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## Modeling of heat transfer in a fuel pellet based on uranium dioxide and ceramics (beryllium oxide)

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### ABSTRACT

The results of heat transfer mathematical model calculations in the "UO<sub>2</sub>-BeO" pellet are presented. The fuel pellet consists of uranium dioxide (UO<sub>2</sub>) and beryllium oxide (BeO) ceramics. Modeling of heat transfer was carried out by a system of generalized heat conduction equations with variable thermophysical properties. The calculated data of the temperature field in the fuel pellet were obtained using the COMSOL Multiphysics software code. The results of temperature calculations were compared with the data of other authors. The agreement of the calculated data shows the mathematical model and the COMSOL Multiphysics code algorithms correctness. Various arrangements of beryllium oxide ceramics BeO in a fuel pellet are considered. The arrangement of the BeO ceramics in the centre of the fuel pellet showed a noticeable decrease in temperature in the energy release zone. Calculations have shown that the composite fuel "UO<sub>2</sub>-BeO" is the most effective for regulating the thermal regime of fuel elements.

**Keywords:** heat transfer modeling, fuel pellet, uranium dioxide, beryllium oxide ceramics.

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## Introduction

Currently, in many countries, work is underway to create a tolerant fuel ATF (Accident Tolerant Fuel) [1], since the increased resistance of the fuel to emergencies becomes more relevant, in particular, the prevention of the superheated steam and zirconium shell interaction reaction with the release of explosive hydrogen. A solution to this problem can be achieved by modifying the zirconium cladding or fuel, by replacing the cladding material or using a new fuel.

As a nuclear fuel in the most nuclear reactors, among which the most widespread are water-moderated reactors PWR, BWR, VVER, etc., pellets of sintered uranium dioxide UO<sub>2</sub> enriched in isotope <sup>235</sup>U within 2-5% are used. Despite such advantages

of uranium dioxide as a nuclear fuel, a high melting point, chemical stability, satisfactory compatibility with fuel element cladding materials, radiation stability, technologically convenient crystalline properties, its significant disadvantage is its low thermal conductivity, which decreases with increasing temperature. This feature leads to the appearance of high-temperature gradients in the fuel pellets, which leads to cracking of the fuel, the interaction of the fuel with the cladding and the release of gaseous fission products [2-4].

Reducing the fuel temperature can be achieved by doping the uranium dioxide material with high thermal conductivity and compatibility with the fuel element materials. The main additive candidates are SiC, BeO, Cr<sub>2</sub>O<sub>3</sub>. Modified fuel with increased thermal conductivity due to lower thermal expansion and low thermal stresses will experience less interaction with the cladding [5-9]. In addition,

lower temperatures reduce the mobility of fission products, thereby reducing fission gas evolution, grain boundary swelling and stress corrosion cracking. This would increase fuel burnup and improve reactor safety due to faster thermal response, less grain storage at fission product boundaries, and less thermal energy in the fuel rods.

Studies to increase the thermal conductivity of  $\text{UO}_2$  were carried out by adding to the composition of such compounds as BeO and SiC [10-26].  $\text{UO}_2$ -BeO composite has better temperature stability compared to  $\text{UO}_2$ -SiC. BeO was chosen as the high thermal conductivity material for  $\text{UO}_2$  because it was found that, BeO is most compatible with  $\text{UO}_2$  fuel as a thermal conductivity enhancing additive in nuclear fuel materials. BeO is one of the highest temperature ceramic elements and can withstand radiation environments and does not react with  $\text{UO}_2$  up to  $2200^\circ\text{C}$ . Most of the  $\text{UO}_2$ -BeO fuel developments were carried out to determine the thermal conductivity of  $\text{UO}_2$ -BeO when the content of BeO in the composition (0.3; 0.6; 0.9; 1.2 and 13.6 wt.%) [21]. The results showed a significant improvement in the thermal conductivity of  $\text{UO}_2$ -BeO with the addition of BeO with a continuous distribution in the composition of  $\text{UO}_2$ .

The article [27] presents the design of a fuel pellet “ $\text{UO}_2$ -BeO fuel sandwich”. The pellet was a combination of  $\text{UO}_2$  fuel and beryllium oxide ceramics BeO. Three types of  $\text{UO}_2$  and BeO zone locations were considered. A quantitative advantage of the  $\text{UO}_2$ -BeO fuel sandwich in a light water reactor has been obtained using multiphysics simulation. The authors consider the results as preliminary study of sandwich fuel with increased thermal conductivity [27].

This article discusses thermal modeling in a pellet consisting of  $\text{UO}_2$  fuel with beryllium oxide ceramics BeO.

### Physical model

In fuel rods, fission of heavy  $^{235}\text{U}$  or  $^{239}\text{Pu}$  nuclei occurs, accompanied by the release of thermal energy, which is then transferred to the coolant. The fuel element provides heat removal from the fuel to the coolant and prevents the spread of radioactive products. The fuel element is a sealed tube made of steel or zirconium alloys with an external diameter of about a centimetre and a length of hundreds of centimetres, filled with  $\text{UO}_2$  tablets [28]. Uranium dioxide tablets with a height of 11.9 mm and a diameter of 8.2 mm are placed in a tube with a gap of 0.08 mm in diameter. The length of the fuel rod

tube is 3800 mm, the position of the fuel pellets is fixed by stainless steel rods and a spring.

We are studying the design of a “ $\text{UO}_2$  fuel with BeO ceramics” pellet in a fuel element (see Fig. 1) to determine its efficiency in comparison with a “ $\text{UO}_2$ -BeO fuel sandwich” [27].

### Mathematical formulation

There are more than 200 fuel pellets in the fuel element, periodically located one after another. Therefore, we consider the problem statement for one pellet (Fig. 1).

Because of the process symmetry, a region is considered, along the length, limited with the length  $l$ , and along the radius  $r_0$  from the central axis of the rod to the zirconium cladding. In the  $\text{UO}_2$  fuel, fission of heavy uranium nuclei occurs with the release of thermal energy with a density of  $q_0$ . On the outer wall of the zirconium cladding, water is cooled with a temperature  $T_f$ .

It is required to determine the temperature distribution over time in the “ $\text{UO}_2$  fuel with BeO ceramics” pellet.

Consider the generalized heat equation in a cylindrical coordinate system:

$$\rho_i(T_i)c_{pi}(T_i)\frac{\partial T_i}{\partial t} = \frac{\partial}{\partial z}\left[\lambda_i(T_i)\frac{\partial T_i}{\partial z}\right] + \frac{1}{r}\frac{\partial}{\partial r}\left[r\lambda_i(T_i)\frac{\partial T_i}{\partial r}\right] + q_i, \quad i=1,2,3, \quad (1)$$

The generalization of equation (1) is that in fuel, the density, heat capacity, thermal conductivity is equal to the  $\text{UO}_2$  parameters. In ceramics, they are similar to the BeO parameters and the annular gap to the parameters. The temperature dependences of the thermophysical properties of  $\text{UO}_2$ , BeO, He were found from experimental data [29]. For example, Figs. 2 - 4 show the dependencies of the thermophysical properties of  $\text{UO}_2$  and BeO. It is easy to notice a significant difference in the thermal conductivity of  $\text{UO}_2$  and BeO (see Fig. 2).

The density of the heat flux of energy release in the fuel zone is  $q_1 = q_0$ , and in the zones of ceramics and helium is equal to 0.

The system of equations (1) is solved under the initial and boundary conditions.

At the initial moment  $t = 0$ , the following conditions are set:

$$\begin{aligned} T(z, r, 0) &= T_1(r) \quad \text{in the domain of } \text{UO}_2; \\ T(z, r, 0) &= T_2(r) \quad \text{in the domain of BeO}; \\ T(z, r, 0) &= T_3(r) \quad \text{in the domain of He.} \end{aligned} \quad (2)$$

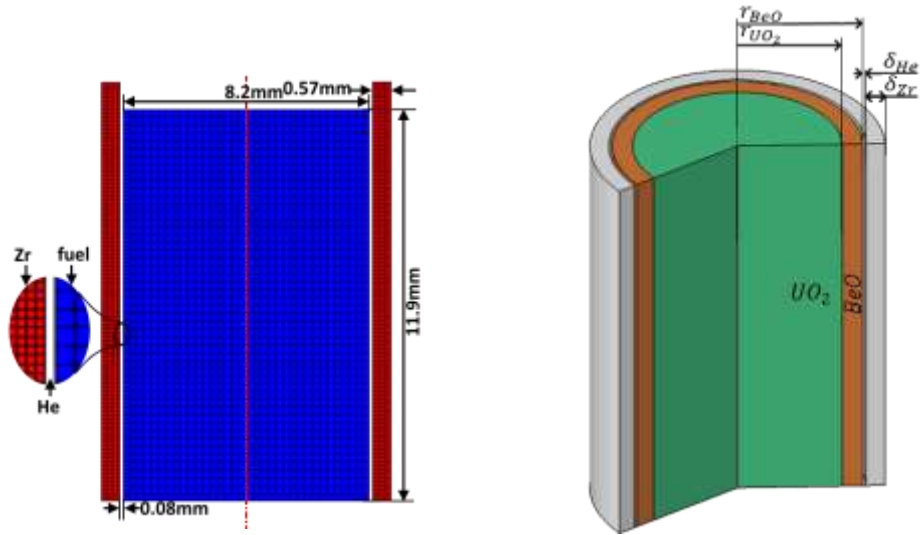


Fig. 1. The layout of the “UO<sub>2</sub> fuel with BeO ceramics” pellet and the computational domain

Symmetry conditions are set on the axis of the computational domain:

$$\frac{\partial T_i}{\partial r} = 0, \text{ at } r = 0; \quad (3)$$

Heat transfer conditions are set on the wall of the zirconium cladding [29]:

$$-\lambda_3 \frac{\partial T_3}{\partial r} = k(T_3 - T_f), \text{ at } r = r_0 \quad (4)$$

Where  $\lambda_3$  is the thermal conductivity of helium,  $k$  is the heat transfer coefficient,  $T_f$  is the cooling water temperature.

The periodic arrangement of fuel pellets in the fuel element can lead to the absence of heat transfer at the contacts along the length. Then the boundary conditions along the length of the computational domain are as follows:

$$\frac{\partial T_i}{\partial z} = 0, \text{ at } z = 0 \text{ and } z = l \quad (5)$$

On the contact surface of UO<sub>2</sub>/BeO and BeO/helium, the conditions of conjugation of the heat fluxes and temperature equality are satisfied:

$$\lambda_i \frac{\partial T_i}{\partial n} = \lambda_j \frac{\partial T_j}{\partial n}, T_i = T_j, i = 1, 2 \text{ and } j = 2, 3 \quad (6)$$

Where  $n$  is normal to the interface.

The system of equations (1) with conditions (2)-(6) and empirical formulas for the thermophysical properties of UO<sub>2</sub>, BeO, He was solved numerically using the COMSOL Multiphysics code.

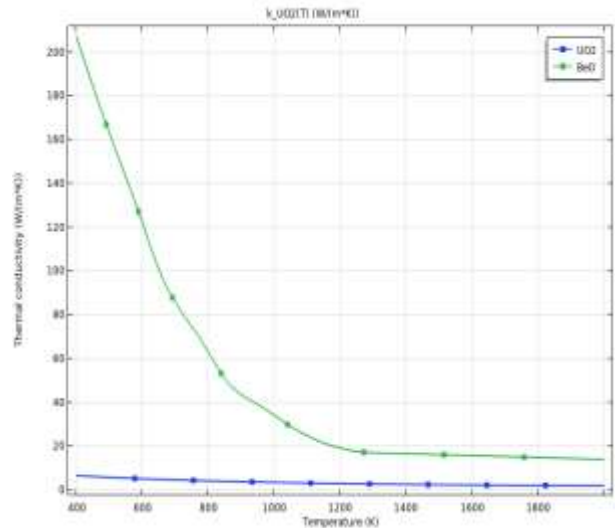


Fig. 2. Dependences of thermal conductivity of UO<sub>2</sub> and BeO on temperature [29].

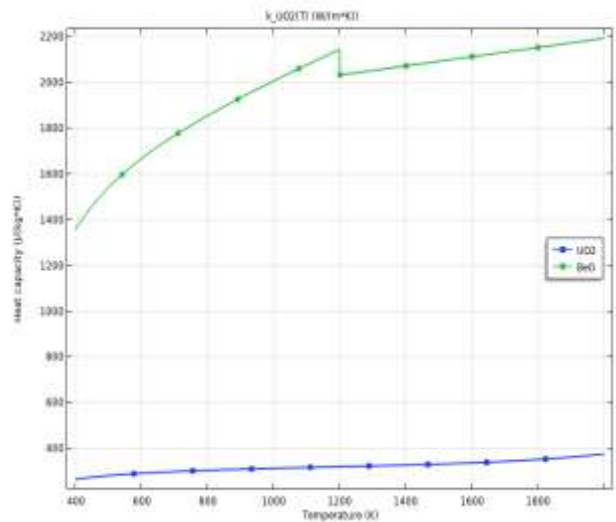


Fig. 3. Dependences of the heat capacity of UO<sub>2</sub> and BeO on temperature [29].

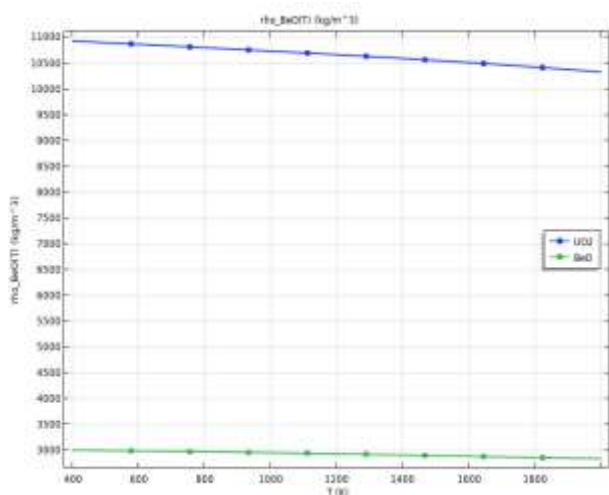


Fig. 4. Dependences of the density of UO<sub>2</sub> and BeO on temperature [29].

### Comparative calculations with the data of other authors

To assess the correctness of the model and calculation methods, relative calculations with the data of other authors were carried out.

Fig. 5 shows comparisons of calculations with the data of [30] when the pellet consists only of UO<sub>2</sub> fuel. The calculations were carried out at two values of the heat flux density  $q_1 = 200$  W/cm, 400 W/cm and other identical operating parameters [30].

At a heat flux density  $q_1 = 400$  W/cm, the temperature in the core increases to 2360 K, and at  $q_1 = 200$  W/cm – to 1340 K. The difference between the calculations at  $q_1 = 400$  W/cm is 2.5%, and at  $q_1 = 200$  W/cm the temperature calculations practically coincide (Fig. 5).

The next series of comparative calculations were carried out according to the article's data [27]. Table 1 shows operating parameters [27]: power source, gas pressure, coolant temperature, etc.

Fig. 6 shows the calculation of the temperature of a fuel pellet consisting only of UO<sub>2</sub>. These temperature calculations [27] are designated as actual data in the helium zone and the centre of the pellet.

Figs. 7 and 8 show the calculations of the temperature of the “UO<sub>2</sub>-BeO fuel sandwich” [27] when the BeO ceramics are located in the central part (c) and the middle part of the pellet (a). In the calculations, the BeO ceramics occupies 36.4 vol.% of the pellet volume. It also shows the calculated temperature [27], as actual data, in the helium zone and the centre of the pellet (Figs. 7 and 8).

It can be noted that our calculations of the “UO<sub>2</sub> - BeO fuel sandwich” in key areas of the pellet coincide with the actual data [27].

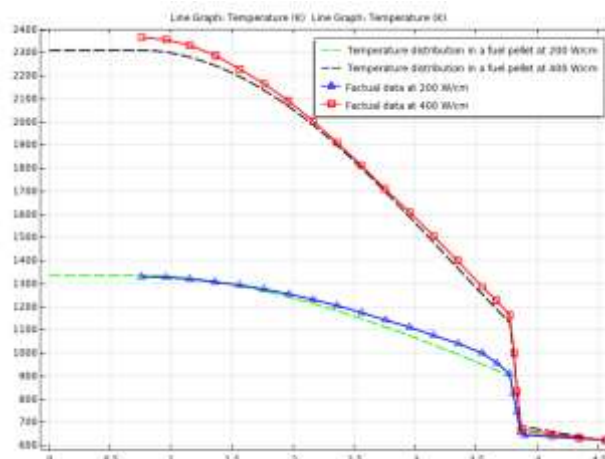


Fig. 5. Temperature distribution in the UO<sub>2</sub> fuel pellet

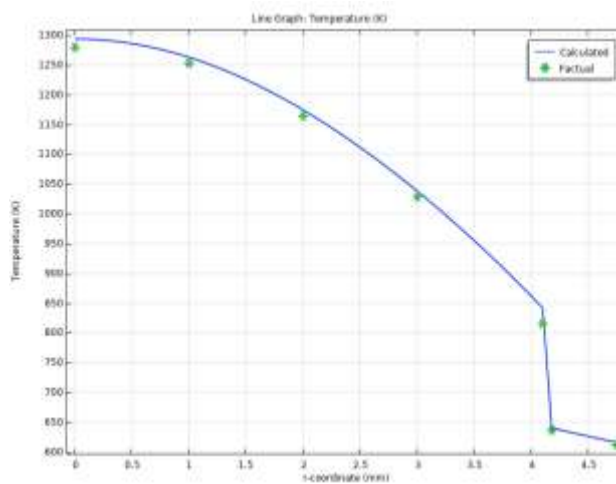
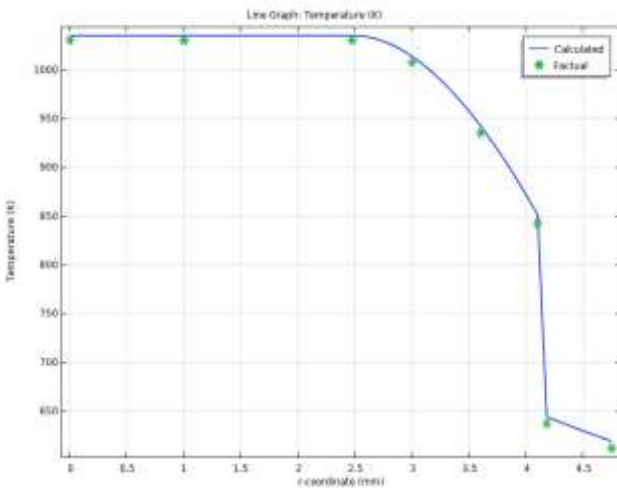


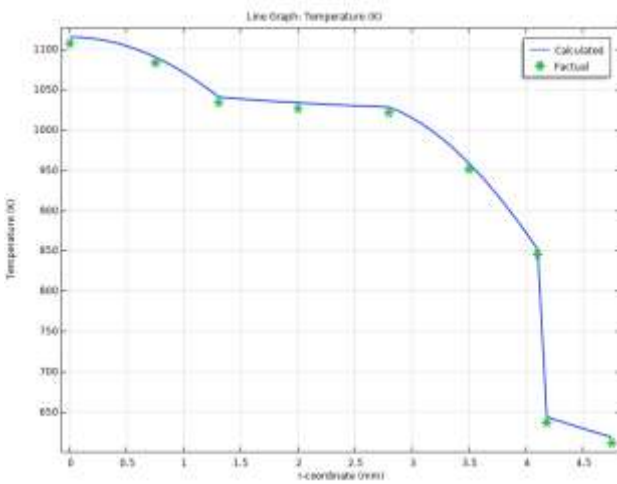
Fig. 6. Temperature distribution in the UO<sub>2</sub> fuel pellet

Table 1 - Operating parameters of the pellet calculations [27]

Linear average power (W/cm)	200
Coolant pressure (MPa)	15.5
Coolant temperature (K)	530
Coolant convection coefficient (W/m <sup>2</sup> K)	7500
Rod fill gas	Helium
Fill initial gas pressure (MPa)	2.0

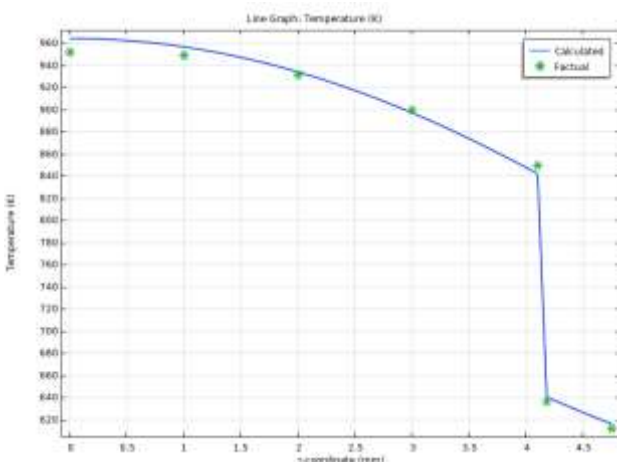


**Fig. 7.** Temperature distribution in the pellet “UO<sub>2</sub>-ceramic BeO fuel sandwich” option (c) [27]



**Fig. 8.** Temperature distribution in the pellet “UO<sub>2</sub> fuel sandwich - BeO ceramic” option (a) [27]

Composite fuel consists of uniformly mixed particles of uranium dioxide UO<sub>2</sub> and beryllium oxide BeO. Fig. 9 shows the calculations of the temperature of the composite fuel 63.6 vol.% UO<sub>2</sub> and 36.4 vol.% BeO.



**Fig. 9.** Temperature distribution in a pellet of composite fuel UO<sub>2</sub>-BeO [27]

Calculations show that when the fuel pellet consists only of uranium dioxide UO<sub>2</sub>, the temperature in the core due to the release of energy reaches 1293.7 K (see Fig. 6). Radial temperature decreases to 841.6 K due to heat removal by highly heat-conducting helium. In the helium annular gap, the temperature drops to 640.1 K. Heat transfer through the zirconium cladding wall results in a coolant temperature of 615.8 K.

Calculations of the UO<sub>2</sub>-BeO fuel sandwich pellet temperature show a decrease in the core to 1035.2 K (Fig. 7) and to 1115 K (Fig. 8).

Composite fuel calculations show that the core temperature drops to 964.5 K (Fig. 9).

As shown in Fig. 6-9, the calculated data agree with the actual calculation data [29]. The settlement agreement is no more than 2.5%.

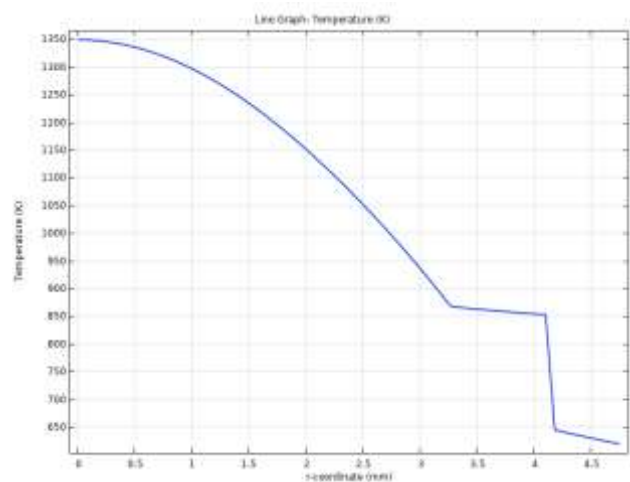
### Discussion of calculations of the “UO<sub>2</sub> fuel with BeO ceramics” pellet

The calculations were carried out by the pellet “UO<sub>2</sub> fuel – BeO ceramics” (Fig. 1). Such a design can be technologically advantageous for the manufacture of a tablet.

The operating parameters were selected in the same way as in Table 1 for ease of comparison with the results of [27].

Ceramics BeO occupies 36.4 vol.% of the pellet volume, and fuel UO<sub>2</sub> – 63.6 vol.%. Fig. 10 shows the temperature distribution along the radius of the pellet “UO<sub>2</sub> fuel with BeO ceramics”.

The temperature in the zone of the BeO ceramics changes insignificantly. In the UO<sub>2</sub> energy release zone, the temperature rises from 865.1 to 1349.3 K (Fig. 10).



**Fig. 10.** Temperature distribution in the “UO<sub>2</sub> fuel with BeO ceramics” pellet

Calculations show that such a design of heat removal from the core turns out to be ineffective compared to the design of heat removal "UO<sub>2</sub>-BeO fuel sandwich" [27].

### Conclusions

Generalized heat conduction equations carry out modeling of heat transfer in a fuel element pellet with nonlinear coefficients of thermophysical properties UO<sub>2</sub>, BeO, He.

Numerical calculations of the mathematical model were obtained using the COMSOL Multiphysics software code.

The validation of the mathematical model and the calculation method were compared with the

calculations [27], [30]. The agreement of the calculated data expresses the correctness of the model and the calculation method.

Among the design of pellets "UO<sub>2</sub>-fuel with BeO-ceramics", the arrangement of the ceramics in the centre of the fuel pellet turned out to be effective. This result is consistent with the data [27].

In the pellet with the composite fuel "UO<sub>2</sub>-BeO", the greatest temperature decrease was obtained, which shows that such a fuel is promising.

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## Уран диоксиді мен керамика (бериллий оксиді) негізіндегі отын таблеткасындағы жылу тасымалдауды модельдеу

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### ТҮЙІНДЕМЕ

Мақалада "UO<sub>2</sub>-BeO" таблеткасындағы жылу тасымалдаудың математикалық моделін есептеу нәтижелері келтірілген. Отын таблеткасы UO<sub>2</sub> уран диоксидінен және бериллий BeO керамикасынан тұрады. Жылу тасымалдауды модельдеу ауыспалы жылу физикалық қасиеттері бар жалпыланған жылу өткізгіштік теңдеулер жүйесімен жүзеге асырылады. Отын таблеткасындағы температуралық өрістің есептік деректері COMSOL Multiphysics бағдарламалық кодын пайдалана отырып алынды. Температураны есептеу нәтижелері басқа авторлардың деректерімен салыстырылды. Есептеу деректерінің келісімі COMSOL Multiphysics бағдарламалық кодының математикалық моделі мен алгоритмдерінің дұрыстығын көрсетеді. BeO бериллий оксиді керамикасының отын таблеткасында орналасуының әртүрлі нұсқалары қарастырылған. BeO керамикасы отын таблеткасының ортасында орналасқанда энергия шығару аймағында температураның айтарлықтай төмендегенін көрсетті. Есептеулер көрсеткендей, " UO<sub>2</sub>-BeO " композициялық отыны жылу режимін реттеу үшін ең тиімді болып табылады.

**Түйін сөздер:** жылу тасымалдауды модельдеу, отын таблеткасы, уран диоксиді, бериллий оксидінің керамикасы.

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## Моделирование теплопереноса в топливной таблетке на основе диоксида урана и керамики (оксид бериллия)

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### АННОТАЦИЯ

Приводятся результаты расчетов математической модели теплопереноса в таблетке «UO<sub>2</sub>-BeO». Топливная таблетка состоит из диоксида урана UO<sub>2</sub> и керамики оксида бериллия BeO. Моделирование теплопереноса проведено системой обобщенных уравнений теплопроводности с переменными теплофизическими свойствами. Расчетные данные температурного поля в топливной таблетке получены с использованием программного кода COMSOL Multiphysics. Результаты расчетов температуры были сравнены с данными других авторов. Согласие расчетных данных показывает корректность математической модели и алгоритмов программного кода COMSOL Multiphysics. Рассмотрены различные варианты расположения керамики оксида бериллия BeO в топливной таблетке. Расположение керамики BeO в центре топливной таблетки показало заметное снижение температуры в зоне энерговыделения. Расчеты показали, что композитное топливо «UO<sub>2</sub>-BeO» является наиболее эффективным для регулирования теплового режима ТВЭЛа.

**Ключевые слова:** моделирование теплопереноса, топливная таблетка, диоксид урана, керамика оксида бериллия.

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