Conference Paper

THE VERIFICATION OF THE COMPLEX PROGRAMS SERPENT 2 AND SCALE (SAS2) FOR ANALYSING THE SAFETY CHARACTERISTICS OF FA REACTOR VVER-1000 AT ALL THE OPERATION STAGES

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Abstract

Currently, to estimate the parameters of the Spent Nuclear Fuel (SNF) and their evolution with time many of the international software are used. This work is dedicated to the evaluation, analysis and comparison the safety characteristics of the fuel Assembly which used in reactor types VVER-1000 obtained in the present work and by other authors [1] using different software packages. The result of calculation for the characteristic safety nuclear fuel at many stages of the Nuclear Power Planet (NPP) was also calculated in this work.

Keywords: VVER-1000, FA, K_{eff}, SNF, SERPENT2, SCALE5 (SAS2), safety.

1. Introduction

Verification and validation of the neutron's codes that are used for modeling the behavior of the nuclear power plants (NPPs), is the subject of research since the beginning of the nuclear technology. There are several objects and research reactors, intended for research on these issues, and there are many publications in this field (for example, the authors have been involved in [2–4]).

The countries that want to have nuclear energy should strengthen the possibility of using these calculations. Some of these calculations include neutron codes, such as WIMS-ANL [5], CITATION [6], MCU [7], MCNP [8], SCALE [9] and others.

To confirm the reliability of the analysis model, it's necessary to verify the calculation methods [10-14] by comparing the calculation results with the measurement results.

Verification of complex programs is very important at every stage of the fuel cycle in nuclear power plants, from the initial campaign, operation, storage and transportation.

2. Code and model

In the present work to calculate the characteristic of the spent fuel assemblies of VVER-1000, SERPENT (2.1.28) and the SCALE5 code package (SAS2) codes were chosen.

SERPENT is [15] a software tool (PS) that implements the Monte-Carlo simulations, enabling the calculation of the change of nuclide composition of nuclear fuel during the irradiation in the reactor, and the effective neutron multiplication factor K_{eff} of arbitrarily complex systems, using for their description two - or three-dimensional geometry [15].

The code package SCALE includes computer module (SAS2) that combines programs (BONAMI, NITAWL, XSDRNPM, COUPLE, ORIGEN-S, and XSDOSE) and libraries (ENDF/B-V in different group energies) to calculate a particular problem (the analysis of the criticality, radiation safety, heat transfer, distribution of isotopic composition depending on burnup) [9, 16]. Other programs that were compared with our results are presented in [1].

For analysis, fuel Assembly (FA) for VVER-1000 was used with standard parameters which are presented in table 1 and Figure 1[1]. In addition to the channels of the fuel elements in the model there is a central channel and 18 of the guides channels, which is a water-filled steel pipe with a zirconium clad. The concentration of isotopes, borated water, fuel and clad presented in table 2.

3. Results and Discussions

In the present work the results of the fuel safety characteristics of reactor VVER-1000 in several tasks, storage of fresh fuel, irradiated fuel and the cooling of spent fuel.

3.1. Non-Irradiated fuel

3.1.1. Storage fresh fuel

The pool storage model of the fresh fuel Figure 2 is an infinite lattice with a pitch of 40 cm and with temperature of 300 K for all materials. Effective neutron multiplication factor K_{eff} significantly depends on the choice of lattice spacing. In table 3 and Figure 3,

Table 1: Geometric specification's for FA.

Parameters	FA-A
Длина топливного элемента. мм	3530
Mass UO_2. Kg	453.504
The number of fuel elements 312/FA (pitch=12.75mm)	
Enrichment (%)	4.4%
The outer diameter of the fuel pellet. mm	7.72
Inner/Outer diameter of the clad. mm	7.72/9.1
Clad material/ density (g /cm^3)	Zr
The Central tube	
Inner/Outer diameter	9.6/11.25
Material / density (g / cm^3)	Zr
Guide tube (18)	
Inner/Outer diameter	10.9/12.65
Material / density (g / cm^3)	Zr

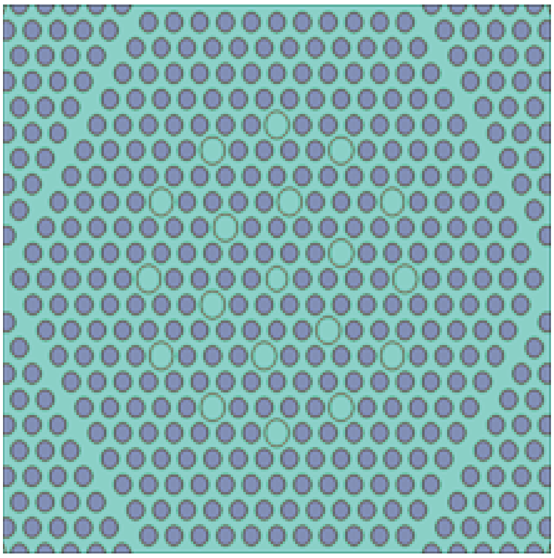

Figure 1: FA geometry.

compared the results of calculation effective neutron multiplication factor K_{eff} according to changes of the density of water (1.0 to 0.0) g/cm^3 by using code SERPENT and the cross section library ENDFB7 with other results by using code (KENO-SCAL4) and the cross section library ENDFB4 presented in work [1].

In the dependent of K_{eff} and the density of water, we can obtain three ranges. In the first range with decreasing the density of water, K_{eff} decreases, because the

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Table 2: Concentrations of isotopes borated water, fuel and clad in units of [atom/(barn·cm)].

	Actinides	UOX (4.4%)
Fuel	^{16}O	3.9235E-2
	^{234}U	8.0000E-6
	^{235}U	8.7370E-4
	^{238}U	1.8744E-2
Clad	Zr	4.2300E-2
Borated water	^{1}H	4.7830E-2
	^{16}O	2.3910E-2
	^{10}B	4.7344E-6
	^{11}B	1.9177E-5

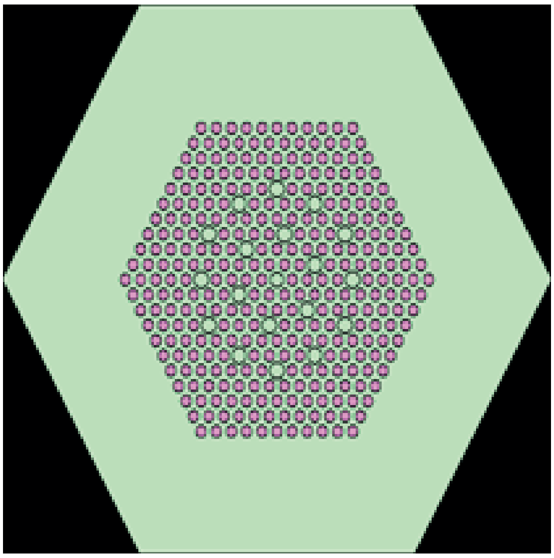

Figure 2: Geometry of the container of the transported fuel.

system has enough water for isolation (independence) assemblies from each other. In the second range with decreasing the density of water, K_{eff}increases, because of the assemblies lost the isolation from other assemblies. And in the third range, with decreasing the density of water, K_{eff} decreases because assemblies are in the conditions of "under-moderated" (between the fuel cells is less than the optimum amount of moderator).

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TABLE 3: The dependence of value K_{eff} for changing the water density.

The density of water (g/cm³)	SERPENT (ENDF/B-VII)	Error	KENO (ENDF/B-V)	Deviation SERPENT-KENO
			238 groups	
1	0.93048	0.00138	0.9254	0.51%
0.9	0.90746	0.00132	0.9031	0.44%
0.8	0.89029	0.00132	0.88530	0.50%
0.7	0.88437	0.00127	0.87950	0.49%
0.6	0.89664	0.00124	0.89160	0.50%
0.5	0.93718	0.00116	0.93250	0.47%
0.4	1.01874	0.00114	1.01400	0.47%
0.3	1.13786	0.00103	1.13500	0.29%
0.2	1.27083	0.00087	1.26900	0.18%
0.1	1.28051	0.00094	1.28700	-0.65%
0 (without pitch)	0.65480	0.0005	0.66360	-0.88%

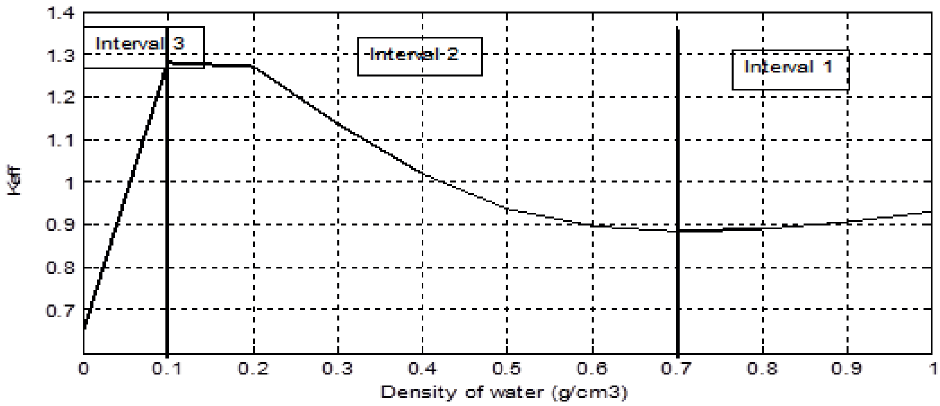


Figure 3: The dependent of values K_{eff} for changing the water density.

3.1.2. The spectrum of gamma ray from the fresh fuel

In Table 4 and Figure 4a and *Figure 4b* presented the spectrum of gamma ray for fresh fuel. Code SERPENT examines and calculates the continuous energy spectrum (Figure 4a). However, to compare it with the result in work [1] it must be converted in the groups of energy (Figure 4b).

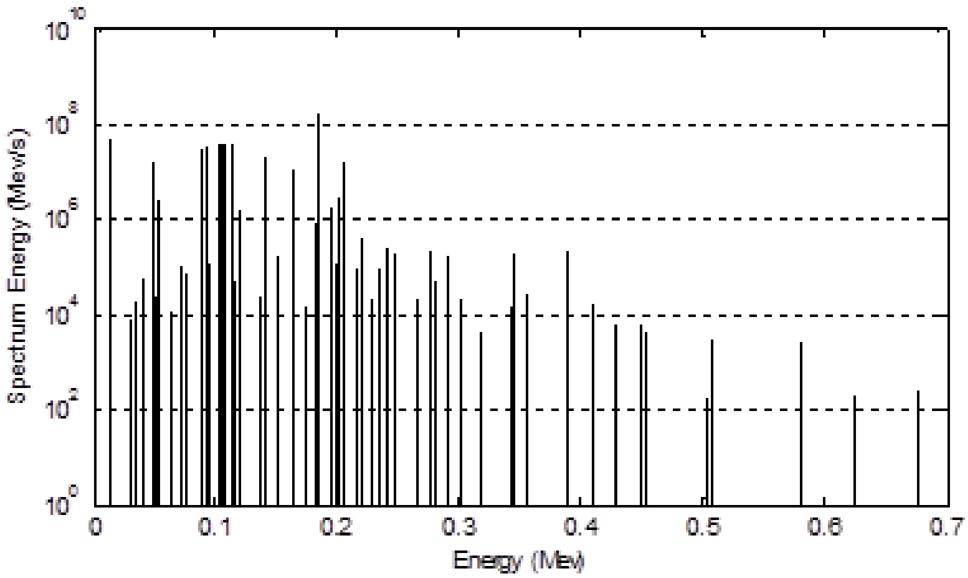
Spectrum of gamma radiation consists of photons resulting from the decay of various isotopes and spontaneous fission of actinides.

Table 4: Spectrum of the gamma for fresh fuel by SERPENT and from work *[1]* by SCALE4.

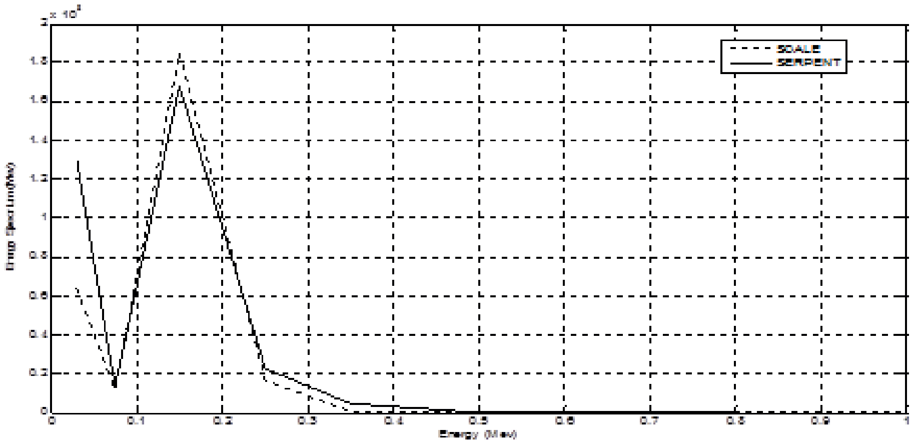
Energy interval	SERPENT		SCALE	
(Mev)	1/c	Mev/s	1/s	Mev/s
От 1.0E-2 до 5.0E-2	4.35E+9	1.30E+8	2.13 E+9	6.40E+7
От 5.0E-2 до 1.0E-1	1.77E+8	1.32E+7	1.56 E+8	1.17E+7
От 1.0E-1 до 2.0E-1	1.12E+9	1.68E+8	1.23 E+9	1.85E+8
От 2.0E-1 до 3.0E-1	9.17E+7	2.29E+7	6.55 E+7	1.64E+7
От 3.0E-1 до 4.0E-1	1.32E+6	4.62E+6	1.95 E+6	6.83E+5
От 4.0E-1 до 6.0E-1	9.13E+4	4.56E+4	1.75 E+5	8.73E+4
От 6.0E-1 до 8.0E-1	5.74E+2	4.02E+2	2.42 E+4	1.70E+4
От 8.0E-1 до 1.0E00			3.72 E+3	3.35E+3
От 1.0E0 до 1.3E00			5.07 E+3	5.91E+3
От 1.3E0 до 1.6E00			2.83 E-22	4.23E-22
От 1.6E0 до 2.0E00			2.21 E+3	4.04E+3
От 2.0E0 до 2.5E00			1.34 E+2	3.01E+3
От 2.5E0 до 3.0E00			7.73 E+2	2.13E+3
От 3.0E0 до 4.0E00			6.93 E+2	2.43E+3
От 4.0E0 до 5.0E00			2.33 E+2	1.05E+3
От 5.0E0 до 6.5E00			9.35 E+1	5.38E+2
От 6.5E0 до 8.0E00			1.83 E+1	1.32E+2
От 8.0E0 до 1.0E+2			3.88 E0	3.49E+1
total	5.74E+9	3.35E+8	3.59E+9	2.78E+8

By SERPENT, the spectrum includes gamma photons with energies not more than 0.7 Mev, and does not include photons generated from spontaneous fission. The main contribution to the spectral radiation gives photons with energies in the range of 0.1-0.2 MeV. The mean free path of these photons in the fuel is 0.04 to 0.08 cm, and the radius of one pin fuel equal to 0.386 cm, which means that, photons have a low probability of exit from the FA.

SERPENT 2 calculates only the total rate of the spontaneous fission (2.57865 E+05 decay/s), which is significantly less than the integral spectrum of gamma radiation (5.74 E+9 1/s). Therefore, the spontaneous fission does not make a significant contribution to the integral spectrum of radiation. But the photons from spontaneous fission with much higher energies have a substantially higher probability of exit from free



(a)



(b)

Figure 4: (a) Spectrum of gamma radiation from FA by SERPENT, (b) Spectrum of gamma radiation from FA in the group energy.

fuel element and the FA. Therefore, their contribution to the value of dose rate from gamma radiation increases.

3.1.3. The dose rate gamma radiation

The dose rate of gamma radiation calculated for two options, direct from the fresh fuel in the form of the fuel assemblies and from casks which are used for transporting

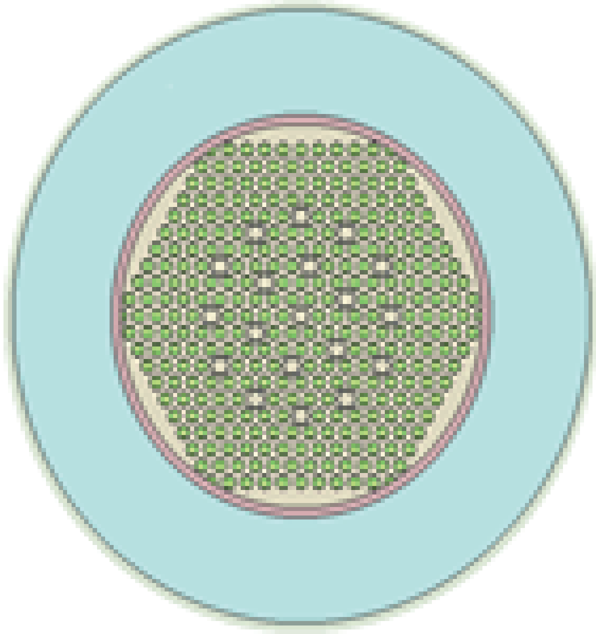


Figure 5: Model of fresh fuel cask.

the fresh fuel (Fig. 5). The isotopic composition of the barrel for fresh fuel in units of [atom/(barn·cm)] is presented in table 5.

Table 5: Composition of the atoms of cask for fresh fuel [atom/ (b·cm)].

Region	fuel	air	Stainless steel	caoutchouc	Stainless steel
radius (cm)	11.8	12.6	13.4	20.4	21.0
Δ R (cm)		12.6	0.8	7.0	0.6
FA	FA				
Zr					
H			0.0001	0.05372	
C				0.01797	0.0001
N					
O				0.00895	
Si				0.00895	
Cr			0.01525		0.01525
Fe			0.06006		0.06006
Ni			0.00847		0.00847
Ti			0.00085		0.00085

The program SERPENT 2 calculates the dose rate only from gamma radiation, and the power of the neutron component of the dose does not take into account. Therefore, Table 6 and Table 7 show the dose rate of gamma radiation for the fresh fuel in the assembly and fresh fuel in the cask (FA, FA barrels) at the surface and at distances 0.5, 1.0 and 2.0 m from the surface with temperature of 300 K. In addition to this, Table 6 and Table 7 compare the data with the author's data and SAS2 [1].

Table 6: Results of the dose rate calculations of the fresh fuel assemblies of VVER-1000 reactors with enriched at 4.4 % UOX fuel.

Detector	SAS1	SERPENT 2	SERPENT-SAS1
Distance from the surface (m)	Gamma dose (μsv/h)		
0.0	2.23	2.33	10.00%
0.5	0.31	0.27	4.20%
1	0.16	0.14	1.90%
2	0.07	0.06	0.53%

Table 7: Results of the dose rate calculations of the fresh fuel assemblies in the cask.

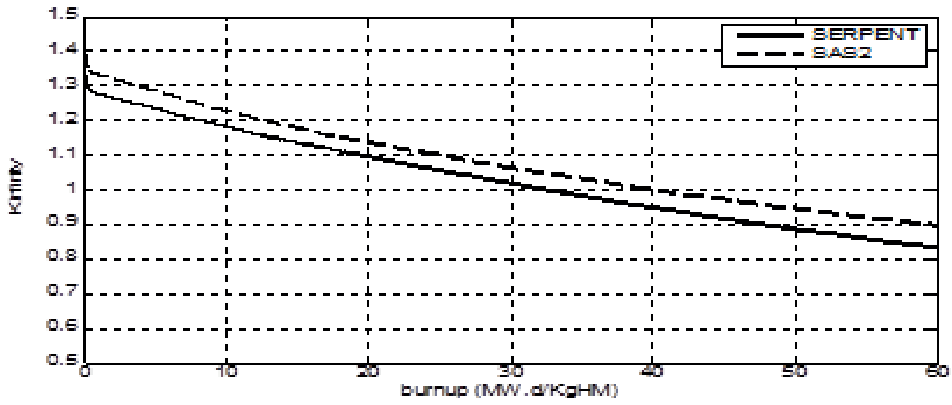
Detector	SAS1	SERPENT	SERPENT-SAS1
Distance from The surface (m)	Gamma dose (μsv/h)		
0.0	8.16E-2	7.86E-02	0.30%
0.5	1.98E-2	1.87E-02	0.11%
1	1.11E-2	1.01E-02	0.10%
2	5.16E-3	4.70E-04	5.11%

Satisfactory agreement between the data in the SERPENT 2 with the calculations results for SCALE 4 [1]. Accordingly, the result of the dose rate from gamma radiation, which calculated by SERPENT 2 are not inferior to similar code.

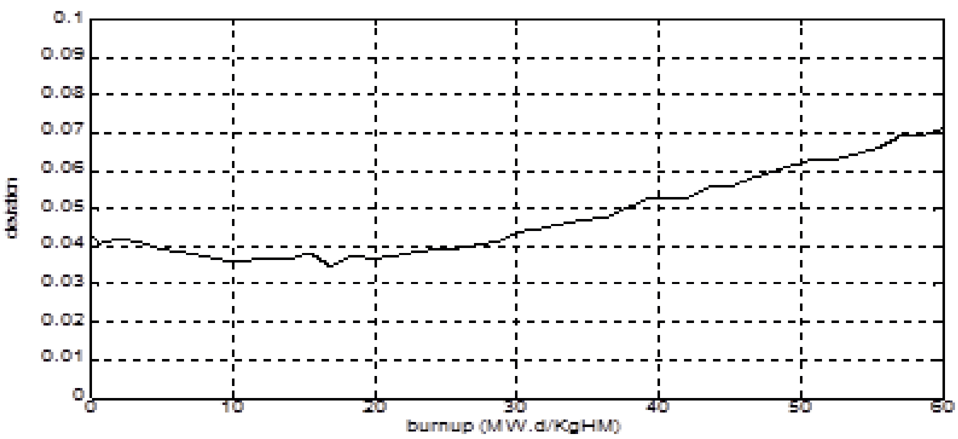
3.2. Irradiated fuel

For analysis irradiated burnable fuel, only the variation of the neutron multiplication factor K_∞ with burnup was calculated, from 0 to 60 (MW.day/Kg HM).

In Figure 6a and, the results of the calculation of the neutron multiplication factor K_∞ were obtained by SCALE5 (SAS2) and SERPENT 2 programs, and the deviation between them was also calculated and presented in Figure 6b.



(a)



(b)

Figure 6: (a) The dependence of K∞ for burnup by using SAS2 (SCALE5) and SERPENT, (b) Deviation between SAS2 and SERPENT for K∞ value in the dependence of burnup.

From *Figure 6a* we can notice that the values of K_∞ were calculated by different programs, are close to each other at different levels of burnup. The deviation results (Fig. 6b) of the burnup 30 [MW.day/Kg HM] was small and almost constant. After burn-in of 30 [MW.day/Kg HM], when K_∞ becomes approximately equal to 1.0, the differences between the results increase.

3.3. Cooling the spent fuel in the pool

3.3.1. The Energy spectrum of gamma-ray

The energy spectrum of the gamma-ray calculated by SAS2 and SERPENT and presented in Figure 7.

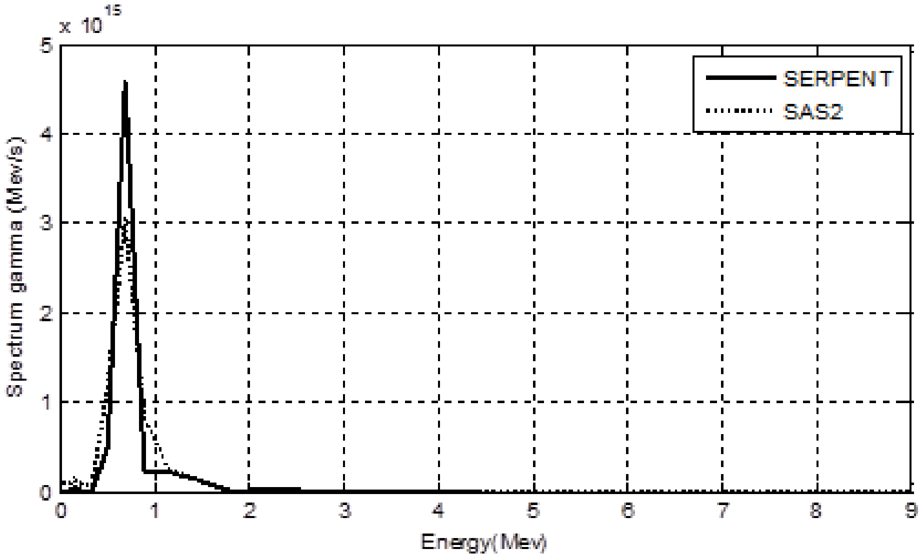


Figure 7: Energy spectrum of SFA photons after 3 years of cooling in 18- energy groups.

Evidently, photons with energies in the range 0.6-0.8 mav give the main contribution to the spectral radiation. And it is known that the main contribution to the spectral radiation is provided by the Cs-134 isotope photons precisely in this energy range. The concentration of the Cs-134 isotope in SERPENT at this time is greater than in SAS2 (4.58E + 01, 4.07E + 01) g / FA, respectively. Because of this, the spectrum of gamma radiation in this range is greater in SERPENT than for SAS2. But the total number of photons by SAS2 is greater.

3.3.2. Dose rates

The dose rate of gamma radiation at distances of 0.5; 1.0 and 2.0 m from SFA after 3 years cooling calculated by SAS2 and SERPENT and compared between others in this work (table 8). The value of dose rate of gamma radiation is related to the gamma radiation spectrum, for that, the values calculated by SAS2 more than SERPENT. The results agreed well with each other and presented in Table 8.

After 3 years cooling of the spent fuel, it can be accommodated in transport containers (Fig. 8). The composition and concentration of the atoms of structural materials in a container for spent fuel is presented in table 9. The total dose rate from gamma radiation and neutrons on the surface of the transport container with 12 SFA and at different distances from its surface, in this work it's calculated only by using program SCALE5 (SAS2). The results are shown in table 10 in comparison with the data obtained by different methods and presented in [1].

Table 8: Comparison of gamma dose rates [μSv / h] after 3 years of exposure, calculated by the programs SERPENT 2 and SCALE5.

The distance from the surface of the fuel assemblies (m)	The power of the gamma dose (μsv/h)		Deviation
	SCALE5	SERPENT2	
0.0	7.08E+8	5.79E+8	18%
0.5	7.89E+7	7.01E+7	11%
1	3.85E+7	3.34E+7	13%
2	1.53E+7	1.33E+7	13%

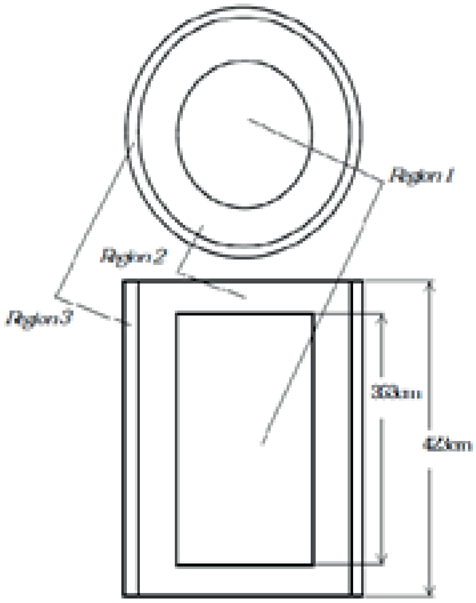


Figure 8: Model the storage of fresh fuel.

There is quite a significant and chaotic scatter of results later program SCALE with the previous versions of the calculations.

3.3.3. Activity and Residual heat generation of spent fuel

The dependence of the residual heat and activity of spent fuel for cooling time were calculated by SERPENT and SCALE5 (SAS2) and presented in Figure 9 and Figure 10 and Tables 11 and 12.

From Table 11 and Figure 9 we can notice that, the activity of the spent fuel which calculated by SAS2 and SERPENT2 with the time of cooling were very close, and the variances between them were not more than 1.4 %.

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Table 9: Состав и концентрация атомов конструкционных материалов в контейнере для отработавшего топлива [атом/ (барн см)].

Область	1	2	3
Диаметр, см	132	200	225
T, K	523	300	300
Zr	0,002216		
Fe	0,0027	0,061	
Cr	0,0007	0,016	
Ni	0,0004	0,008	
B	0,00029		
O	0,0054		0,026
C			0,014
H			0,065

Table 10: Comparison of dose rate [μsv/h] from gamma radiation and neutrons after 3 years of cooling, calculated by different methods.

The distance from the surface (m)	SAS2 SCALE5	SAS2 SCALE4	Z(2-D)	Z(1-D)	K	L
0.0	508	391	473	490	550	630
0.5	277	219	250	278	310	460
1.0	187	150	174	210	234	350
2.0	98	82	91	139	155	230

The results of the decay heat of the spent fuel are compared and presented in Table 12 and Figure 10.

It shows that in the beginning of the cooling time, the residual heat in the SERPENT is more than SAS2, and the deviation between the results is increased to 1.5 years of cooling. Furthermore, the deviation begins to decrease, and it continues to 4 years of cooling SERPENT becomes smaller than for SAS2. This is due the different concentrations of the fission products and actinides, which are presented in Table 13.

From Table 13 it is seen that the concentration of long-lived actinides in the SAS2 is more than SERPENT, so with cooling time, the residual heat in the SAS2 becomes more than the SERPENT. The contribution of actinides and the fission products in the residual heat of the spent fuel with cooling time are presented in Table 14.

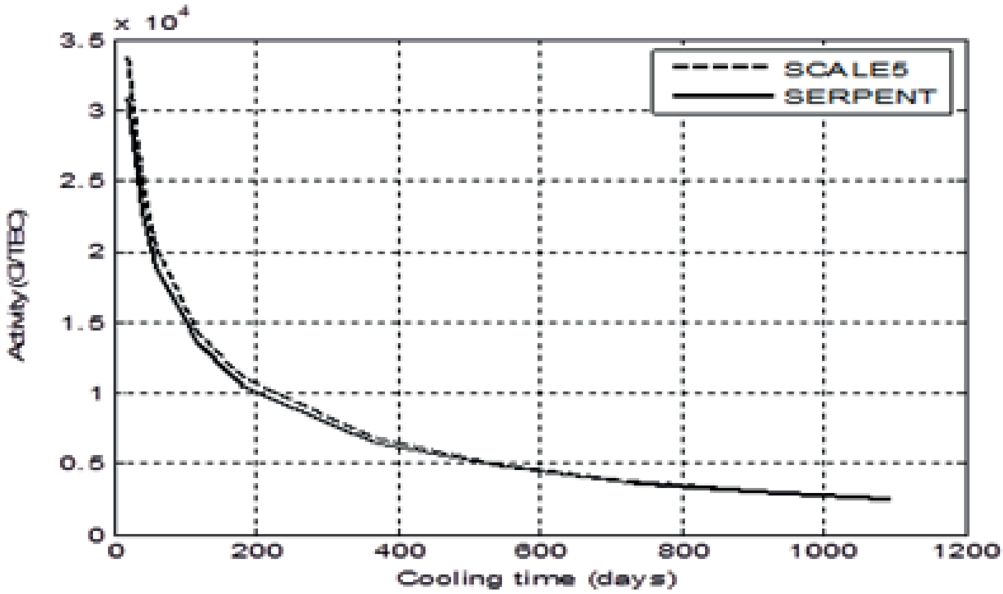

Figure 9: The dependence of the activity of SFA from the time of cooling.

Table 11: The dependence of the activity of SFA from the time of cooling (Ci/FA).

Cooling time (years)	SERPENT (Ci/FA)	SAS2 (Ci/FA)	deviation
0.05	7.87E+06	7.92E+06	-0.65%
0.11	5.87E+06	5.92E+06	-0.76%
0.16	4.84E+06	4.87E+06	-0.74%
0.33	3.26E+06	3.28E+06	-0.50%
0.50	2.47E+06	2.48E+06	-0.20%
1.00	1.54E+06	1.53E+06	0.35%
1.50	1.14E+06	1.14E+06	0.41%
2.00	9.00E+05	8.96E+05	0.35%
2.50	7.36E+05	7.34E+05	0.21%
3.00	6.21E+05	6.21E+05	0.02%
4.00	4.79E+05	4.82E+05	-0.48%
5.00	4.02E+05	4.06E+05	-0.96%
6.00	3.56E+05	3.61E+05	-1.40%

4. Conclusions

We can observe from comparing the different values, the deviation of the data received by SCALE program with the results of SERPENT 2 program. The main reason for

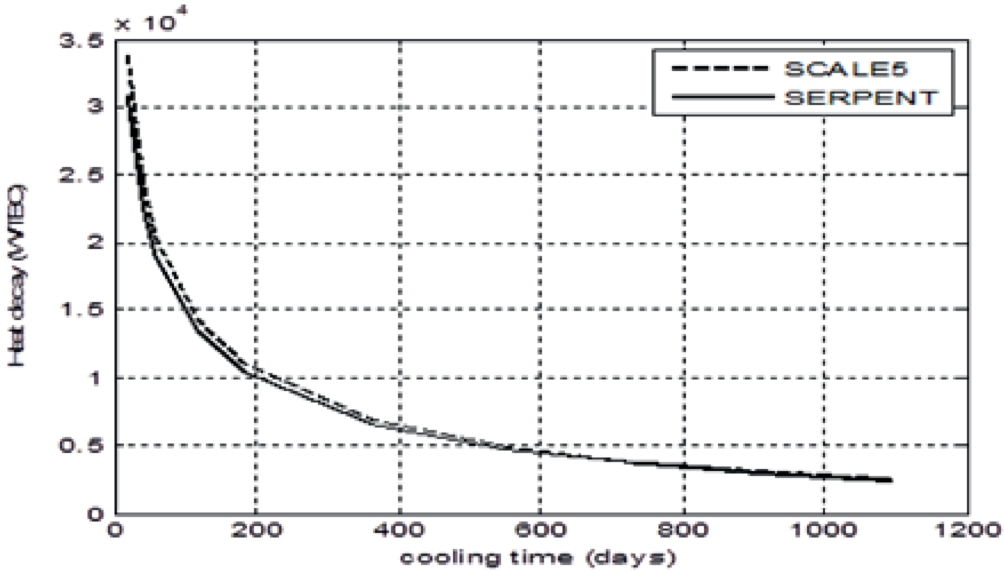

Figure 10: The dependence of the residual heat of SFA from the time of cooling.

Table 12: The dependence of the residual heat of SFA from the time of cooling (W/FA).

Cooling time (years)	SERPENT	SAS2	deviation
0.05	3.41E+04	3.41E+04	0.16%
0.11	2.50E+04	2.50E+04	0.17%
0.16	2.07E+04	2.06E+04	0.23%
0.33	1.45E+04	1.45E+04	0.51%
0.50	1.13E+04	1.12E+04	0.78%
1.00	6.95E+03	6.85E+03	1.34%
1.50	5.02E+03	4.94E+03	1.45%
2.00	3.85E+03	3.79E+03	1.35%
2.50	3.06E+03	3.03E+03	1.18%
3.00	2.52E+03	2.49E+03	0.91%
4.00	1.84E+03	1.84E+03	0.14%
5.00	1.48E+03	1.49E+03	-0.77%
6.00	1.27E+03	1.29E+03	-1.62%

this difference is the approximation space and energy which are used in deterministic program SAS2.

The geometric FA in SAS2 does not contain the guide channels, which contained water. But in SERPENT the geometric FA contained them. This water will effect on the energies of neutrons, and that will change various values such as K_∞, choice of cross

Table 13: Concentrations of isotopes spent fuel after three years cooling.

Isotopes	SERPENT (g/FA)	SAS2 (g/FA)	deviation (SA2-SR)/SA2
U234	7.18E+01	6.97E+01	-3.02%
U235	2.15E+03	2.52E+03	14.63%
U236	2.45E+03	2.43E+03	-0.79%
U238	3.65E+05	3.64E+05	-0.29%
Np237	3.37E+02	3.57E+02	5.65%
Pu238	1.73E+02	1.94E+02	10.80%
Pu239	2.42E+03	2.87E+03	15.73%
Pu240	1.25E+03	1.32E+03	5.35%
Pu241	6.76E+02	7.63E+02	11.40%
Pu242	4.92E+02	4.98E+02	1.15%
Am241	1.28E+02	1.46E+02	12.29%
Am242m	2.55E-01	6.19E-01	58.82%
Am243	1.43E+02	1.48E+02	3.31%
Cm242	1.22E-01	1.21E-01	-1.58%
Cm243	3.73E-01	4.52E-01	17.32%
Cm244	6.51E+01	7.39E+01	11.93%
Cm245	5.93E+00	6.29E+00	5.77%

section reaction and concentration of isotopes. Due to of changing these values, the characteristics of the SFA will be different.

Also, multi-group approximation, applied in the simulations SCALE contribute in the deviation. In work [17] shown that, the differences of the values were found for the typical LWRs lattices when comparing them with the multi-group Monte-Carlo code and continuous energy Monte Carlo.

Despite these reasons, the results calculated by SERPENT and SCALE5 for all the values were closed, and the results coincide well with each other. The discrepancy between the results of dose rate of the gamma radiation between the SERPENT and SCALE from our point of view due to the following reasons:

On the surface of TVs - due to the spatial approximations.

At various distances from the surface of the FA – due to different spectra of gamma radiation.

Table 14: Contribute of the actinides and fission products in the residual heat of the spent fuel with cooling time.

Cooling time (years)	Percent contribution of actinides	Percent contribution of fission product
0.05	5.81%	93.21%
0.11	6.65%	92.19%
0.16	7.47%	91.33%
0.33	8.81%	90.20%
0.50	9.48%	89.83%
1.00	10.00%	89.84%
1.50	10.32%	89.65%
2.00	11.29%	88.70%
2.50	12.87%	87.13%
3.00	14.86%	85.14%
4.00	19.23%	80.77%
5.00	23.27%	76.73%
6.00	26.55%	73.45%

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