

# CALCULATION OF THERMAL REACTIVITY COEFFICIENTS FOR NPP MOCHOVCE-3,4 START-UP CONDITIONS BY MCNP5

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## ABSTRACT

In general a reactor is initially started up from a precondition stage (200°C) by withdrawing control rods or by changing the boron acid concentration in primary circuit coolant until the reactor is slightly supercritical, thus producing an exponentially increasing neutron population on a very long period. As the neutron population increases, the fission heating and thus the reactor temperature increases. This increase in temperature produces a decrease in reactivity. That would lead to the slowdown of increasing the neutron population and the reactor power should saturate at certain higher level. Generally, core loading patterns are designed in such way that isothermal reactivity coefficient should already be negative at the Cold Zero Power (CZP). For VVER 440 reactors CZP is equal to 200 °C. To meet this requirement could be problematic, particularly for the first core loading, when all fuel assemblies are fresh. Due to the first criticality start-up of the Nuclear Power Plant (NPP) Mochovce units 3 and 4 in the near future, detailed analyses of core parameters are required by the Slovak Regulatory Authority to support safe operation of the nuclear facility. The article introduces determination of the thermal reactivity coefficients, especially summary (isothermal) and moderator (density) reactivity coefficients between 200°C and 260°C with step of 2 °C. The work presents calculated critical parameters, especially critical boron acid concentrations at given coolant temperatures and position of the 6<sup>th</sup> control assembly group. Numerical iteration procedure was applied to calculate the critical parameters as a substitute for a critical experiment. Geometrical and material models were created in compliance with the reactor design and the first fuel loading of the NPP Mochovce 3 and 4. All mentioned calculations were performed by computational code MCNP5 1.60 supported by NJOY99.364 microscopic sections processing system and our control scripts.

## 1 INTRODUCTION

Considering the first planed criticality start-up of the NPP Mochovce 3 and 4 units in the near future, detailed core analyses required by the Slovak Regulatory Authority were performed to support the licence process. Normally, the VVER-440 reactor type is initially started up by critical experiment method. The reactor start-up is realized by boron acid

regulation and withdrawing of control assembly groups from the core until the reactor is slightly supercritical, thus producing an exponentially increasing neutron population on a very long period. As the neutron population increases due to the fission heating, the reactor temperature increases. Increase of the temperature than produces a decrease in reactivity which could result in the fall of neutron population and the reactor shut down. An increase in fuel temperature will broaden the effective resonance absorption (and fission) cross section, generally resulting in increase of neutron absorption and corresponding reduction in reactivity — the Doppler effect. In terms of the increased moderator temperature, it will cause a change in the local fuel–moderator properties as well as change in both the moderator absorption and the flux disadvantage factor. In addition, a decrease in moderator density will reduce the moderating effectiveness and produce a hardening (shift to higher energies) in the neutron energy distribution. This will have an effect on the effective energy-averaged absorption cross sections for the fuel. The reduction in moderator/coolant density increases the diffusion of neutrons, which will cause of the increased leakage from the system [1]. This article introduces methodology for determination of the thermal reactivity coefficients related to the first start-up of the NPP Mochovce 3 and 4. Especially, isothermal (summary) and moderator (density) feedback reactivity coefficients were calculated between 200°C and 260°C with step of 2°C. Evaluation of the critical boron acid ( $\text{H}_3\text{BO}_3$ ) concentrations was performed for the given coolant temperatures as a precondition of the thermal coefficients calculation. All of calculated values should support the safe start-up of the new reactor units and help to predict behaviour of these systems.

## 2 CALCULATION METHOD AND MODEL

### *Definition of the system conditions*

As mentioned above, VVER-440 core model with the given start-up fuel loading pattern was used. Investigated condition is defined by the minimal controlled power level with  $k_{eff}$  equal to 1, coolant temperature of the primary loop between 200°C and 260°C with 2°C step and position of the 6<sup>th</sup> control assembly group of 125 cm or 200 cm. Because the coolant temperature increase in the core is sufficiently small during the time of interest, we assumed a uniform spatial temperature distribution of the reactor internals - so called isothermal condition.

### *Geometrical and material model*

Considering the complicated geometry of the VVER-440 internal parts, reliable neutron transport calculation can only be performed using a technique enabling the treatment of complex three-dimensional geometry. Therefore the MCNP5 1.60 code [2] based on the transport Monte Carlo method was chosen and applied. Regarding the objective of the work to determine the temperature coefficients of reactivity with high accuracy and reliability, the geometrical and material part of the reactor model had to be created in the finest possible details. The model enables significant level of flexibility to define a given core configuration and reactor operational conditions. The calculation model was optimized after subsequent testing, validation and verification for effective calculation of critical conditions and the thermal reactivity coefficients based on the requirements of the NPP operator. The created

whole-core VVER-440 model consists of the reactor in-vessel components such as fuel assemblies (including fuel rods, upper spacer grid, intermediate spacer grids, supporting grid, mixing grid, central tube, casing, head and bottom, channel with self-powered neutron detectors), control assemblies (absorber and fuel part), core basket, barrel (including irradiation channels) and the reactor pressure vessel, Fig. 1. Regarding the working fuel assemblies FA and the control assemblies CA, two main model variants were created – the 1<sup>st</sup> generation type (NPP Mochovce 2 commissioning) and the 2<sup>nd</sup> generation type (NPP Mochovce 3 and 4). The differences between these two types of FAs/CAs are mainly in geometrical characteristics (fuel pitch, fuel length, head and the bottom part). Fuel pins are located in a triangular lattice with step of 12.2 mm (the 1<sup>st</sup> generation type) or 12.3 mm (the 2<sup>nd</sup> one).

The boundaries of the created VVER-440 whole-core model are given by the outer surface of the reactor pressure vessel, the upper and lower edge of the FA construction. The reactor barrel model consists of vertical cylindrical vessel including six pairs of channels to insert irradiation chains with samples of reactor pressure vessel materials. The irradiation channels were modelled with no internal filling.

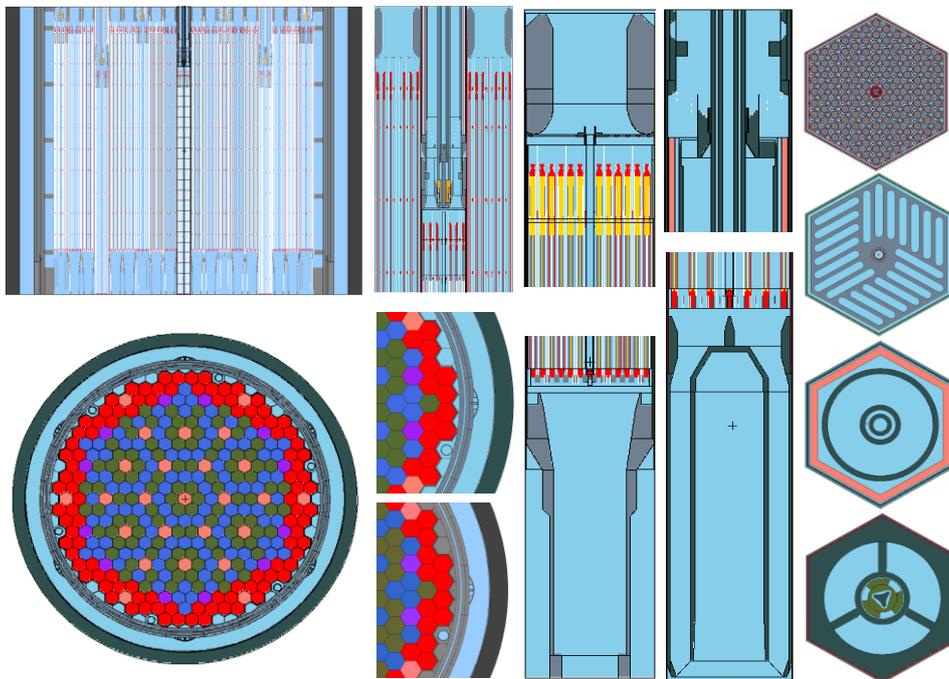


Figure 1: Plots from the 3D whole-core model of the VVER-440 reactor in MCNP5

Libraries of the microscopic effective cross sections and probability tables entering the calculation code MCNP5 1.60 were prepared using NJOY99.364 code system [3]. Code system NJOY is a modular calculation system where each module is intended for solving a specific assignment. Verified library of microscopic effective cross sections ENDF/B-VII distributed by OECD NEA Data Bank consisting of 381 materials was used as an input for the NJOY99.364 calculation [4]. The whole library preparation process was verified [5] using benchmark tasks based on the International Handbook of Evaluated Criticality Safety Benchmark Experiments [6]. To process the microscopic effective cross sections by NJOY99.364 Moder, Reconr, Broadr, Unresr, Leapr, Therm, Heatr, Purr, Gaspr, Viewr and Acer modules were used. Principal simplified process of creating libraries of effective cross sections is demonstrated in the Fig.2.

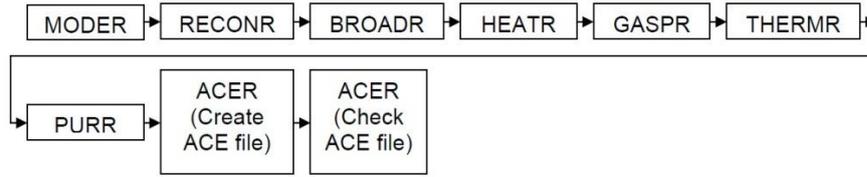


Figure 2: Main simplified process of creating libraries of effective cross sections using NJOY99.364 code system.

### Determination of critical boron acid concentration

The MCNP5 1.60 code used to calculate the critical boron acid ( $\text{H}_3\text{BO}_3$ ) concentration does not have the direct output of this value. The critical boron acid concentration corresponds to the value, at which the calculated  $k_{\text{eff}}^{\text{MCNP}}$  is equal to 1 with the defined accuracy. The result can be obtained in at least two ways: simulation of the critical experiment or using the iteration method. Taking into account the computation time to evaluate the critical boron acid concentration, the iteration method was chosen for the analyses. This approach is capable of shortening the calculation time by more than half due to no need to analyse the partial calculation results. Moreover, the applied method allows automatic termination of the computation when the specified result's accuracy is reached. The numerical iteration procedure used for evaluation of the critical boron acid concentration uses the bisection method and the Newton's iteration method. Control script in the scripting language *csh* was prepared to control the calculation. For the validation of the criticality calculations (critical boron acid concentration), the first critical conditions of the NPP Mochovce 2 start-up were used. [7] The stabilised critical parameters are the following: position of the 6<sup>th</sup> control assembly group of 144.4 cm; primary circuit temperature of 200.3 °C; pressure in the primary circuit of 12.09 MPa; the median of critical boron acid concentration of 8.11 g/kg. In order to validate the calculation of the critical boron acid concentration, experimental values obtained by three more independent measurement methods were considered. The values coming from the different experimental methods are:

- potentiometric method,  $c_{\text{Bcrit1}}=8.12$  g/kg;
- coulometry method,  $c_{\text{Bcrit2}}=8.14$  g/kg [3];
- titration method used in NPP Mochovce,  $c_{\text{B3crit}}=8.08$  g/kg;
- 716 DMS Titrino method, used in NPP Mochovce as well,  $c_{\text{B4crit}}=8.11$  g/kg.

These boron acid concentration measurement methods provide the values with uncertainty of  $\pm 0.05$  g/kg. In relation to the above described conditions, the MCNP5 input file was created, taking into account all the materials and geometric arrangement of the first fuel loading of the NPP Mochovce 2.

The critical  $\text{H}_3\text{BO}_3$  concentration was calculated for the first fuel loading of the Mochovce 2 according to the described conditions by means of the iteration method. During the calculation, the accuracy of the  $k_{\text{eff}}^{\text{MCNP}}$  calculation was adjusted to the value better than  $\xi_N = 0.00005$ . The calculated critical  $\text{H}_3\text{BO}_3$  concentration  $c_{\text{Bcrit}}^{\text{MCNP}}=8.45023$  g/kg differs from the experimentally obtained value of  $c_{\text{Bcrit}}^{\text{exp}}=8.11$  g/kg. This deviation is considered to be a systematic error of the calculations, which will be reflected in the results as a correction  $\Delta_{c_{\text{Bbias}}}$ . The value of the correction is:

$$\Delta_{c_{Bbias}} = c_{Bkrit}^{exp} - c_{Bkrit}^{MCNP} = -0.34023 \text{ g/kg} \quad (1)$$

The median of the measured critical  $\text{H}_3\text{BO}_3$  concentration was  $c_{Bcrit} = 8.11 \text{ g/kg}$  obtained with the tolerance of  $\pm 0.05 \text{ g/kg}$ . For purpose of the systematic bias value  $\Delta_{bias}$  determination, we considered the above value to be the experimentally specified value of the critical boron acid concentration  $c_{Bkrit}^{exp}$  with the known tolerance. Conservatively, we assumed a uniform distribution of the  $c_{Bkrit}^{exp}$  value in the whole interval of tolerance, and specified the standard uncertainty:

$$\sigma_{c_{Bkrit}^{exp}} = \frac{a+b}{2\sqrt{3}} = \frac{0,05+0,05}{2\sqrt{3}} = 0.02887 \text{ g/kg}. \quad (2)$$

In the described conditions, the reactor is critical, that is  $k_{eff}^{exp} = 1$  with the uncertainty of  $\sigma_{exp}$ , obtained by MCNP5 1.60. During the calculation, we took into account a postulated uniform occurrence of the critical  $\text{H}_3\text{BO}_3$  concentration in the whole tolerance interval from 8.05 to 8.16 g/kg. The calculated values of  $k_{eff}^{MCNP}$  and  $k_{eff}$  corresponding to the uniform occurrence of the value of boric acid critical concentration were the following:  $k_{eff} = \langle 1.00114; 0.99925 \rangle$  and  $k_{eff}^{MCNP} = \langle 1.0078 \pm 0.00008; 1.00592 \pm 0.00006 \rangle$ . For the stabilized median of the critical  $\text{H}_3\text{BO}_3$  concentration 8.11 g/kg, the  $\Delta_{bias}$  value defined by term (3) is equal to 0.00667.

$$\Delta_{bias} = k_{eff}^{exp} - k_{eff}^{MCNP} \quad (3)$$

The uncertainty of bias  $\Delta_{bias}$  will be determined by the relation:

$$\sigma_{bias} = \sqrt{\sigma_{MCNP}^2 + \sigma_{exp}^2} = 6.14 \cdot 10^{-4} \quad (4)$$

Using the  $\Delta_{bias}$  from the calculated  $k_{eff}^{MCNP}$  we can determine the effective multiplication coefficient value as follows:

$$k_{eff} = k_{eff}^{MCNP} + \Delta_{bias}. \quad (5)$$

The uncertainty of the  $k_{eff}$  value can be determined as:

$$\sigma = \sqrt{\sigma_{MCNP}^2 + \sigma_{bias}^2} \quad (6)$$

In accordance with above conditions and used methodology, the critical boron acid concentration drops from  $c_{B1krit200} = 7.09898 \text{ g/kg}$  to  $c_{B2krit200} = 7.05211 \text{ g/kg}$  at the position of the 6<sup>th</sup> CA group:  $h_6 = 200 \text{ cm}$ . Similarly, with an increase of the coolant temperature from 200 to 260°C, the critical boron acid concentration falls from  $c_{B1krit125} = 6.92121 \text{ g/kg}$  to  $c_{B2krit125} = 6.81498 \text{ g/kg}$  at  $h_6 = 125 \text{ cm}$ .

## Determination of thermal reactivity coefficients

The calculation of summary (isothermal)  $a_{PO}$  and moderator (density)  $a_M$  thermal reactivity coefficients using MCNP5 1.60 can be performed by two approaches: the realistic or the combined conservative one, which differ from each other in the preparation of input parameters and the evaluation of the resulting uncertainty of the calculation results. The realistic approach assumes the use of realistic model with real parameters and conditions. The computation result must be carried out with the assessment of the uncertainty, which is the result of the sensitivity analysis of uncertainty components affecting the simulated process. The sensitivity analysis requires the precise determination of tolerances and uncertainties of all the input parameters relevant for the calculation. The mean isothermal reactivity coefficient  $a_{PO}$  (all equations below are relevant for evaluation of density thermal reactivity coefficients  $a_M$ ) is determined according to the relation:

$$a_{PO_i} = \frac{\Delta\rho_i}{T_i - T_{i-1}} = \frac{k_{eff_i}^{MCNP} - k_{eff_{i-1}}^{MCNP}}{2(k_{eff_i}^{MCNP} + \Delta_{bias})} \quad (7)$$

Where  $\Delta\rho_i$  is the reactivity effect caused by the change of temperature of the core materials within the range of  $T_i - T_{i-1}$ . The magnitude of the temperature change is 2 °C in the whole interval of interest.  $k_{eff_i}^{MCNP}$  and  $k_{eff_{i-1}}^{MCNP}$  are the effective multiplication coefficient values determined by MCNP5 calculation for temperatures  $T_i$ ,  $T_{i-1}$ , and  $\Delta_{bias}$  is the systematic bias of  $k_{eff}$  value. The uncertainty of the evaluation of isothermal reactivity coefficient  $\sigma_{PO_i}$  is:

$$\sigma_{PO_i} = \sqrt{\left(\frac{\partial a_{PO_i}}{\partial k_{eff_i}^{MCNP}}\right)^2 \sigma_i^2 + \left(\frac{\partial a_{PO_i}}{\partial k_{eff_{i-1}}^{MCNP}}\right)^2 \sigma_{i-1}^2 + \left(\frac{\partial a_{PO_i}}{\partial \Delta_{bias}}\right)^2 \sigma_{bias}^2} \quad (8)$$

$$\sigma_{PO_i} = \sqrt{\left(\frac{\Delta_{bias} + k_{eff_{i-1}}^{MCNP}}{2(k_{eff_i}^{MCNP} + \Delta_{bias})}\right)^2 \sigma_i^2 + \left(-\frac{1}{2(k_{eff_i}^{MCNP} + \Delta_{bias})}\right)^2 \sigma_{i-1}^2 + \left(-\frac{k_{eff_i}^{MCNP} - k_{eff_{i-1}}^{MCNP}}{2(k_{eff_i}^{MCNP} + \Delta_{bias})^2}\right)^2 \sigma_{bias}^2} \quad (9)$$

where  $\sigma_i$  and  $\sigma_{i-1}$  are the uncertainties of calculated effective multiplication coefficients using MCNP5 1.60 for the temperature  $T_i$  or  $T_{i-1}$ .  $\sigma_{bias}$  is a combined uncertainty of the  $\Delta_{bias}$ . The calculations of summary (isothermal) thermal reactivity coefficients were realized without consideration of power feedback.

## 4 RESULTS

For the calculation of  $k_{eff}$  values entering the expression of the thermal reactivity coefficient (7) we used the code MCNP5 1.60 with the libraries ENDF/B-VII.0, as well as the bias  $\Delta_{bias}$  and the uncertainty  $\sigma_{exp}$  values. In each case, the critical boron acid concentration at given coolant temperature was added to the system definition.

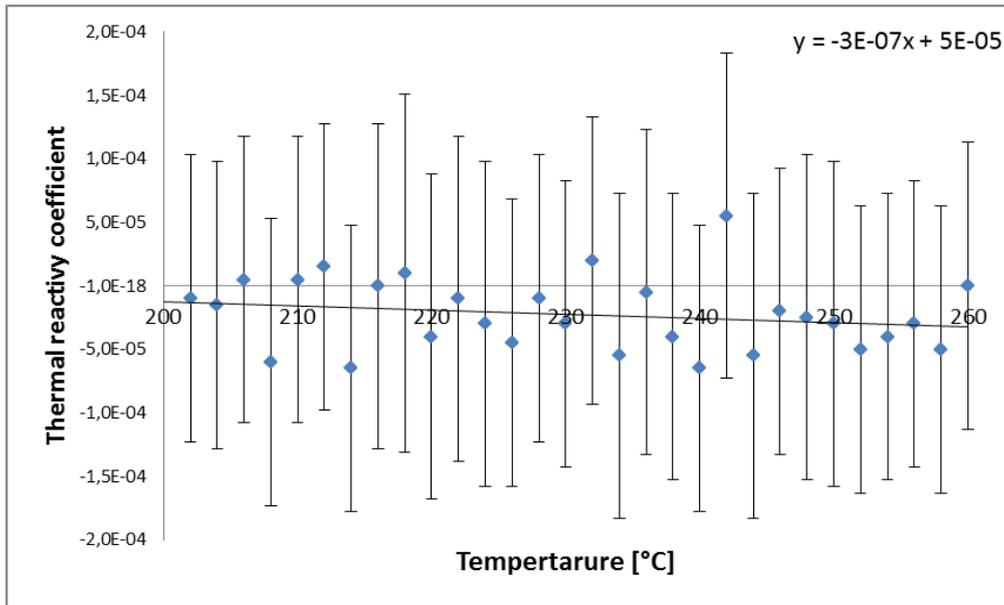


Figure 3: Isothermal reactivity coefficients (RC temperature from 200°C to 260°C and position of the 6<sup>th</sup> CA group of 125 cm).

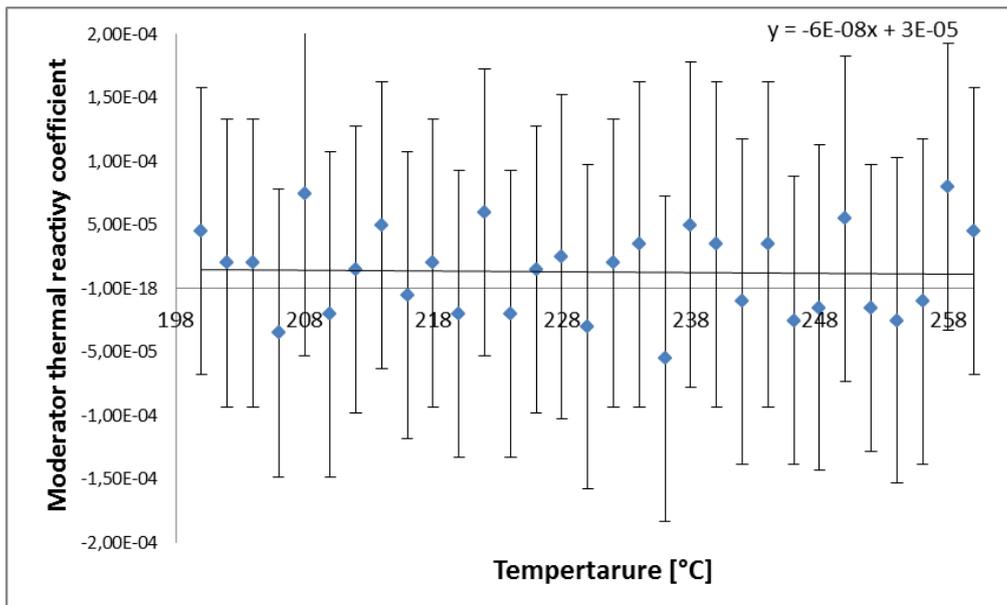


Figure 4: Moderator thermal reactivity coefficients (position of the 6<sup>th</sup> CA group of 200 cm, preservation of temperature of the other core components at 200°C).

## 5 CONCLUSION

The drop of the critical boron acid concentration between 200°C and 260°C indicates the expectation of negative summarized thermal reactivity coefficient values related to the first fuel loading using the 2<sup>nd</sup> generation type of FA. Implementation of the iteration method based on automatic computation of the given critical parameter can be used for the calculation of other variables including control rod position, or appropriate coolant density.

The analysis of the summary thermal reactivity coefficient  $a_{pO}(T)$  in the given temperature interval (for the 2<sup>nd</sup> generation type of FA) proved that the obtained summary thermal reactivity coefficient  $a_{pO}(T)$  has the trend line (Fig.3) in the negative area. With growing coolant temperature, the absolute value of  $a_{pO}(T)$  is increasing, corresponding to the theoretical assumptions. The moderator thermal reactivity coefficient, as demonstrated in the Fig.4, has the trend line in positive area, but it is still close to zero. With increasing moderator temperature the value of  $a_M$  is decreasing, according to expectations. Based on the computed results presented in Fig.3 and Fig.4 we can claim that the 2<sup>nd</sup> generation type of FA satisfies the safety criteria for the reactor start-up process.

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