Conference Paper

CALCULATION OF NEUTRON-CAPTURE REACTIONS CONTRIBUTION TO ENERGY RELEASE IN VVER-1000 USING SERPENT CODE

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Abstract

Calculating the energy release in fuel elements is an important aspect of the modeling and design of nuclear reactors. Most of the energy is produced by fission, but a non-negligible percentage is coming from neutron capture reactions, such as (n, γ) or (n, α). We implement a previously developed method for the calculation of effective energy release using Serpent Monte Carlo code. We investigate the percentage of capture component in effective energy release for various models of VVER-1000 fuel: firstly, an equivalent cell, then fresh fuel assemblies of different compositions, differing in fuel enrichment and the presence of burnable absorbers. The results are compared to similar calculations previously done in MCNP 4 and MCU 5.

Keywords: capture energy, fission energy, nuclear reactor, Monte-Carlo, Serpent, VVER

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1. Introduction

Calculation of physical characteristics of nuclear power reactors is a complicated task. The precision of the calculation strongly depends on the used methods and nuclear data. Nowadays high computational powers of supercomputers give the possibility to perform complex and precise calculations. Using Monte-Carlo codes one can obtain results with very low statistical errors. However, final bias of the calculated physical value depends not only on the Monte-Carlo statistical error, but also on the table data used in the calculation. This kind of errors could be caused by error in effective energy release values. They could appear in the calculation of nuclear fuel burn-up and spent nuclear fuel characteristics. In addition, precise effective energy release values are needed for reactors antineutrino spectrum predictions.

In this work using Serpent Monte Carlo code we repeated the calculations executed previously [1], because it is essential for model and codes cross verification. The new results showed agreement with the previously obtained ones.

2. Calculation method

The effective energy release can be expressed as:

$$E_{efe} = E_f - \Delta E_n - \Delta E_{\beta\gamma} + E_{capt} \quad (1)$$

where: E_f –fission energy, ΔE_n – adjustment considering the loss of fission neutrons kinetic energy after an absorption which leads to fission, $\Delta E_{\beta\gamma}$ – adjustment considering that energy release from fission fragments decay is delayed and E_{capt} – energy released in neutron-capture reactions.

The effective energy released depends on geometrical and material composition of neutron-multiplying system (an investigated model). The energy values on the right-hand side of (1) are proportional to fission and capture reaction rates by a respective energy yield.

We used the Serpent Monte-Carlo transport code [2] with cross section and thermal scattering libraries based on ENDF/B-VII database [3] to obtain reaction rates. For calculating effective energy release components, we used energy yields table values based on data from ENDF/B-VII.I. and Nubase2012 [4].

3. Models

The simplest VVER-like model is an equivalent cell. The geometrical parameters of the model are like a fuel pin and its vicinity in a VVER-1000 fuel assembly (Fig 1.) and material composition is a simplified version of regular VVER fuel assemblies' material compositions (Table 1.) with no fission products. The moderator contains boric acid in such amount that makes the multiplication factor equal one while using reflective boundary conditions. The calculation was carried out for two different temperatures, a 'cold state': T_{fuel} = 293.6 K, $T_{cladding}$ = 293.6 K, $T_{moderator}$ = 293.6 K with boric acid concentration 15.5 g (H_3BO_3) / kg (H_2O); and a 'hot state': T_{fuel} = 1200 K, $T_{cladding}$ = 900 K, $T_{moderator}$ = 600 K with boric acid concentration 17.8 g (H_3BO_3) / kg (H_2O).

For performing more complex calculations, two modified VVER-1000 fuel assemblies were modeled: 13ZS, which consist of 312 UO_2 fuel pins and 19 steel guide channels, to

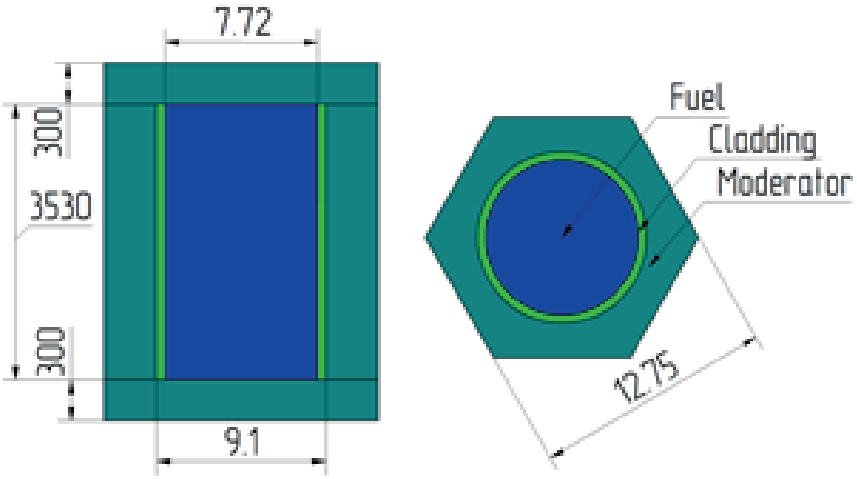

Figure 1: Equivalent cell geometry (mm).

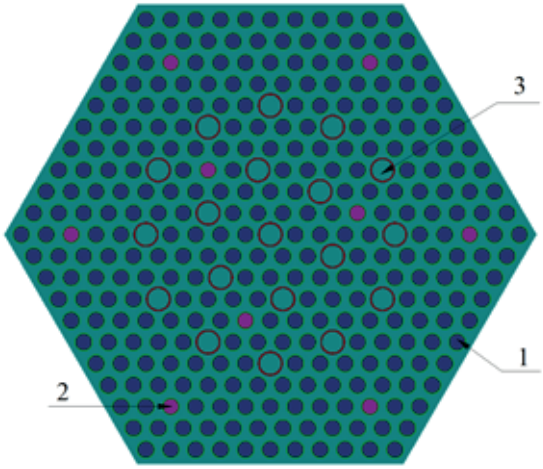

Figure 2: 30ZSV fuel assembly: 1-fuel rod, 2-fuel rod with gadolinium, 3-steel guide channel. The 13ZS fuel assembly is the same, if 2s are replaced by 3s.

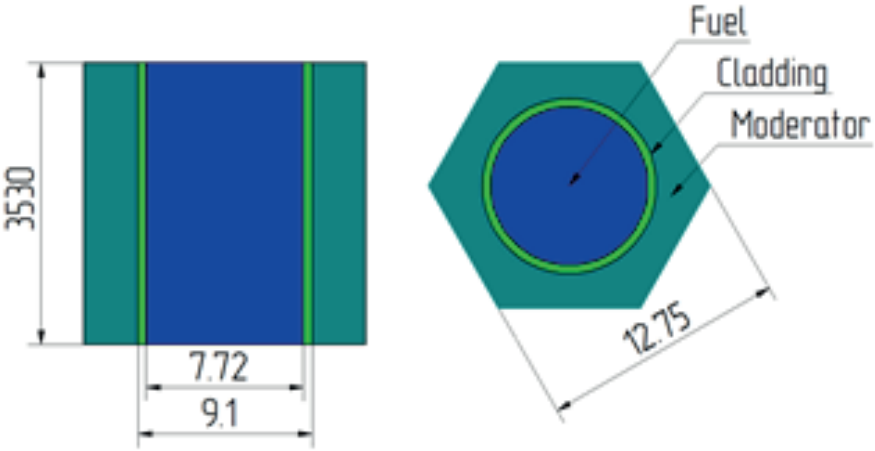

Figure 3: Geometry of a fuel rod (mm).

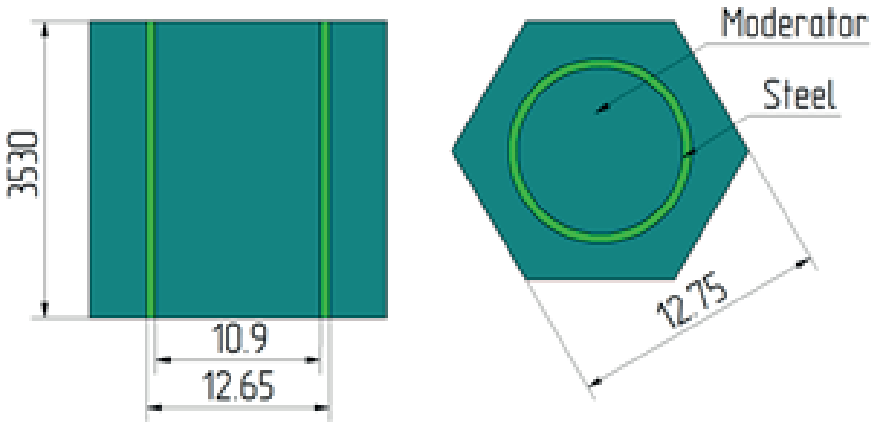

Figure 4: Geometry of a guide channel (mm).

Table 1: Material compositions for equivalent cell [5].

Material	Composition	Density (g/cm^3)
Fuel	UO_2 (3% ^{235}U)	10.0
Cladding	Zr + 1% ^{93}Nb	6.6
Moderator	$H_2O + H_3BO_3$	/ 0.715[a]
a.cold state / hot state		

Table 2: Results for equivalent cell model calculations in cold state. Energy values are in MeV/fission.

Funct.	Serpent	MCU	Relative difference	MCNP	Relative difference
K_{eff}	1.0171	1.0171	0.00%	1.0161	0.10%
ΔE_n	0.07	0.07	0.00%	0.07	0.00%
$E_{capt.}$	6.25	6.19	0.96%	6.15	1.60%
E_{efe}	198.5	198.4	0.05%	198.4	0.05%
E_{capt}/E_{efe}	3.15%	3.12%	0.95%	3.10%	1.59%

Table 3: Results for equivalent cell model calculations in hot state. Energy values are in MeV/fission.

Funct.	Serpent	MCU	Relative difference	MCNP	Relative difference
K_{eff}	1.0038	1.0027	0.11%	1.0075	-0.37%
ΔE_n	0.086	0.08	6.98%	0.08	6.98%
$E_{capt.}$	6.76	6.77	-0.15%	6.69	1.04%
E_{efe}	199.0	199	0.00%	199	0.00%
E_{capt}/E_{efe}	3.40%	3.40%	0.00%	3.36%	1.18%

Table 4: Material compositions for fuel assembly models [5].

Material	Composition	Density (g/cm^3)
Fuel	UO_2 (3% ^{235}U)	9.5
Fuel with gadolinium	UO_2 (2.4% ^{235}U) + 6.4% Gd_2O_3	9.5
Cladding	Zr + 1% ^{93}Nb + 4% Fe + 0.6% Ni + 1% Cr + 0.06% Ti + 0.01% C	6.6
08X18H10T steel	Fe + 18.5% Cr + 10.5% Ni + 1% Ti + 0.1% C	7.7
Moderator	H_2O + H_3BO_3	1.0 / 0.715[a]
a. cold state / hot state		

Table 5: Results for the fuel assembly models in cold state. Energy values are in MeV/fission.

Funct.	Serpent	MCU	Relative difference	MCNP	Relative difference
13ZS					
K_{eff}	1.0085	1.0072	0.13%	1.008	0.05%
ΔE_n	0.075	0.074	1.33%	0.076	-1.33%
$E_{capt.}$	6.65	6.72	-1.05%	6.64	0.15%
E_{efe}	198.9	199	-0.05%	198.9	0.00%
E_{capt}/E_{efe}	3.34%	3.38%	-1.20%	3.34%	0.00%
30ZSV					
K_{eff}	1.0077	1.0038	0.39%	1.0027	0.50%
ΔE_n	0.073	0.074	-1.37%	0.076	-4.11%
$E_{capt.}$	7.59	7.64	-0.66%	7.6	-0.13%
E_{efe}	199.8	199.9	-0.05%	199.8	0.00%
E_{capt}/E_{efe}	3.80%	3.82%	-0.53%	3.80%	0.00%

study the effect of a more complex geometry on the capture energy release component; and 30ZSV, which is identical to the previous one, except that 9 fuel pins contain gadolinium, so on this model, the effect of the presence of burnable absorbers can be shown. Figures 2., 3. and 4. present the geometrical characteristics of these fuel assemblies. The fuel assembly pitch in a VVER-1000 core is 236 mm.

The material compositions in these models are more accurate as well (Table 4.).The calculations were carried out with two temperature settings: 'cold state': T_{fuel} = 293.6 K, $T_{cladding}$ = 293.6 K, T_{steel}= 293.6 K and $T_{moderator}$= 600 K with boric acid concentration

Table 6: Results for the fuel assembly models in hot state. Energy values are in MeV/fission.

Funct.	Serpent	MCU	Relative difference
13ZS			
K_{eff}	1.0084	0.9998	0.86%
ΔE_n	0.075	0.075	0.00%
$E_{capt.}$	6.79	6.83	-0.59%
E_{efe}	199.0	199.1	-0.05%
E_{capt}/ E_{efe}	3.41%	3.43%	-0.59%
30ZSV			
K_{eff}	1.0095	1.0007	0.87%
ΔE_n	0.073	0.073	0.00%
$E_{capt.}$	7.71	7.73	-0.26%
E_{efe}	200.0	200	0.00%
E_{capt}/ E_{efe}	3.86%	3.86%	0.00%

15.7 g (H_3BO_3) / kg (H_2O) for the 13ZS and 9.5 g (H_3BO_3) / kg (H_2O) for the 30ZSV fuel assembly; and a 'hot state': T_{fuel} = 1200 K, $T_{cladding}$ = 600 K, T_{steel}= 600 K and $T_{moderator}$ = 600 K with boric acid concentration 14.17 g (H_3BO_3) / kg (H_2O) for the 13ZS and 7.7 g (H_3BO_3) / kg (H_2O) for the 30ZSV fuel assembly.

4. Results

The investigated functionals were: the effective multiplication factor K_{eff}, to check the consistency of the models; effective energy release components ΔE_n and E_{capt}; E_{efe} itself and the E_{capt}/ E_{efe} ratio as a most expressive value for the calculations.

The results for the equivalent model calculations are shown in tables 2. and 3 and the results for fuel assembly model calculations are shown in tables 5. and 6. Results obtained by MCNP and MCU are cited for comparison from [1]. The relative differences are calculated as:

$$\frac{(value\ from\ Serpent) - (value\ from\ MCNP\ or\ MCU)}{(value\ from\ Serpent)} \quad (2)$$

For the hot state of fuel assemblies, there were only MCU calculations to compare with.

From the result tables we can see that the results obtained using Serpent are in the same order of magnitude as the result of previous calculations: the relative differences

are less than or around 1%, similar to differences between MCU and MCNP results in [1] (aside from few instances, which is to be blamed on the round-off).

The various phenomena observed in [1], can be observed in the Serpent results as well:

- The contribution of capture reactions to the effective energy release is larger in hot state than in cold state in the equivalent cell model: 3.40% vs. 3.15%. This is due to the increment of neutron capture probability in ^{238}U by Doppler resonance broadening after heating the fuel.
- The aforementioned effect presents itself in smaller magnitude in the fuel assembly models than the equivalent cell models: in the 13ZSV fuel assembly is 3.41% vs. 3.34% and in the 30ZSV it is 3.86% vs. 3.80%. The reason for this is the presence of guide tubes filled with moderator and the difference in the densities of fuel.
- The presence of gadolinium makes the capture energy release contribution larger (3.86% vs 3.41% in hot state and 3.80% vs. 3.34% in cold state), because the energy release of (n,γ) reaction in gadolinium is three times higher than of (n,α) reaction in boron.

5. Conclusions

We can conclude that using Serpent, we get similar values for the investigated quantities and the results behave qualitatively the same as results obtained by using other transport codes. This fact supports the credibility of the results.

We assured that Serpent is as valid tool for these kind of calculations as MCU and MCNP, so one may choose to use Serpent instead of the latter two codes.

We could see that capture reactions account to 3-4 % of the effective energy release in the investigated models, which is not a negligible amount. Therefore, in the modelling and calculations of VVER reactors, one should consider these reactions beside the fission.

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