Total fission energy depending on VVER-1000 fuel burnup

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Abstract. To calculate the energy deposition in a nuclear reactor’s core, it is necessary to calculate the value of the energy released per one fission act. Simplified methods for calculating the total fission energy are still used in many computer codes. They do not take into detailed account some of the physical phenomena occurring in nuclear fission and their time dependence. In this work, we used a calculation method that takes into account these physical features in order to obtain the dependence of the total fission energy and its components on the fuel burnup of VVER-1000. The calculation for the model of 16ZSH type fuel assembly using the methodology of the Fisencor.pl program (based on the MCU-PTR code) demonstrated that total fission energy increases with the fuel burnup. During the interval between refuelling, total fission energy increases by 3% from 199.7 to 206.4 MeV per one fission. Application of the proposed method for calculating the total fission energy will allow to enhance the precision of nuclear fuel isotopic composition calculations.

1. Introduction
An important task of design and operation of nuclear reactors is the calculation of the energy distribution in the core. Many modern calculation programs use methods for calculating the energy release and deposition, which do not take into account some of the components of the total fission energy and possible corrections to it (e.g. MCNP, SERPENT, MCU-PTR, RAINBOW, TVS-M, JARFR).

The use of the method of calculation of energy release, which takes into account the above mentioned features, will increase the accuracy of the calculation of the neutron characteristics of nuclear reactors.

The total fission energy along with its components was calculated depending on the fuel burnup for fuel assembly of 16ZS type of VVER-1000 using the method, which was developed in previous works [1-5] and improved in the present work. To perform the calculations, the script Fisencor.pl was developed on the base of MCU-PTR code. The script was intended to obtain total fission energy using the rates of nuclear reactions calculated in MCU-PTR. Application of the script allows also to adjust values of the total fission energy in the library of the MCU-PTR code and maintain the critical state of the model.

2. Method of total fission energy calculation
It is recommended to calculate the total fission energy taking into account all components according to the formula [6,7].
\[ E_{\text{total}} = E_{\text{f}} - E_{\text{0}} - \Delta E_n - \Delta E_{\beta\gamma} + E_{\text{nc}}, \]

where \( E_{\text{f}} \) is fission energy, \( E_{\text{0}} \) is kinetic energy of antineutrino, \( \Delta E_n \) is the correction to the kinetic energy of neutrons, \( \Delta E_{\beta\gamma} \) is the correction to the delayed energy release, \( E_{\text{nc}} \) is the capture component of the fission energy. When calculating the components of the total fission energy, one should take into account the dependence of the fission energy and corrections to the kinetic energy of neutrons on the energy of the fissioning neutron, the dependence of the delayed energy release from the previous work regime of a reactor, the dependence of the capture component on the isotopic composition of materials in the core. All of them were taken into account in the developed method [1–5].

The accuracy of calculating the total fission energy directly affects the accuracy of the calculation of the neutron flux density and therefore the accuracy of the calculation of the change in the isotopic composition of nuclear fuel during the operation of a reactor.

The scheme adopted in many programs for calculating the change in the isotopic composition of nuclear fuel consists in the sequential solution of the stationary neutron transport equation and the system of isotopic kinetics equations (adiabatic approximation [8, 9]). In this combination, the Monte Carlo method is used to obtain the spatial distribution of the neutron flux at a fixed point in time. The system of equations of isotopic kinetics is solved to obtain changes in the isotopic composition during a given period of time at a constant neutron flux.

Some programs allow to take into account the dependence of the change in the neutron flux during a time step. For example, in the module for solving the equations of isotopic kinetics, which is included in the MCU-PTR code (module BURNUP), it is taken into account that the neutron flux depends linearly on time. The fuel burnup is calculated using the predictor-corrector method, in which the isotopic composition at the end of the step is calculated twice: first without taking into account the dependence of the neutron flux on time, and then taking into account the linear dependence obtained from the first calculation. The use of linear interpolation of the flux reduces the error of the effective multiplication factor, fuel burnup, and the isotopic composition of the burnt out nuclear fuel [10].

With the help of the Monte-Carlo code, it is possible to obtain only the values of tallies normalized to a unit neutron production rate [11]. To translate them into real values, they should be normalized to the reactor power using the normalization factor [12], called the scaling factor:

\[ S = \frac{P \bar{\psi}_f}{K_{\text{eff}} E_{\text{tot}}}. \]

where \( \bar{\psi}_f \) and \( E_{\text{tot}} \) are the average number of neutrons produced in one fission reaction, and the total fission energy averaged over all fissile isotopes, \( P \) is the integral thermal power of the reactor.

It is obvious that the error in the total fission energy directly affects the magnitude of the scaling factor, which is proportionally related with the neutron flux density. When calculating the change in the isotopic composition of nuclear fuel, an error in the neutron flux density gives an error in the resulting composition of the burned fuel.

3. Implementation of the method on the basis of the MCU-PTR code

To correct the total fission energy in the calculations of the change in isotopic composition of nuclear fuel using the MCU-PTR code, a program Fisencor (fission energy correction) in the PERL scripting language was created. This program implements the previously developed method for calculation of the total fission energy and corrects the values of the total fission energy used in the MCU-PTR code for normalization of the neutron flux density to the reactor model power. The program can also adjust the concentration of boric acid or the depth of the control rods immersion in order to maintain the critical state of the model (Figure 1).
Algorithm of the program Fisencor includes three parts.

1. Bringing the model to a critical state by changing the concentration of boric acid or moving the control rods (Borcor and Rodcor subroutines).

   The model is brought to a critical state by changing the mass fraction of boric acid in the moderator.

   Before the calculation, the value of the mass fraction of boric acid at the first time step and its primary increment is specified. The critical value of boric acid is calculated from two values of the multiplication factor obtained in the calculation of the MCU-PTR with different fractions of boric acid. It is assumed that the multiplication factor is linearly dependent on the mass fraction of boric acid. If the multiplication factor does not correspond to the unity with the accuracy specified by the user, then additional calculations are carried out until an acceptable deviation from the unity is reached. If the user-specified accuracy is lower than the statistical calculation error, then the program increases the number of simulated histories.

   At each time step, more than one calculation is performed with modified mass fraction of boric acid. For subsequent time steps, the mass fraction of boric acid from the previous step is used as an initial value, and the difference between the mass fraction values in the two previous steps is used as an increment. To bring the model of VVER-1000 reactor to a critical state with an accuracy of $\Delta K_{\text{inf}} = 0.01$ (pin cell and fuel assembly models), about two calculations with different mass fractions of boric acid are required. It is necessary to ensure that the concentration of boric acid does not exceed the critical value (about 7-8 g per 1 kg of water), otherwise the model will not correspond to the operating state of the reactor.

   Also, for bringing to a critical state, the subroutine Rodcor can be used, with the help of which the immersion depth of the control rods is changed. This subroutine was not used in this work.

2. Calculation of the time step.

   The program deletes the files remaining from the calculation of the previous time point, adjusts the time step value (if required), calculates one step in the MCU-PTR. The calculation consists of three steps in time according to the predictor-corrector method. The 2nd step is taken as the result. Then the program creates a file with an extension REZ, containing the values of the multiplication factor, the delayed energy release, the concentration of isotopes. The file with an extension PDC_B1 is saved to the PDC file to transfer the isotopic composition to the next time step.

3. Calculation of $E_{\text{total}}$.

   At this stage, with the subroutine Etotal, the calculation and adjustment of the total fission energy in the library of the MCU-PTR code is carried out (contains 20 fissile isotopes). To obtain the components of the total fission energy, the integrated over the volume fission and neutron capture

![Figure 1. The scheme of the program Fisencor](image-url)
reaction rates in a given number of energy intervals are calculated with MCU-PTR. In this work, we used 29 energy intervals. The tabular values of the fission energy components are taken from ENDF/B-VII.I (taking into account the dependence on the incident neutron energy), neutron-capture reactions energy yields are from [13], obtained on the basis of the mass excess of the reaction products taken from AME2016 [14]. After calculating the total fission energies of individual fissile isotopes, an adjustment could be made to the ENERGY.FIS file. In this paper, the calculations were carried out without adjusting the ENERGY.FIS.

4. Dependence of total fission energy components on the reactor operation time
The calculation of the total fission energy depending on the fuel burnup was performed for the 16ZS fuel assembly model with oxide fuel having 2% enrichment of $^{235}$U [4]. The total power of the model was 18405 kW. The time scale was divided into uneven intervals. The step was smaller at the beginning of the reactor operation. A total of 30 steps were considered. The total number of histories for each time step was 1.2 million. The average time for calculating one step on the PC (2 cores), taking into account the bringing into critical state was 4 hours. All isotopes with concentrations below $10^{-8}$ were included into the artificial summarized isotope. Exceptions were $^{10}$B, $^{235}$U, $^{238}$U, $^{239}$Np, $^{239}$Pu, $^{240}$Pu, $^{241}$Pu, $^{242}$Pu, $^{242}$Am, $^{242}$Cm, $^{135}$Xe, $^{135}$I, $^{149}$Pm, and $^{149}$Sm.

The dependence of the total fission energy and its components on the time of the reactor operation is presented in Figures 2 and 3. The fuel burnup after 325 days is 14 MWd/kg. The accuracy of the transfer to the critical state was set to $\Delta K_{inf} = 0.01$.

![Figure 2](image_url)

**Figure 2.** Dependence of the total fission energy and its components on the VVER-1000 fuel burnup. $E_{\beta\gamma}$ is the delayed energy per fission event, $Q_{nc}$ is the average energy release when a single neutron is captured.
Figure 3. Dependence of the components of the total fission energy on the VVER-1000 fuel burnup

The results show that during the interval between refueling, the total fission energy increases by 3%. This is explained by the fact that the capture component increases by 32% (due to the increase in captures on fission products) and the average fission energy increases by 2% (due to the increase in the number of fissions of $^{239}$Pu). The average energy release in neutron capture also increases by 17% and the correction for the kinetic energy of fission neutrons increases by 10%, but its average value is small (0.25 MeV / fission). As the contribution of plutonium fissions increases, the amount of delayed energy per one fission decreases by 8%. Hereby the correction for delayed energy changes its sign (approximately 25 days after the start of the reactor operation).

5. Conclusions

The calculation of the spatial distribution of power density is one of the most important tasks in modeling of the processes occurring in the cores of nuclear reactors. To obtain it, it is necessary to know the amount of energy released in a fission event. The accuracy of the calculation of the total fission energy is determined by the detailing of the considered physical phenomena occurring during nuclear fission. However, many calculation programs still use simplified methods for calculating the total fission energy.

This paper describes the application of the developed method of energy deposition calculation for calculating the dependence of the total fission energy on the fuel burnup for fuel assembly 16ZS of the VVER-1000. The calculation takes into account the components of energy release associated with the fission of heavy nuclei and neutron capture, the correction for the delayed energy release, the correction for the kinetic energy of fission neutrons, the continuous dependence of the fission energy on the energy of the incident neutron. When calculating the correction for delayed energy release, the change in the isotopic composition of nuclear fuel during the reactor operation is simulated, taking into account transformations of isotopes occurring due to fission, neutron capture and radioactive decay. When calculating the correction for the kinetic energy of fission neutrons, their leakage outside the core is taken into account.
To implement the calculation methodology based on the MCU-PTR code, program Fisencor.pl was developed, which allows to bring the model to a critical state, calculate and adjust the total fission energy in the MCU-PTR code’s library.

The results show that during one interval between refuelling, the total fission energy increases by 3%, the capture component increases by 32%, the correction for the kinetic energy of fission neutrons increases by 10%, the amount of delayed energy and the correction for delayed energy are reduced.

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