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Neutronic Analysis of Various Fuels for the TEPLATOR HT

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ABSTRACT

In the light of a new world's approach focusing on energy decentralisation and decarbonisation, the development of Small Modular Reactors is crucial. The new small reactor TEPLATOR produces low-cost heat for various purposes, such as district heating or process heat. To supply process heat, a high temperature is required. For this reason, a high-temperature version of the TEPLATOR with corresponding fuel is under development. TEPLATOR HT with high output temperature assumes using the organic coolant, which affects the possibility of using contemporary fuels available on the market. This paper focuses on preliminary neutronic analyses that evaluate the coupling of an organic coolant with various available fuel geometries and assesses the feasibility of using certain fuels assuming minimal design changes. All fuel material combinations and geometries were tested in TEPLATOR geometry to choose an appropriate candidate for TEPLATOR HT that can withstand higher operational parameters. Based on the results, it will be decided whether existing fuel can be used for TEPLATOR HT or whether a new fuel type needs to be developed.

1 INTRODUCTION

The new reactor concept TEPLATOR is designed for using already irradiated VVER-440 fuel with optimal burnup and is designed for district heating, and other purposes described previously in [1][2]. At the same time, there is a possibility of operating TEPLATOR with slightly enriched fresh VVER-440 fuel or with some alternative fuel like natural uranium [3][4]. This article focuses on the new idea of modification to high-temperature TEPLATOR (HT). Standard TEPLATOR is designed to max. 150 MWth output power and heavy water coolant temperature close to 170 °C. Higher output temperatures of the coolant can be used for various purposes, not only for district heating. With increasing output temperature, the potential number of applications for this reactor increases. The possibility of using alternative fuel in combination with alternative coolant is described in this article. Using the Monte Carlo code, a set of calculations was investigated. Main TEPLATOR parameters such as the reactor calandria vessel, graphite moderator, fuel channel pitch, and other parameters are the same as for standard TEPLATOR. Modified parts will be described in detail for each modification.

1.1 Main challenges of the TEPLATOR HT coolant

The main issue and the most severe complication of high temperatures reactors, in general, is to ensure sufficient and reliable heat removal from the nuclear fuel to another circuit and, at the same time, fuel and other construction material properties and behaviour under this temperature. Regarding current power reactors, primarily water-based reactors are in operation (PWR, BWR, PHWR), several sodium-cooled fast reactors (BN-600), and the last groups are gas-cooled reactors, which have been operated mainly in the past (MAGNOX) [5]. If we want to operate a reactor with output temperatures higher than 400 °C, the light water or heavy water cannot be used due to exceeding their critical point (for light water, critical parameters are T = 374 °C, p = 22.14 MPa, and for heavy water T = 370.7 °C, p = 21.94 MPa) [6]. Super-critical coolant applications are now under investigation. However, many complications, such as high pressures, negatively affect the thicknesses of construction components such as reactor vessels and heat exchangers.

For high-temperature reactor cooling, CO_2 or helium has already been successfully tested and operated in several reactor concepts. The main disadvantage of gas is its low heat capacity and low heat transfer from fuel assembly to the coolant. The use of gas as a coolant requires a special design of the fuel assembly with special heatsinks on the surface of the fuel assembly, and in combination with a large amount of gas required for sufficient cooling, a significant amount of energy needs to be supplied to the gas blowers, thus negatively affecting the efficiency of power generation. In the case of heat production only, the gas coolant is very uneconomical [7].

Other alternatives to high-temperature gas coolant are liquid metals such as sodium or lead-bismuth. Sodium-cooled fast reactors are currently successfully operated in Russia, and lead-bismuth reactors are considered IV. Gen reactors. These types of coolants found usage for temperatures higher than 600 °C. Although the thermohydraulic properties of liquid metal coolant are much better than those of gas, some disadvantages can also be found. Liquid sodium is highly reactive with water and air humidity and spontaneously burns when exposed to air. In extreme cases, the hydrogen produced by the reaction with water can explode. Lead-bismuth fast reactors were used on nuclear submarines, and regarding melting point, the eutectic alloy of lead-bismuth is better than pure lead. On the other hand, the main disadvantage is the enormous density of this coolant, which complicates the production of components and the whole reactor in case of its large volume. Last but not least is the activation of bismuth to polonium, which is a strong alfa emitter. The main advantage in both cases is a high boiling point at atmospheric pressure [8],[9].

A possible alternative of TEPLATOR HT coolant can be considered organic aromatic hydrocarbons or molten salts. Organic coolant was previously successfully tested in experimental and power reactors (Piqua, Ohio USA) [10]. Regarding hydrocarbons, there are plenty of combinations and types with various advantages and disadvantages. The formerly used and tested were marked as Santowax OM, Santowax OMP, HB-40, Dowtherm A, Syltherm 800 and PFPE-1 [11]. All these candidates are based mostly on terphenyl, biphenyl, polydimethylsiloxane, their combinations and other hydrocarbons. The main advantage of the hydrocarbons can be noted as the higher boiling temperature at atmospheric pressure compared to pressured water, which makes them suitable for high-temperature use up to 550 °C [11]. The second advantage is that they are non-corrosive compared to water, which means that standard non-stainless materials can be used. The disadvantage is, as in other cases, their typical flammability and toxicity. The biggest weakness is that all hydrocarbons are subject to radiolysis and thermolysis, so a particular circuit is needed to clean and refill the degraded coolant. However, regarding the advantages, this issue can be covered by standard operating costs [12]. For the preliminary study, the organic coolant Santowax OM was chosen. The main properties of Santowax OM can be seen in Table 1.

Table 1. Main properties of organic coolant – Santowax OM [11]

Chemical formula	$C_{18}H_{14}$
Freezing point [°C]	~ 85
Atm. boiling point [°C]	~ 315
Autoignition temperature [°C]	~ 578
Specific heat capacity [J/kg·K]	2529 (371°C)
Density [kg/m^3]	813 (371°C)

2 FUEL MATERIAL AND GEOMETRY TESTING

Based on the preliminary study, the TEPLATOR HT output temperature of the coolant is designed to be 450 °C. This temperature can be used for multiple technological processes such as chemical, petrochemical or electricity production. Using Santowax as a new coolant material requires deeper analyses of fuel assemblies, which could be used. For this reason, the three different geometries were tested in combination with four different fuel materials.

2.1 Fuel materials

High temperature places certain specific demand on the fuel material. Using organic coolant based on light hydrogen negatively affects the heavy water moderator properties. For this reason, fuel material should be enriched. Therefore, using fuel made of natural uranium is not possible in this case. Higher operating temperature affects the temperature in the fuel material. The temperature in the fuel layer must be sufficiently lower than the melting point of the fuel material. Combining these facts led us to test five different fuel materials – Uranium Metal (U metal), Uranium Dioxide (UO_2), Uranium Carbide (UC) and Uranium Nitride (UN). The main crucial properties of these fuels can be found in Table 2.

Table 2. Main properties of chosen fuel types [13],[14]

Material	U metal	UC	UN	UO_2
Melting point [°C]	1132	2507	~ 1100	2850
Density [kg/m^3] (500 °C)	~ 18500	~ 13270	~ 14310	~ 10800
Thermal conductivity [W/(m·K)] (500 °C)	33,53	23,10	14,60	4,28

Table 2 shows that uranium carbide and uranium metal have the most promising properties for high-temperature fuel applications. In contrast, due to very low thermal conductivity, Uranium Dioxide cannot be used in thick fuel layer thicknesses. Using Uranium Metal raises certain issues that complicate its capability for commercial nuclear reactors. The main issue is Metal Uranium swelling with increasing burnup. This phenomenon is becoming essential with burnup higher than approx. 8 MWd/kgU [15]. Based on material properties, Uranium Carbide could be a good candidate for TEPLATOR HT usage.

2.2 Fuel geometries

Three different fuel geometries were tested for this preliminary study. The standard TEPLATOR is designed to use VVER-440 fuel assemblies. Therefore, the geometry of this fuel was tested first for the TEPLATOR HT. Using VVER-440 geometry may be advantageous because the additional modification of the reactor core is not necessary. After that, the RBMK reactor fuel geometry was placed and tested in the TEPLATOR HT core, and fuel channels were modified to the RBMK assembly diameter. RBMK assemblies have been tested because this geometry is well proven in real operating conditions. Finally, the cylindrical tubular geometry of fuel assembly with different fuel layer thicknesses was tested. The fuel channel was modified to a cylindrical shape corresponding to the VVER-440 dimensions. The following fuel layer thicknesses were tested: 1 mm, 2 mm, 4 mm, 6 mm, and 8 mm. For better imagination, the modelled fuel geometries can be seen in Figure 1. Blue means heavy water moderator, green is Santowax coolant, orange means fuel material, purple stands for Zircaloy-4, and yellow is CO_2 gas.

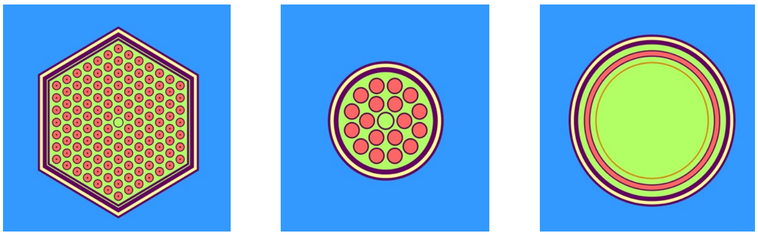

Figure 1. VVER-440 fuel geometry (left), RBMK reactor fuel geometry (centre), tubular geometry (right)

In all three cases of the fuel geometries, the fuel channels were modified in terms of increased mechanical resistance and reduction of heat transfer between the cooling and moderator circuits. The internal channel has a 4 mm thickness, the gap filled with low-pressure CO_2 is 3 mm thick, and the outer tube has a 2 mm thickness in these cases. All parameters were chosen according to engineering estimates, and their exact dimensions and thicknesses will be the subject of further analyses and calculations, which are not essential for this article.

3 CALCULATIONS AND MODELS

All calculations of HT TEPLATOR with different variants of the fuel were performed using Serpent 2.1.30 Mote Carlo code [16]. Models were created in 3D geometry, with all dimensions being the same as the real case. Calculations were performed using ENDF/B-VII.1[17] nuclear data library with corresponding TSL matrixes. The materials have been modelled with the appropriate temperature, so the temperature of heavy water moderator and other calandria materials and structures was set to 371 K, and fuel cladding, coolant and internals of the fuel channel were assumed to 723 K, and fuel material to 900 K. The polyethylene TSL matrix was used as the TSL matrix for the Santowax coolant as the first approximation. This simplification was made because of the missing TSL matrix for Santowax.

Criticality calculations were simulated with 40 000 neutrons per generation in 1000 active and 100 inactive generations for sufficient convergence of the neutron sources in the reactor core. In all calculated cases, the uncertainty is lower than 11 pcm, which is satisfying for these analyses. For each fuel geometry (VVER-440, RBMK and tubular), all combinations of the fuel materials were considered and calculated, and various fuel enrichment has also been investigated. The enrichment was set from natural uranium (0,72% of ^{235}U) to 3% enrichment of ^{235}U in the 1% step.

After criticality analyses, the burnup calculations sequence was performed for all modifications. Burnup sequences were carried out with 25 000 neutrons per generation, 500 active and 75 inactive generations. Calculations uncertainty is below 20 pcm for all cases. Based on the results, the most promising candidate can be chosen from the neutronic point of view.

4 RESULTS

Regarding the *keff* results, the most promising combinations were chosen and deeply investigated based on criticality calculations. The case of the tubular geometry was modified by adding a graphite moderator to the centre of the coolant displacer after the first part of the calculations performed without graphite. This graphite displacer significantly increased the multiplication coefficient *keff*. The highest obtained results of multiplication coefficient depending on fuel enrichment and other parameters can be seen in Table 3.

Table 3. Results of *keff* for various calculations

Material	**Thickness**	**Enrichment**				**Mass of fuel loaded to the core [kg]**
		***keff* for 0.72 %**	***keff* for 1 %**	***keff* for 2 %**	***keff* for 3 %**	
U metal	**2mm**	0.68630	0.82047	1.10266	1.24819	2220.7
	4mm	0.83283	0.96632	1.22355	1.34557	4370.8
	6mm	0.89369	1.02307	1.26338	1.37402	6450.5
	8mm	0.92534	1.05073	1.28004	1.38336	8459.7
UC	**2mm**	0.59043	0.71965	1.00778	1.16641	1610.7
	4mm	0.75742	0.89242	1.16487	1.29934	3170.3
	6mm	0.83386	0.96689	1.22312	1.34408	4678.8
	8mm	0.87632	1.00649	1.25051	1.36291	6136.1
UO2	**2mm**	0.49589	0.61654	0.90213	1.06939	1219.9
	4mm	0.67463	0.80871	1.09220	1.23898	2401.0
	6mm	0.76537	0.90052	1.17090	1.30386	3543.5
	8mm	0.81890	0.95265	1.21183	1.33488	4647.2
UN	**2mm**	0.52735	0.65056	0.93691	1.10101	1694.8
	4mm	0.64905	0.78014	1.06159	1.20937	3335.8
	6mm	0.70059	0.83192	1.10404	1.24242	4923.0
	8mm	0.72790	0.85750	1.12193	1.25387	6456.4
Material	**Geometry**	**Enrichment**				**Mass of fuel loaded to the core [kg]**
		***keff* for 1 %**	***keff* for 2 %**	***keff* for 3 %**	***keff* for 5 %**	
UO2	**RBMK**	0.88349	1.13247	1.25227	1.36968	2933.3
	VVER-440	0.96410	1.21459	1.33284	1.44859	8738.2
UC	**RBMK**	0.94153	1.17622	1.28531	1.39087	3873.1
	VVER-440	1.00536	1.24055	1.34923	1.45418	11537.8

Results for 1 mm fuel layer thickness are not shown in Table 3 due to very low values of multiplication coefficient *keff*. One can notice from Table 3 that reaching criticality with sufficient excess of the reactivity for reactor operation is achieved only with fuel enrichment higher than 2 % of ^{235}U. The second effect observed is increasing criticality with an increasing amount of uranium in the core, indicating a high degree of reactor over-moderation. This assumption was confirmed by the one randomly chosen fuel type and geometry calculation. The behaviour of the *keff,* depending on the fuel assembly pitch, can be seen in Figure 2. Figure 2 shows that the optimal fuel assembly pitch is around 30 cm. Detailed determination of the optimum fuel assembly pitch for each specific fuel type depends on enrichment and other parameters with optimisation of reactor core layout will be the subject of further research.

Table 3 shows that the behaviour of *keff* in cylindrical fuel assembly for metal uranium and uranium carbide fuel is relatively close. However, considering UC and U metal properties, the UC seems a better candidate for this fuel type. A higher value than 3 % of enrichment was not calculated because HT TEPLATOR considers heavy water as the moderator, so using higher enrichment than 3% of ^{235}U seems unnecessary. In this case, it would be better to change the complete geometry of the designed TEPLATOR HT and avoid the use of expensive heavy water.

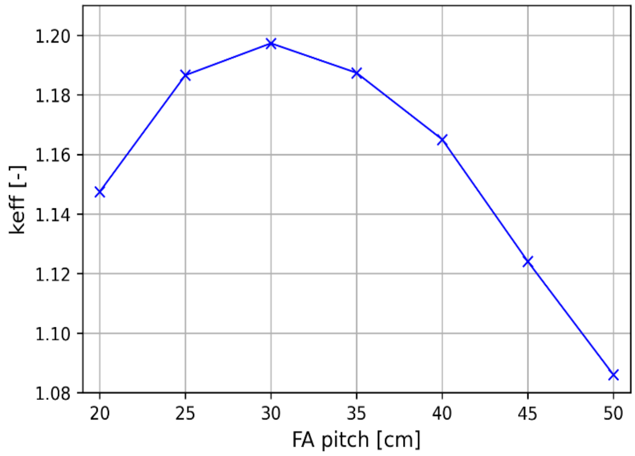

Figure 2. Behaviour of *keff* depending on FA pitch - Cylindrical UC fuel material with 4 mm thickness and 2% enrichment

Table 4 presents results for burnup calculations that better describe the behaviour of the fuel in the reactor core than the critical calculation. For all fuel designs, a power density was calculated. Considering the relatively significant metal uranium swelling with higher burnup, the cases only with UC and UO_2 are examined. The U metal always reaches slightly higher burnup than UC. Modification of UO_2 tubular fuel with 8 mm fuel layer thickness was not calculated due to the high temperature in the fuel layer regarding the temperature of the coolant. For all cases, the fuel burnup for the same enrichment rises with an increasing amount of fuel in the core, which is evident from the VVER-440 fuel modification. VVER-440 geometry with UC fuel has almost two times larger amounts of fuel than cylindrical fuel with the thickest 8 mm fuel layer.

Table 4. Results of operating time and fuel burnup for more promising modifications

Modification	Enrichment	keff BOC	EFPD [days]	Burnup [MWd/kg]
CYL - U metal 4 mm	3 %	1.34562	1769.7	20.2
CYL - U metal 6 mm	3 %	1.37381	2163.0	23.1
CYL - UC 4 mm	2 %	1.16505	479.0	7.6
	3 %	1.29971	1069.0	16.9
CYL - UC 6 mm	2 %	1.22302	992.8	10.6
	3 %	1.34430	1905.7	20.4
CYL - UC 8 mm	2 %	1.25003	1525.3	12.2
	3 %	1.36327	2701.8	22.0
CYL - UO_2 4 mm	3 %	1.23889	634.8	13.2
CYL - UO_2 6 mm	3 %	1.30374	1224.0	17.3
VVER-440 UC	2 %	1.24021	3191.4	13.8
	3 %	1.34922	5430.4	23.5
	4 %	1.41265	7547.0	32.7
	5 %	1.45417	9585.7	41.5
RBMK UO_2	2 %	1.13223	363.6	6.2
RBMK UC	2 %	1.17644	683.5	8.8

Maximal obtained fuel burnup for cylindrical tubular geometry with 2% enrichment was reached in the case of UC with the 8 mm layer. The burnup was 12,2 MWd/kgU, with an operational time more than 4,1 years, which is equal to 1525,3 Effective Full Power Days (EFPD) meaning full output power per all days. For 3% enrichment, the highest burnup value is 22 MWd/kgU for UC with an 8 mm layer thickness case with, an operational time of 7,4 years. Based on these calculations, the case with 2% UC in the 8 mm layer seems more economical due to the highest fuel burnup for the lowest fuel enrichment.

In the case of VVER-440 fuel, the modifications with higher enrichment were evaluated. This was done to determine the usability of standard NPP fresh fuel assemblies. As was mentioned before, using higher than approx. 3% enrichment is the subject of a more in-depth economic analysis. On the other hand, for the 50 MW_{th} HT TEPLATOR unit, the case with 3% enrichment reaches more than 14,8 years of operation without refuelling. For 4% enrichment, the operational time rises to 20,6 years, and for 5% enrichment, the operating time is longer than 26 years. This operating time is very long and helps to resolve the issue of storing spent fuel at the site of the TEPLATOR. Considering 5% enrichment, only one refuelling is required over the lifetime of the TEPLATOR, reducing the financial cost of building an intermediate spent fuel storage facility on site. Designed lifetime of the TEPLATOR is approx. 50 years.

To understand the operational conditions in the reactor, the average heat flux for various fuel assemblies was calculated, see Table 5. It can be noticed that VVER-440 fuel has the lowest temperature load, which favourably supports the possibility of its long-term operation. The heat flux for the RBMK assembly is the highest but is not critical. For instance, the average heat flux for the VVER-1000 energetic reactor is approx. 576 kW/m^2.

Table 5. Calculated heat flux for fuel assemblies

Fuel geometry	**Average heat flux [kW/m^2]**
VVER-440	92,3
RBMK	434,6
Tubular – 2 mm fuel layer	232,2
Tubular – 8 mm fuel layer	243,8

5 CONCLUSIONS

Preliminary analyses of coolant and possible fuel for TEPLATOR HT were performed. A potential suitable organic coolant was chosen, i.e., the chemical compound marked as Santowax OM. After modelling three different fuel geometries with four other fuel materials, the most promising fuel was chosen. In the case of tubular fuel, the modification with 2% Uranium Carbide with 8 mm fuel layer thickness, which reaches 12,2 MWd/kgU burnup with an operational time of 4,1 years, was chosen as a better candidate due to the highest burnup for lowest fuel enrichment. From all aspects, Uranium Carbide appears to be the most promising fuel material in terms of thermal conductivity, swelling, melting point and density from all examined candidates in this paper. In the case of VVER-440 fuel, all fuel enrichments reach higher burnup, which means better fuel cycle economy. This result is caused because the core is almost two times more fuel than in the case of cylindrical fuel. The calculated operational time for VVER-440 with UC fuel material is 14,8 years for 3% enrichment, for 5% enrichment more than 26 years. This can be advantageous as it eliminates the need for periodic refuelling. During the lifetime of the TEPLATOR HT, it would only be necessary to change the fuel once, which positively affects the nuclear safety of operation and reduces the cost of handling and storing spent nuclear fuel stored on site. Further research will focus on optimisation the whole reactor core and deeper analyses of neutronic and thermohydraulic properties of all fuel geometries and fuel behaviour during reactor operation.

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