A large change in the structure, density, and chemical and phase composition occurs in nuclear fuel with deep burnup, and an edge zone is formed. Simulation of the formation of an edge zone in a fuel kernel of thermal reactors will make it possible to suggest ways to decrease its influence on the characteristics of a fuel element. In the present work, the neutron-physical processes occurring in the peripheral layer of a fuel kernel are simulated. The distribution of nuclear reaction rates along the radius of a fuel pellet is calculated using the SCALE-4.3, MCNP-4B, and UNK computer programs. The radial dependence of the local breeding ratio is calculated. It is shown that for fresh fuel $BR > 1$ for fissile nuclei in a 100 µm thick layer, while the initial $BR$ averaged over a pellet is no more than 0.5. The volume energy distribution in a 100 µm thick peripheral layer is 30% higher than the average value over a pellet. A combined pellet, where the central part possesses the standard enrichment (4–5% $^{235}$U) and the peripheral layer contains less than 0.7% $^{235}$U, is proposed to decrease the influence of the edge zone on the properties of fuel.

The main goal of scientific and technical development work in fuel-cycle power reactors is increasing fuel burnup and the reliability of fuel assemblies under operating conditions. This is achieved mainly by increasing the initial fuel enrichment and by using consumable absorbers. However, an increase of burnup leads to the development of processes that affect the integral characteristics of fuel elements. One such process gives rise to an edge zone with an easily distinguishable altered microstructure on the periphery of the fuel pellets. The structure of the edge zone is characterized by the presence of many fine gas bubbles, vanishing of the initial grain structure, and formation of new, much smaller subgrains (<1 µm) [1, 2].

It has been found experimentally that an edge zone starts to form in uranium dioxide fuel pellets in thermal reactors at burnup higher than 45–50 MW·days/kg. This layer is 100–200 µm thick and is characterized by much higher burnup than the main part of the fuel pellet. Thus, for average burnup 50 MW·days/kg the burnup in a 100 µm thick peripheral layer will reach 80 MW·days/kg, and the burnup directly on the surface of a pellet will reach 150 MW·days/kg.

The formation and development of an edge zone where the porosity is 3–5 times higher than the initial porosity creates a barrier for heat flow from fuel to cladding and degrades the thermal conductivity of the fuel–cladding gap with emission of gaseous fission products. An increase of the fuel temperature and the emission of gaseous fission products from the edge zone will increase the pressure on the cladding of a fuel element, which can have a large effect on the characteristics of the fuel element. Simulation of the processes resulting in the formation of an edge zone will make it possible to suggest ways to decrease the effect of such a zone on the characteristics of a fuel element.
Development of a Mathematical Model. Different approaches to simulating the distribution of nuclear reaction rates along the radius of a fuel pellet are possible. For example, a novel model, based on a simplified description of the characteristics of the neutron spectrum using the hardness parameter, has been developed at the Troitsk Institute of Innovative and Thermonuclear Research (TRINITI) to determine the burnup of nuclear fuel along the radius of a fuel pellet. There is still no physical model of the mechanism of the formation of this structure. Specifically, it is not entirely clear whether this process is solely determined by elevated burnup or whether other parameters, such as, the fission rate, temperature, grain size, and so forth, also have an effect. One model which is often used at the present time is based on the concept of critical burnup, i.e., it is assumed that a fine-grain structure is formed when the local burnup reaches a certain critical level [3, 4].

The increase in the speed of modern PCs makes it possible to simulate fuel burnup using programs which perform neutron calculations on the basis of multi-group deterministic methods – methods of discrete ordinates and first-collision probabilities – as well as Monte Carlo stochastic methods. The use of different programs makes it possible to evaluate the uncertainties in a result which are associated with methodological and systematic errors. The calculations whose results are presented in the present article were performed using the following programs:

- **SCALE-4.4** [5] – multi-group calculation based on the method of discrete ordinates in a one-dimensional cylindrical geometry with automatic preparation of the constants for calculating burnup with the ORIGEN-S program, solving the equations of burnup on the basis of the spectrum average for some region, 238-group constants library based on ENDF/BV evaluated nuclear data;
- **MCNP-4B** [6] – calculation of the neutron field in an arbitrary geometry on the basis of the Monte Carlo method, library of constants with a continuous energy dependence based on ENDF/BVI evaluated nuclear data;
- **UNK** [7] – multigroup calculation based on the method of first-collision probabilities in a one-dimensional cylindrical geometry with automatic adjustment of the constants for calculating burnup with the BARNUP program, solving equations of burnup on the basis of the spectrum average for a certain region, 134-group library of constants based on ENDF/BV evaluated nuclear data; a special multi-group calculation is performed in resonance region for $^{235}\text{U}$ and $^{238}\text{U}$ to take account of the resonance blocking effect.

Spatial-Energy Distribution of the Neutron Field in a Fuel Pellet. Rate of Neutron-Physical Processes in the Edge Zone. A series of cellular calculations was performed to analyze the formation of an edge zone. It is well known that nonuniform burnup is associated with radial nonuniformity of plutonium production, which, in turn, is caused by the blocking of resonance neutron capture by $^{238}\text{U}$ [4].

The spatial distribution of neutron fluxes with different energy was calculated using the SCALE program to evaluate the thickness of the layer where resonance blocking will result in elevated accumulation of plutonium, and to analyze the energy-release nonuniformity due to the distribution of heat flux over the radius of a fuel pellet.

The neutron spectrum does not change along the radius of a fuel pellet, with the exception of the region of $^{238}\text{U}$ resonances. The flux of neutrons with resonance energy changes sharply along the radius of a pellet (the flux is much higher near the boundary of a pellet than at the center). As a result, plutonium accumulation changes substantially along the radius of a pellet. At the start of burnup, the energy release is uniform along the radius of a fuel pellet. An elevated plutonium accumulation in the peripheral layer of a pellet results in the appearance of substantial energy-release nonuniformity along the radius with average burnup 10 MW-days/kg.

A three-zone cylindrical model of a VVER-1000 cell was used in the calculations. The radius of a uranium dioxide fuel pellet with density 10.27 g/cm$^3$, equal to the inner radius of the cladding, was 0.386 cm, the zirconium cladding was 0.069 cm thick, and the outer radius of the cell corresponded to the triangular lattice spacing 1.25 cm. The working state of a cell with water temperature 573 K and density 0.71 g/cm$^3$ was studied. The enrichment of the $^{235}\text{U}$ fuel was chosen to be 5.5% in order to reach deep burnup.

As Fig. 1 shows, a neutron flux with resonance energy changes the most along the radius. As a result of this behavior, plutonium accumulation in the peripheral layers of a fuel pellet is higher than in the central layers. As a result of resonance absorption, the rate of capture of neutrons by $^{238}\text{U}$ is 34% higher in a 400 µm thick peripheral layer than in the rest of the region. In addition, the smaller the thickness of the peripheral layer, the greater the difference is.