440 and VVER1000 types using the NESSEL/PYTHIA and CASMO/SIMULATE code systems.

A short description of the codes used in the calculation is given. The calculations and the results are presented.

On the basis of the calculations carried out it can be concluded that nuclear calculations for reactor cores with a large amount of fuel assemblies with gadolinium as burnable absorber require a careful selection of the fuel pin model during the preparation of few group cross section libraries. To improve the models used in the calculations further benchmarks and comparison with operational data are necessary.

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## INTRODUCTION

One of the developments of fuel within the framework of modernization of NPPs with VVER type reactors is the use of burnable absorbers by integration of Gadolinium ( $Gd_2O_3$ ) into the nuclear fuel.

In order to determine nuclear characteristics and parameters of reactor cores of VVER type in the Ukrainian NPP's the utilities use calculational codes, developed in Russia (by RSC „Kurchatov Institute“, ASRI of NPP etc.). In this connection, the use of calculational codes developed by other organizations is expedient for independent qualitative nuclear safety analysis of core loading patterns of VVER reactors by the expert organization of the Ukrainian NRA.

One of the alternative instruments for the safety evaluation of reactors of VVER type is the code system PHYBER developed at K.A.B. Berlin. The features and possibilities of the code system are comparable to the Russian codes in use and are, in some points at least, even better. The system comprises codes which enable:

- to prepare few group libraries of neutron cross sections - NESSEL-4;
- to calculate micro- and macroscopic distributions of power density, burnup etc. - DERAB, PYTHIA.

Primarily, the code system PHYBER was developed for reactor physics calculations necessary during the operation of reactors of VVER440 and VVER1000 type. After the installation of the code system in Ukraine, various test calculations were carried out and the results obtained were compared to operational data from Ukrainian NPP with VVER type reactors. This confirmed the possibility to use the code system for modeling VVER reactor cores.

In connection with the beginning of the insertion of fuel assemblies (FA) with Gd fuel at Ukrainian NPP the task was to test the application of the code system and of the pertinent libraries of neutron cross sections for modeling operational characteristics of the new fuel type. Taking into account that experimental benchmark data and approved operational data are not yet available, tests can be carried out by comparison of calculational results by application of verified and validated reactor physics codes.

In German PWRs and BWRs, Gd fuel has been in use for more than 15 and 25 years respectively. German experts obtained a lot of experience in calculational modeling of reactor cores with Gd fuel. The following reactor physics codes are broadly used for these purposes:

- CASMO – to prepare few group libraries of FA-averaged neutron cross sections;
- SIMULATE – to model the characteristics of reactor cores for PWRs and BWRs.

The paper deals with the modeling of cores of pressurized water reactors of PWR and VVER type using Gd fuel with the code systems CASMO – SIMULATE and NESSEL - PYTHIA – DERAB.

## SHORT DESCRIPTION OF THE CODES CASMO AND NESSEL

The codes CASMO and NESSEL [1, 2] are used for the preparation of few group neutron cross sections taking into consideration the reactivity characteristics of FA with square and hexagonal geometry of the fuel pin lattice specific for nuclear reactors of PWR and VVER type, respectively. The starting multigroup libraries of neutron cross sections for the various isotopes of the reactor and fuel materials are obtained for codes on the basis of well known files of approved neutron data ENDF-B. Multi group neutron spectra are determined by solution of the one dimensional transport equation for cylindrical geometry with the first collision probability method. For these purposes, during the calculation process the real structure of the fuel system to be modeled is transformed stepwise into cylindrical zones equivalent in area. Condensation and homogenization of the neutron cross sections are carried out on the basis of the multi group spectra for the calculational zones and two dimensional few group lattice transport calculations.

During the calculations the following results are defined:

- critical eigenvalues of the modeled systems ( $k_{\infty}$ ,  $k_{eff}$ );
- few group diffusion coefficients of multiplying areas (which contain fuel) and non multiplying areas (e.g. control rods);
- the change of the isotopic content in the calculational zones dependent on the fuel burnup;
- few group (two group) libraries of neutron cross sections in dependence on fuel burnup.

The short description given above shows that both codes are sufficiently similar to each other with regard to the problems solved and the solution methods. Both programs were developed nearly at the same time and were based on approximately the same stage of development of computing techniques and of calculational methods. The code CASMO was intended mainly to be used for nuclear calculations of lattices of PWRs and BWRs in quadratic geometry whereas the code NESSEL was designed for calculations of hexagonal lattices for VVER reactors.

## PREPARATION OF LIBRARIES OF FEW GROUP CONSTANTS WITH THE CODES CASMO AND NESSEL

The codes CASMO and NESSEL are used for the preparation of libraries of few group neutronic constants needed for the modeling of fuel loadings of PWR and VVER reactors using the codes SIMULATE and PYTHIA respectively.

Even though each of the codes CASMO and NESSEL is designed to be able to make calculations for systems with quadratic as well as hexagonal geometry, the code CASMO is better suited for quadratic lattices whereas the code NESSEL targets systems with hexagonal lattices. For this reason, the comparison was drawn for both types of geometrical systems.

During preparation of two group constant libraries, both codes calculate the infinite multiplication factor  $k_{\infty}$  for the modeled system dependent on the burnup. This parameter is chosen for the comparison. Calculations were carried out for standard FAs of PWRs of KONVOI type (i.e. quadratic lattice of 18x18-24 fuel pins) and FAs used in Ukrainian nuclear reactors of VVER440- and VVER1000 types. A more detailed description of the three FA types modeled and their main characteristics can be found in numerous publications (e.g. [3]). Therefore we will not present these data explicitly in the paper.

Results of the test calculations are shown in the figures 1 - 4 and 7 - 10. At first, calculations for FA lattices of PWR, VVER440 and VVER1000 types without burnable absorber rods (BAR) were performed (see figures 1 - 4). These calculations aimed to demonstrate the possibility of the codes to model the respective lattice types. Deviations of the results for all investigated FA types do not exceed the range of 1 % in  $k_{\infty}$ . As can be seen in figure 2, where results for small values of burnup are represented, a good agreement is obtained in the whole range of operational parameters including the starting phase of Xenon build up.

In the case of FAs with BAR for the comparative analysis, the following typical FAs were chosen:

- For PWRs - quadratic lattice geometry 18x18-24 (24 guide tubes for control rods) with 288 Uranium fuel pins with an enrichment of 3.45 % U235 and 12 BARs with 2.3 % U235 and 7 % gadolinium (see Fig. 5);
- For VVER1000 - hexagonal lattice geometry with 240 Uranium fuel pins with an enrichment of 4.6 % U235, 60 peripheral fuel pins with an enrichment of 4.0% U235 (so-called profiled FA) and 12 BARs with an enrichment of 3.6 % U235 and 5 % gadolinium (see Fig. 6).

Results of the burnup calculations are represented in figures 7 - 10. The very good compliance of the results in the range of burnup greater than 15 MWd/kgHM was to be expected because the gadolinium is completely burnt out and cannot furthermore influence the FA characteristics.

From the point of view of analysis of the gadolinium influence, the burnup range 0 - 15 MWd/kgHM is more interesting (see figures 8 and 10). Here we notice unsatisfactory large deviations of the calculation results especially for the quadratic PWR FAs (see figure 8). If the fuel pellet for the calculations with the code NESSEL is modeled as one cylindrical homogeneous zone with uniform isotopic composition and neutron physical characteristics, deviations of the results calculated with the codes CASMO (which automatically selects the number of zones in dependence on whether gadolinium is contained in the fuel or not) and NESSEL are especially substantial. This effect is due to the shielding of the inner layers of the fuel pellet by the outer ones during the burnup of the gadolinium. In fact, the gadolinium burns up not uniformly in the pellet volume but in a layer which shifts from outer to inner pellet parts in the burnup process, which, in fact, is specifically taken into account in CASMO.

Increasing the number of layers explicitly taken into consideration to 2 or more leads to a sufficiently better agreement of the calculated infinite multiplication factors  $k_{\infty}$ . The maximum deviation does not exceed the range of 1 % of  $k_{\infty}$ .

It is of interest that the calculations of FAs of VVER1000 type with BARs don't show the shielding effect mentioned above. The increase of homogenization zones for the NESSEL calculations has no remarkable effect on the results. This may be connected with the higher enrichment and the lower content of gadolinium in the fuel. Another possible reason may be that the influence of the gadolinium burnup on the FA characteristics is weaker during the homogenization of the FA cross sections due to the greater dimensions of the fuel rod lattice. The deviation between CASMO and NESSEL results is not greater than 1.5 % of  $k_{\infty}$ . Nevertheless, the effect of shielding of the inner parts of the fuel pellet can become more remarkable also for FAs of VVER type reactors if the number of BARs or the content of gadolinium (i.e. the weight fraction) is increased.

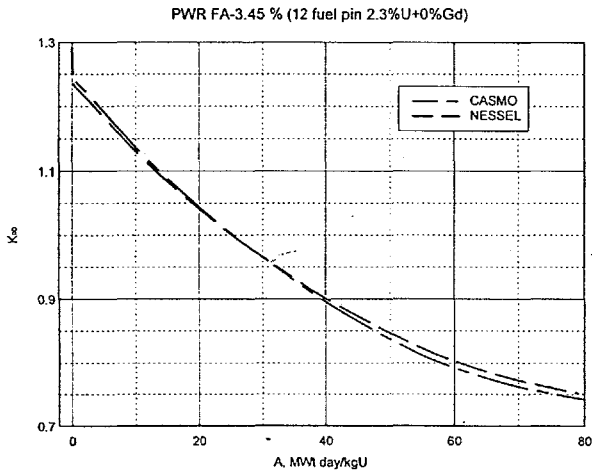


Figure 1: Infinite multiplication factor vs. burnup for fuel assembly PWR 18x18, 3.45 % without Gd

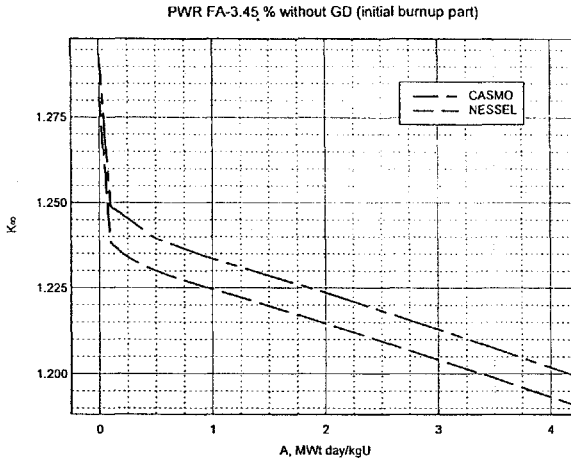


Figure 2: Infinite multiplication factor vs. burnup for fuel assembly PWR 18x18, 3.45 % without Gd (detail of figure 1)

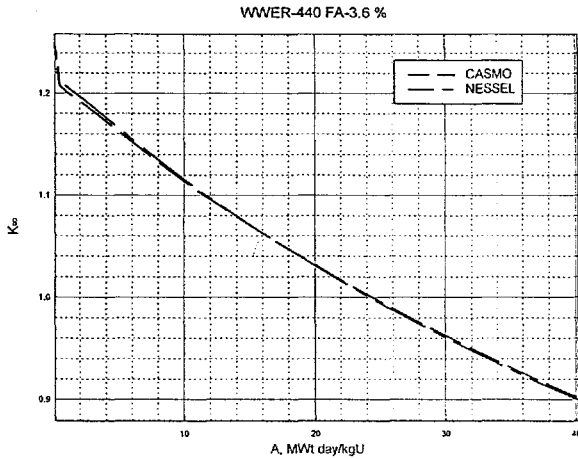


Figure 3: Infinite multiplication factor vs. burnup for fuel assembly VVER-440, 3.6 % without Gd

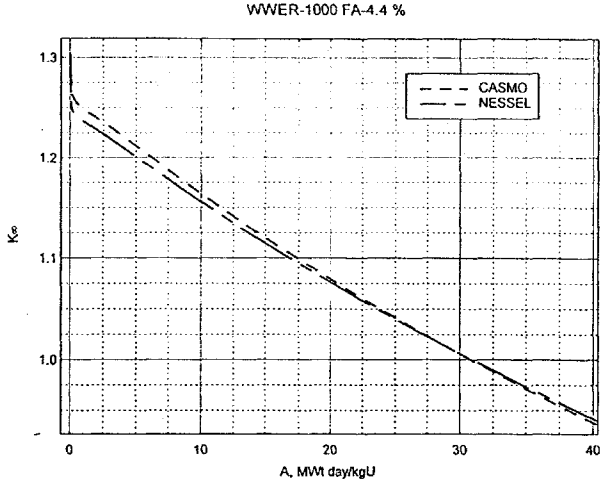


Figure 4: Infinite multiplication factor vs. burnup for fuel assembly VVER-1000, 4.40 % without Gd

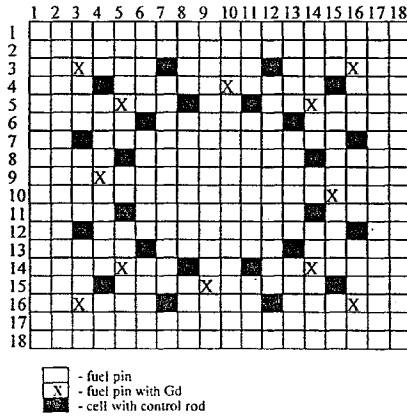


Figure 5: Layout pattern of the fuel assembly PWR 18x18 with 12 Gd fuel pin

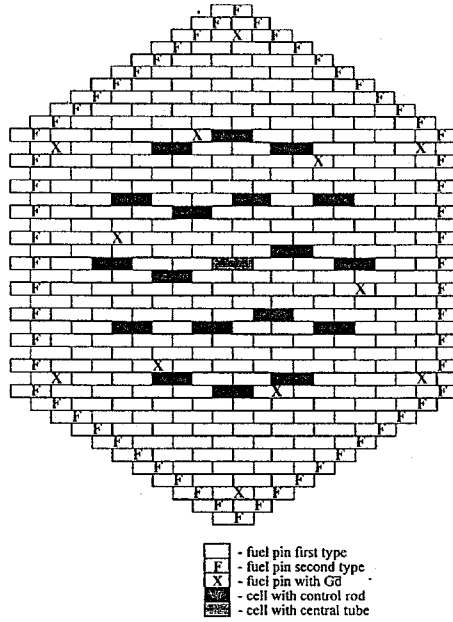


Figure 6: Layout pattern of the fuel assembly VVER-1000 with 12 Gd fuel pin

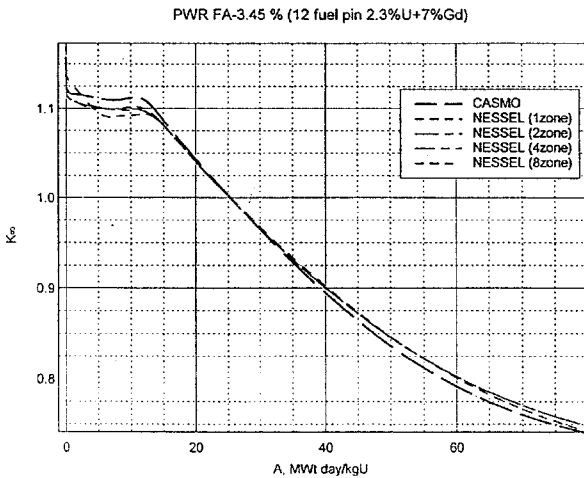


Figure 7: Infinite multiplication factor vs. burnup for fuel assembly PWR 18x18, 3.45 % with 12 Gd fuel pins



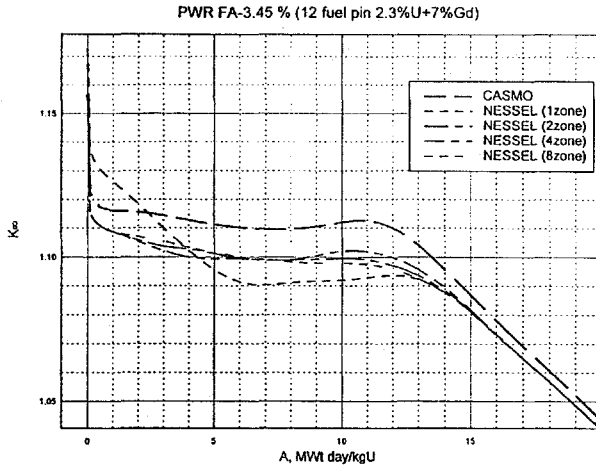


Figure 8: Infinite multiplication factor vs. burnup for fuel assembly PWR 18x18, 3.45 % with 12 Gd fuel pins (detail of figure 7)

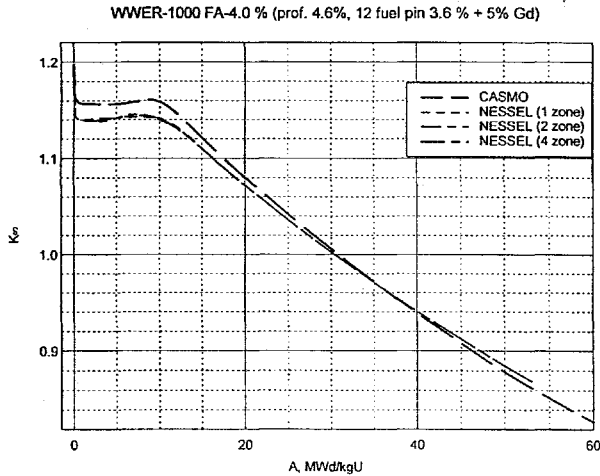


Figure 9: Infinite multiplication factor vs. burnup for fuel assembly VVER-1000, 4.00 % with 12 Gd fuel pins

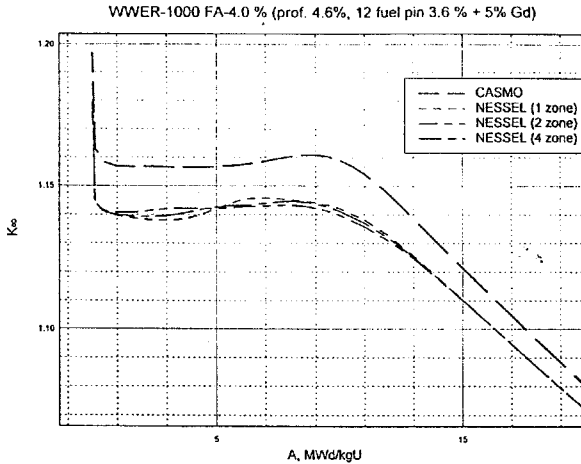


Figure 10: Infinite multiplication factor vs. burnup for fuel assembly VVER-1000, 4.00 % with 12 Gd fuel pins (detail of figure 9)

## CALCULATIONS OF NUCLEAR CHARACTERISTICS OF REACTOR CORES

As mentioned in the previous paragraphs, the calculations of  $k_{\infty}$  for FAs containing BARs with gadolinium show differences between the codes NESSEL and CASMO. In order to assess the influence of the obtained deviations on nuclear reactor core parameters, comparative calculations were carried out with the codes PYTHIA [3] and SIMULATE [4].

### Short description of the codes PYTHIA and SIMULATE

The codes PYTHIA and SIMULATE are used to calculate macroscopic nuclear characteristics of reactor cores during the burnup process of fuel loads. The following properties can be determined:

- the cycle length and the change of the boron acid concentration during the fuel cycle;
- the power density distribution in the FA's and in the core;
- the control rod worth;
- reactivity coefficients.

Both codes are similar with regard to the solved problems, but different in the application fields.

The code PYTHIA was developed by K.A.B., Berlin, and applies to the modeling of reactor cores with hexagonal fuel lattices (reactors of VVER type, in which hexagonal fuel cassettes are used). As an additional option, the possibility to model reactor cores with quadratic fuel lattices is realized.

The code SIMULATE is provided by Studsvik Scandpower and can be used for the modeling of reactor cores with quadratic fuel lattices (Western nuclear reactors of PWR and BWR types).

On this basis and taking into account the possibilities of the codes PYTHIA and SIMULATE and the availability of operational data, the cycles No. 1 - 3 of a NPP with PWR were chosen for the test calculations. Also, the fact that FAs with BARs were inserted into the core starting from the first cycle needs to be considered. Until now, no operational data of core loadings with FAs containing BARs for VVER type reactors are available. This is especially important for the design of first core loading patterns and fuel cycles. Such projects are interesting because for Ukrainian NPPs in construction (Khmelnitsky NPP, unit 2 and Rovno NPP, unit 4) first core loadings with BA might be realized.

In general, the choice of the NPP and of the cycles is based on the following facts:

- the codes PYTHIA and SIMULATE allow modeling of reactor cores with quadratic fuel lattice geometry;
- the reactor core loadings of the NPP starting with the first cycle comprise a great fraction of FAs with BARs;
- the availability of operational data for the chosen cycles.

#### Calculations of reactor-physical parameters of fuel cycles

In the calculations of nuclear core parameters, the following core properties were chosen for comparison:

- concentration of boron acid dependent on core average fuel burnup;
- cycle length;
- power density of the FAs and the hot spot power density.

With regard to these comparisons it must be mentioned that the code PYTHIA has not been validated for the calculation of quadratic fuel lattices. Therefore the main interest is focused not on the absolute values, but on the behaviour of the properties calculated for the fuel cycles.

#### Cycle No. 1

The results of the calculations for the first cycle are presented in figure 11 and 12. Figure 11 shows the change in boron concentration during the cycle calculated with PYTHIA and SIMULATE. There are also results of the calculations given which were carried out by order of the NPP with the code MEDIUM. For the calculation with the code PYTHIA two different few group libraries were used. The libraries differ in the way of the burnup calculations for fuel containing Gadolinium. The first library (in figure 1 - calculations with the so-called „Old lib“-library) was prepared using a model of one cylindrical zone for the

fuel pellet. For the preparation of the other library (marked as „New lib“) the fuel pellet was modeled by several cylindrical zones. The modeling of Gadolinium fuel pellets is described above in more detail.

- In figure 11 it can be seen that the time behaviour of the calculated boron concentrations compared at several time points of the cycle differs more or less. In the range 0-100 full power days (FPD), the boron concentration decrease calculated by the code PYTHIA is faster compared to that calculated by the other codes. In the range of 100-200 FPD this change of boron concentration is slowed down a little and corresponds in the dynamic behavior with the results of the other codes. In the last range from 200 FPD to the end of cycle (EOF), the agreement between the compared calculations is satisfactory.

In our opinion, these differences are caused by the different modeling of the Gadolinium burnup in the codes NESSEL and CASMO. The use of several cylindrical zones for the calculations to prepare libraries of few group constants (NESSEL, PYTHIA) improves the situation, but not sufficiently. This is emphasized also by the results concerning the FA power density. In figure 12, the changes in maximum relative FA averaged power density  $K_q$  and in maximum relative local value of the FA power density (in an axial layer)  $K_v$  in the course of the cycle are presented. One can see that the values  $K_q$  and  $K_v$ , calculated by the different codes, are similar quantitatively. In the range  $\approx 100-200$  FPD, however, the  $K_q$  and  $K_v$  calculated by the code PYTHIA show a peak. This (similar to the boron concentration change) is due to the probably overestimated fast burn out of gadolinium at this moment of the cycle and to the redistribution of the power density between the FAs in the reactor core.

### Cycle No. 2 and No. 3

Analogous results are obtained during the calculations for the second and third cycle. In figure 13 and 14, the boron concentration  $C_B$  and the FA power density  $K_q$ ,  $K_v$  in the course of cycle 2 are presented, respectively, and in figure 15 and 16 for cycle 3. Here we can see the same differences in the time behaviour of  $C_B$ ,  $K_q$  and  $K_v$  as described for cycle 1.

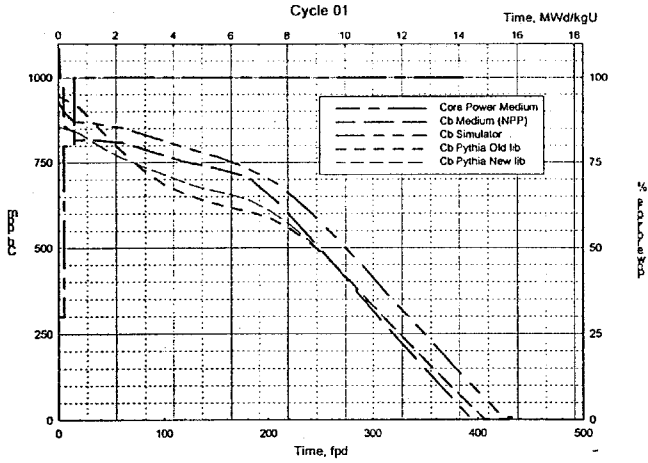


Figure 11: Change of the boron concentration  $C_B$  in the coolant during cycle 1

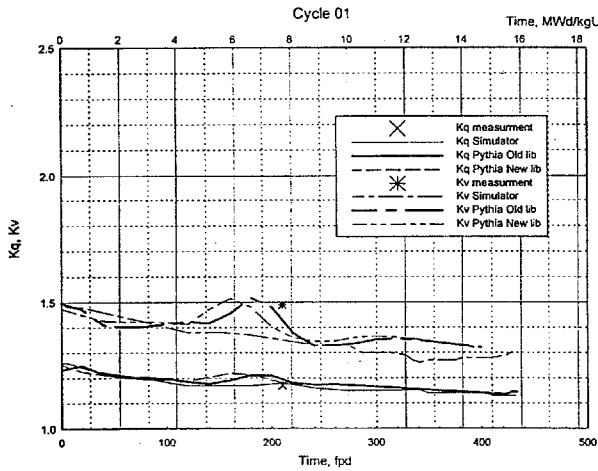


Figure 12: Change of the maximum power density of the FA  $K_q$  and  $K_v$  during cycle 1

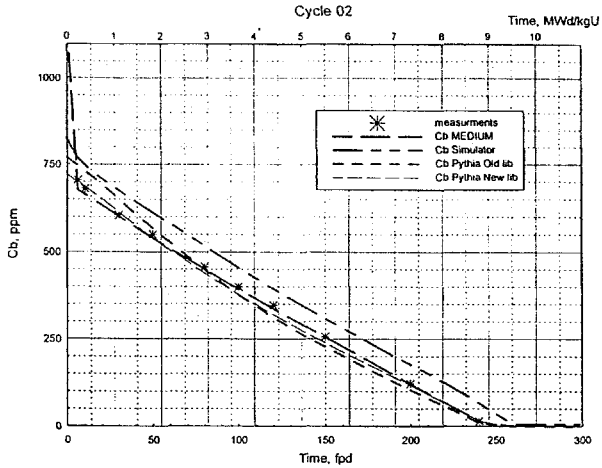


Figure 13: Change of the boron concentration  $C_B$  during cycle 2

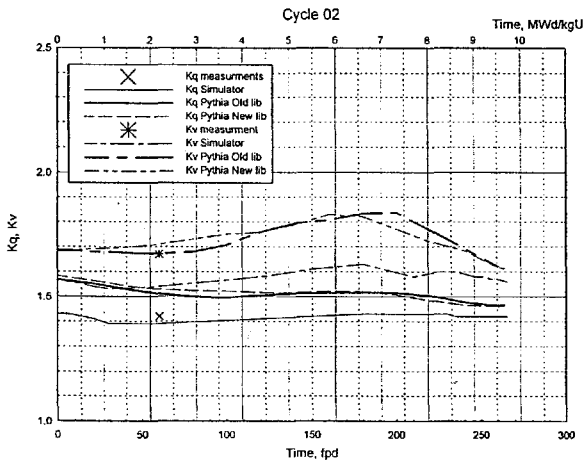


Figure 14: Change of the maximum power density of the FA Kq and Kv during cycle 2

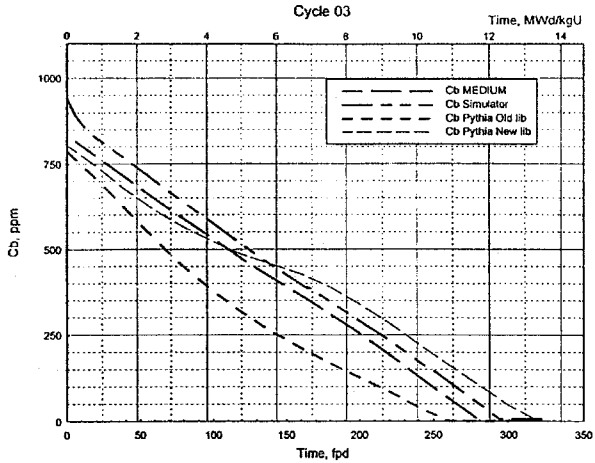


Figure 15: Change of the boron concentration  $C_B$  during cycle 3

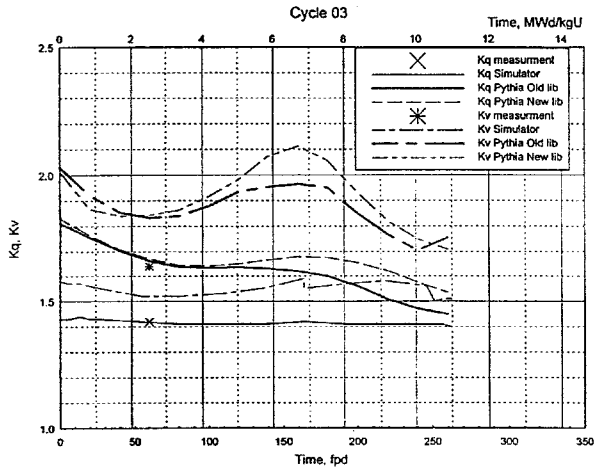


Figure 16: Change of the maximum power density of the FA Kq and Kv during cycle 3

## CONCLUSION

On the basis of the explanation given above it can be concluded that nuclear calculations for reactor cores with a large amount of FA's with Gd as burnable absorber require careful selection of the optimal model for the fuel pellet in the stage of the preparation of few group constant libraries. This has to be taken into account for the assessment and selection of alternative nuclear design of first reactor core loadings for the reactors of Khmel'nitsky NPP (unit 2) and Rovno NPP (unit 4) under construction.

It has to be mentioned that the presented results are the very first of their kind. Some differences in the time behaviour of calculated core characteristics have to be analyzed in more detail to clarify the reasons. In the context of this work it could only be stated that in principle the codes used calculated sensible core parameters and that there are some differences which can be connected with the mathematical models of the codes PYTHIA and SIMULATE and especially with the differences in the specific models for calculating the space and time dependent gadolinium concentration in the fuel rod by the codes NESSEL and CASMO.

To improve the agreement of the results, deeper investigations of the mathematical and physical models used in the different codes are necessary. Further benchmark calculations and comparisons should be carried out.

Finally, the quality of a model can be assessed on the basis of approved operational data. For this reason, the creation of approved operational data libraries which do not yet exist is necessary. This is significant in the case of VVER-1000 with a high fraction of Gd fuel even in the first fuel cycle.

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