SIMULATION OF UO₂ FUEL ROD FAILURE CONDITIONS FOR TRANSIENT POWER REGIMES BY THE RTOP CODE
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ABSTRACT

The paper covers the results of numerical modeling of the pellet-cladding mechanical interaction. An approach to solve the thermal-mechanical problem implemented in the RTOP code is presented. The approach comprises a complex modeling of fuel and cladding: in the 1.5D geometry for the conditions of quasi-steady-state power and in the 3D geometry for detailed calculations of fast power changes. To accelerate the calculations in 3D geometry the current version of the RTOP code makes use of the CUDA technology that uses parallel computing on graphics processing units (GPU). Self-consistent models of the mutual effect of the fuel rod thermal mechanics and gas atoms behavior are developed. These models allow considering the contribution of porosity to the mechanical stresses in the cladding. The analysis of stresses in fuel rod cladding and fuel rod failure conditions is carried out with the account for local non-uniformities of mechanical stress fields for the case of INTERRAMP and Risø3 experiments.

INTRODUCTION

To carry out the safety analysis of nuclear fuel operation it is necessary to predict internal gas pressure of the fuel rod and mechanical stresses in the cladding as it interacts with the fuel pellets. The application of the available correlations to predict the state of the fuel rods under nominal and transient conditions especially at high burnups brings about a considerable scatter in the estimated parameters. Therefore, for calculation of the fission gas release and the stresses in the cladding mechanistic fuel performance codes are applied that make it possible to describe in a self-consistent manner the behavior of fuel pellets and cladding under nominal and transient conditions.

The calculation of the pellet-cladding mechanical interaction (PCMI) with the account for the local non-uniformities of the mechanical stress fields should be carried out in 3D geometry considering the spatial dependencies of radial, axial and angular components of mechanical stresses in the fuel rod. The stresses in the fuel and cladding are determined by temperature distribution across the fuel rod and depend on the geometrical parameters of the pellets and the quantity of cracks in them. The interaction of fragmented pellet with cladding can lead to formation of stress concentrators that are located in the cladding areas adjacent to the crack. High peak tensile stresses in the cladding can accelerate the processes that lead to loss of fuel rod tightness. In particular one of the possible cladding failure mechanisms is iodine-induced stress corrosion cracking.

To model the high burnup fuel one needs to consider its specific physical features. These features include: high content of fission gas in the fuel matrix, intragranular and intergranular porosity; rim-structure formation at the fuel pellet periphery; fuel swelling and irradiation-induced cladding creep; degradation of UO₂ fuel heat conductivity and mechanical properties of the fuel rod cladding. The analysis of the experimental data on fuel behavior in transients [1] has shown the necessity of self-consistent calculation of fuel and cladding mechanical behavior, fission gas release and microstructural changes in the fuel. Microcracking of fuel in a field of mechanical stresses leads to intergranular boundary opening and increase in fission gas release from the fuel matrix. On the other hand, the presence of compressive stresses in the fuel pellet slows down the fission gas release as it suppresses the percolation of intergranular gas bubbles and leads to the closing of gas channels in the deformed pellet. Gas swelling of fuel due to gas bubbles in the intergranular boundaries, in the pores and cracks of the pellet can lead to a considerable increase in the load on the fuel rod cladding. The higher is the burnup of UO₂ and respectively the quantity of fission product atoms the more pronounced is the effect of the interaction of gaseous fission products behavior and mechanical stresses in the fuel and cladding.

The present paper provides the results of modeling the pellet-cladding mechanical interaction using the fuel performance code RTOP. To calculate the stress and strain fields in a fuel pellet a complex approach is elaborated that uses a combination of a one and a half dimensional (1.5D) and a three-dimensional (3D) computational model. The given approach allows both calculating the geometrical variations of fuel at the stage of steady-state irradiation and determining the tensile stresses in the cladding as it contacts with the fuel pellet considering the stress concentrators: radial cracks in the pellet and pellet-to-pellet interface. The models of the mutual effect of the
thermal-mechanical behavior of fuel rods and FGR under nominal and transients conditions are considered. The code takes into account the specific physical features of high burnup fuel.

The paper covers the modeling of the mechanical behavior and failure conditions of fuel rods with the RTOP code for the experiments INTERRAMP and Risø3 from the database distributed by IAEA within the framework of an international project FUMEX-3. The provided comparison of calculated results with the experimental data shows a possibility of correct description of nuclear fuel under nominal conditions and transients with the RTOP code.

MODELING OF FUEL ROD THERMOMECHANICAL BEHAVIOR FOR NOMINAL AND TRANSIENT CONDITIONS

The modeling of thermomechanical behavior of the fuel rod is closely related to the determination of the dynamics of the plastic deformations in the fuel rod during the preliminary irradiation and increases of linear heat rate. The numerical solution of the evolution problem for plastic deformations is connected with multiple calculations of the stress-strain state of fuel and cladding. To determine the evolution of plastic deformations during the entire fuel rod operational period using the 3D model requires a large amount of computations, which is time-consuming. To minimize the computation time the complex approach is implemented in the RTOP code that involves the calculation of the fuel rod deformations evolution in the accelerated 1.5D statement and 3D modeling of the stress fields in the fuel rod at the moments of peak thermal loads.

The thermoelastic problem in 3D statement is solved using the finite-element method [2]. To reduce the computing time the technology of parallel programming using the graphic processing units (Nvidia CUDA platform) [3] is applied. The increase in performance of calculations is achieved due to simultaneous processing of command or data flows in different execution cores while running the computational algorithm.

The solution of the problem of thermomechanical fuel rod behavior within the framework of the RTOP code comprises the modeling of:

- thermoelastic state of pellets and cladding with the account of their mechanical interaction,
- evolution of plastic deformations and relaxation of mechanical stresses in fuel and cladding,
- changes in the geometrical parameters of fuel due to sintering and radiation swelling of UO$_2$-matrix and radiation creep of cladding,
- pressure of the stable fission gases released into the fuel rod free volume.

To calculate the evolution of the fuel rod stress-strain state resulting from plastic deformations in the fuel pellets and cladding the interaction of fuel and cladding is modeled using the axially symmetrical (1.5D) model. Within the framework of the given model the fuel pellet and the cladding are considered as the cylinders with axially symmetrical distribution of temperature and mechanical properties (Young modulus). The stress-strain state is described with radial and axial displacements. To calculate the displacements the simplifying assumption is made that axes of cylindrical coordinate system coincide with principal axes of strain and stress tensors.

The boundary conditions on the lateral surfaces of the fuel and cladding are determined by gas pressure inside the rod, coolant pressure or pressure of pellet-cladding mechanical interaction. On the edge surfaces of fuel and cladding the value of the applied force is assigned. The value of that force is determined by the action of the spring and the friction force between fuel and cladding. Thermal expansion of fuel can lead to axial displacement of the pellets. This displacement is limited by the spring compression force $F_s$ and the friction force $F_f$.

The value of fuel pressure on the cladding $P_{fc}$ depends on the axial force $F_{ax}$, that is summed up from the friction force $F_f$ and the action of the spring $F_s$. In turn the maximum value of friction force $F_f$ depends on the pressure $P_{fc}$ exerted by the fuel on the cladding in the radial direction. The axial distribution of forces is determined iteratively.

To determine the rate of plastic deformations the components of stress deviator $S_{ax}$ are calculated. The rate of fuel and cladding creep is calculated in accordance with the correlation dependencies [4], implemented in the FRAPCON code and using the database MATPRO [5]. The correlation considers the creep of UO$_2$ fuel resulting from the flow of vacancies in the field of mechanical stresses and motion of dislocations. The creep rate caused by the vacancy flow is linearly proportional to mechanical stresses. At high stresses the processes of dislocation motion are activated and the creep rate is described by the power dependence on stresses: $\sim S_{ax}^{4.5}$. The effect of irradiation on the processes of the creep is considered by the vacancy diffusion coefficient. The creep rate depends on the fuel grain size and its porosity. The plastic deformation rate of cladding [4],[5] is determined by the fast neutron flux, temperature and the value of mechanical stresses. The dependence of the fuel and cladding creep rate on temperature is described by Arrhenius functions with appropriate activation energies.
When the reactor is operating at power, the temperature of the fuel column centre is higher compared to the pellet edge which leads to generation of mechanical stresses in fuel. The fuel in the central part becomes compressed and at the edge the tensile tangential stresses arise. The high temperature in the central part of fuel causes the increase in plastic deformations and mechanical stress relaxation. When the thermal load is released residual stresses arise in the fuel pellet. The residual stresses as well as available plastic deformations are considered in calculations of the thermomechanical behavior of fuel rods in 3D geometry.

The statement of the PCMI problem in 3D geometry comprises fuel pellet surrounded by cladding. Cracks can exist along the pellet radius in the fuel. The initial state of the pellet and cladding is described with the defined geometry, the absence of mechanical stresses and uniform temperature. Further on, temperature distribution over the radius, gas pressure inside the rod and coolant pressure in the fuel pellet are specified. The cracks in the fuel pellet are assumed to divide it into equal angular sectors. Temperature distribution over the pellet depends on the radial position. Due to the angular symmetry of the temperature problem and symmetry relative to the plane that divides the pellet in two, the solution is calculated for half-angle of the pellet sector.

To validate the implementation of the proposed methods benchmark tests were calculated for the stress-strain state of fuel and cladding for the conditions of no cracks in the fuel pellets. The mechanical stresses obtained from the RTOP code in 1.5D geometry were compared with the results of the calculations by the 3D module. The history of the linear heat rate in the fuel rod was defined as an interval of pre-irradiation at a constant linear power ($LP = 20$ kW/m), at the end of which the linear heat rate was ramped to $LP = 30$ kW/m within the time of $t = 10^7$ s. The duration of the pre-irradiation stage was $10^8$ s. The initial gap between the fuel and cladding was chosen to be equal to $120 \mu m$. By the moment of linear heat rate ramp the gap between the fuel and the pellet disappeared because of fuel swelling and cladding radiation creep. Coolant pressure was equal to $P_{cool} = 140$ atm.

A comparison of calculated mechanical stresses in fuel and cladding by 3D module and by the 1.5D model for the benchmark tests is shown in Figures 1, 2. One can see that the stress distributions over the radius of the fuel pellet and fuel rod cladding calculated by 1.5D and 3D models show a good agreement.

![Fig.1. A comparison of the radial (to the left) and tangential (to the right) mechanical stresses (MPa) in the fuel pellet calculated by 1.5D and 3D program modules. (O) – 1.5D, (▬) - 3D.](image1)

![Fig.2. A comparison of the radial (to the left) and tangential (to the right) mechanical stresses (MPa) in the cladding, calculated by 1.5D and 3D program modules. (O) – 1.5D, (▬) - 3D.](image2)
MUTUAL EFFECT OF FUEL ROD THERMAL-MECHANICAL BEHAVIOR AND FISSION GAS RELEASE

To model the fuel behavior in transient conditions it is necessary to consider the effect of the fission gas release and the microstructural changes in fuel on the mechanical behavior of fuel and cladding. Gas swelling of fuel can considerably increase pellet pressure on the cladding. It is also necessary to consider the feedback effects: the effect of mechanical stresses on the processes of gas release out of the fuel column. The present section covers the main models of the mutual effect of the fuel rod thermomechanics and fission gas atom behavior, in particular: fuel microcracking, effect of stresses in the fuel on the percolation threshold of the intergranular bubbles and gas blockage in large pores and macrocracks resulting from fuel pellet deformation.

The RTOP code contains a separate calculational module to describe the intergranular microcracking of fuel over the grain boundaries. The mechanical strength at the grain boundaries is lower than inside the grain volume. Therefore, sharp increase in the nonuniform temperature field and consequently gas pressure in the bubbles and the mechanical stresses in the pellet can lead to cracking along the grain boundaries. If the cracks along the intergranular boundaries become sufficiently large, the effect of irradiation-induced resolution of the intergranular gas into the fuel matrix stops and the intragranular gas is released into the crack faster.

The model of cracking along the grain boundaries [1],[6] uses the following criterion:

\[ 3.5 \cdot \delta P + 5.2 \cdot \sigma_{\text{ext}} > \sigma_{\text{crit}}, \]  

(1)

The criterion relates the pressure increase in the intergranular bubble \( \delta P \), a microscopic stress in pellet \( \sigma_{\text{ext}} \) and the ultimate strength \( \sigma_{\text{crit}} \) of the grain boundaries.

There exist two modes of intergranular bubble behavior. The first mode under a quick heating can lead to fuel cracking along the grain boundaries. This case is realized when the effective tensile stress exceeds the critical value. The second mode is observed at a slow temperature rise. In this case the other mechanism of pressure decrease in the bubbles is an increase in their volume due to a diffusion flow of vacancies leading to reduction in the mechanical stresses and increase of the intergranular porosity. If the temperature change is small, the pressure in the bubbles decreases and the criterion for cracking might not be reached. At present the model of microcracking undergoes the stage of additional verification.

Let us determine the relation of threshold concentration of gas at the grain boundary at which the percolation takes place to the hydrostatic pressure in fuel. The intergranular bubbles in the external field of mechanical stresses are described in the RTOP code by the Van der Waals equation of state:

\[ P_{\text{ext}} + 2 \gamma \sin \theta / R = \frac{N K T}{V - Nb}, \]  

(2)

here \( N \) is the number of gas atoms in a bubble; \( V = (4 \pi/3) \phi R^3 \) is the bubble volume; \( b = 8.5 \cdot 10^{-29} \text{ m}^3 \) is the Van der Waals constant for Xe; \( \phi \) is the bubble form-factor, expressed via the contact angle \( \theta \); \( \gamma \) is the surface tension coefficient, \( P_{\text{ext}} = -\sigma_{\text{hyd}} / 3 \) is hydrostatic tension in fuel expressed via the trace of mechanical stress tensor. It is commonly assumed [7], that the percolation limit for the bubbles at the grain boundaries is reached when the fraction of grain surface area occupied with bubbles is equal to some definite value (usually 0.5). Assuming that the number of bubbles on the grain boundaries weakly depends on the external pressure it possible to find the form of dependence of gas threshold concentration at the grain boundary \( c_{\text{tr}} \) at which the percolation occurs on the pressure in fuel:

\[ c_{\text{tr}}(P_{\text{ext}}) - c_{\text{tr}}(0) = P_{\text{ext}} \]  

(3)

As the fuel contacts with cladding compressive stresses arise over the radius and the length of the fuel column. They increase the threshold concentration of gas needed to reach the percolation and thus slow down the gas release into the fuel rod plenum. At power drop the condition of percolation is met and an accelerated gas release into the plenum takes place.

Gas release from the intergranular boundaries into the fuel rod free volume might not occur in case when there are significant deformations in the pellet that block the channels connecting the intergranular porosity and the plenum (cracks in fuel, fuel-to-cladding gap). The solution of the problem of gas flow in a porous medium of \( \text{UO}_2 \) fuel is sufficiently complex, considering a high sensitivity of such a model to the parameters that are difficult to verify experimentally (for example, the dynamics of growth and “healing” of cracks between the fuel fragments). Therefore, a simplified approach to the description of the gas blocked in the macroporosity and cracks of \( \text{UO}_2 \) fuel has been implemented in the RTOP code.

The blocked fission gas can be assumed to situate mainly in radial cracks and radially-oriented pores. It is
confined by the angular component of stress tensor $\sigma_{\theta\theta}$. With the quantity of gas blocked in the porosity known, its volume can be found from the equation of state $-\sigma_{\theta\theta} = NkT/(V - Nb)$, where the overline implies the averaging over the pellet radius. To determine the conditions under which gas is blocked in cracks and the microporosity, a following assumption can be made: gas is released via the channels that are located parallel to the pellet circumference and that are blocked upon radial compression. Then the condition of gas blocking is given by a characteristic parameter that defines the value of elastic radial deformations in the pellet:

$$z = -\frac{\sigma_{\theta\theta}}{E},$$

where $E$ is the Young modulus of fuel. If parameter $z$ is negative, the channels are not blocked and neither is the gas. Otherwise the fraction of gas flowing out of the intergranular porosity that is blocked in cracks and micropores at the present moment of time amounts to:

$$\delta = 0.5 \left[ 1 + \operatorname{erf} \left( \frac{(z - z_0)}{\sqrt{2}z_1} \right) \right],$$

where $z_0$ и $z_1$ are the critical parameters that have meaning of the average parameter of blockage and its dispersion correspondingly and $\operatorname{erf}$ is the function of error integral. Respectively, the fraction of fission gas flow directed to the plenum is $1 - \delta$.

The above effects of increasing the percolation threshold in the intergranular bubbles due to the pressure in fuel and fission gas atom blockage in fuel bring about a slowdown in gas release into the fuel rod plenum under transient power increases. At that, porosity volume increases and the load on the cladding rises. After power drop the porosity opens up and gas pressure in the fuel rod quickly increases. The phenomenon discussed is observed in Risø3 tests [8]. The example of linear power scenario for the rod GE2 from Risø3 series is shown in Fig. 3.

Fig. 3. Scenario of linear heat rate for GE2 test in Risø3 experiments. Linear power, kW/m versus irradiation time, h.

Fig. 4 shows the influence of the considered effects of gas blockage on the kinetics of fission gas release using the fuel rod GE2, Risø3 as an example. A comparison of the basic calculation without consideration of the models that slow down the fission gas release under transients, the calculation with the models included and the measured FGR versus the time shows that the implementation of these models in the RTOP code allows improving considerably the kinetics of FGR predicted by the code. Besides, a good quantitative agreement of the calculated and experimental value of the step in the FGR plot can be seen. Fig. 5 shows the effect of porosity on the magnitude of fuel pellet pressure on the fuel rod cladding. Porosity formation leads to an increase in fuel pressure on the cladding by about 25%.

**MODELING THE FUEL ROD FAILURE CONDITIONS UNDER PCMI**

The developed approach for performing 3D calculations was applied to model the experiments INTERRAMP [9] and SUPERRAMP [10]. Projects SUPERRAMP and INTERRAMP were carried out in order to analyze the effects of the pellet-cladding mechanical interaction, fission gas release as well as the microstructural changes in the fuel under significant power ramps. In the experiments INTERRAMP a pre-irradiation of fuel was performed to the burnup of 10 and 20 MWd/kgU. After the pre-irradiation the fuel rods were subjected to irradiation at a constant heat rate of about 25 kW/m. Then the linear heat rate was increased to the level above 40 kW/m at a rate of about 4 kW/(m·min). After the maximum power had been reached the fuel rod was retained at this level of power for 24 hours or, until activity was detected in the coolant in case of fuel rod failure. In a series of experiments fuel rods were used with different fuel-to-cladding gap and different thermomechanical treatment of the claddings (recrystallization and cold wall plus stress relieve). Projects INTERRAMP and SUPERRAMP incorporated detailed post-irradiation examinations along with the reactor diagnostics: measurements of the fuel column and cladding
geometrical characteristics, measurements of fission gas release and determination of the cesium distribution and microstructure of the fuel (grain dimensions and porosity).

Figs. 4, 5. FGR (to the left), fuel pressure on the cladding (to the right) versus the time for the fuel rod GE2 (Risø3 test). – 1 – inclusion of models of gas blockage in macroporosity and the effect of pressure on the percolation threshold; – 2 – inclusion of the model of the pressure effect on the percolation threshold; – 3 – basic calculation, porosity not considered; – 4 – experimental data.

The calculations by the 3D version of the RTOP code have shown that in the presence of cracks in fuel pellets the tensile stresses in cladding increase considerably. It is related to the fact that the cold layers in the cracked fuel pellet located on the periphery do not prevent the central part of fuel from thermal expansion. If there are more than three cracks in the pellet, the maximum stresses weakly decrease and the average stresses increase as the number of the cracks increases. The average stresses and deformations in the cladding as well as the fuel pressure on the cladding virtually do not depend on the friction coefficient between the fuel and cladding. The peak stresses in the cladding grow with the increase in the friction coefficient.

Fig. 6 shows the 3D distributions of the circumferential stresses in the cladding of fuel rods HR2 and HS1 from the INTERRAMP experiments. The distributions are given in the quarter of a fuel fragment. The angular symmetry plane of the fuel fragment is shown on the right and the symmetry plane with respect to pellet height is shown at the bottom of the figures. In the center of the pellet compressive stresses arise. They reach maximum values close to the middle of the pellet axis due to the bend of a non-uniformly heated pellet with free edges. At the edge of the pellet and in the cladding tensile stresses take place. As a result of the linear heat rate ramp a through-the-wall defect occurred in fuel rod HS1. No activity release was observed at power loading of fuel rod HR2. As one can observe, the distribution of the tangential stresses in HS1 fuel rod cladding has the specific feature in the area of the fuel crack with maximum tensile stresses on the internal surface of the cladding. The formation of stress concentrator in this area is explained by the angular deformations of the fuel pellet fragment at linear heat rate increase and pellet-to-cladding friction.

Fig. 6. Circumferential stresses for fuel rods HR2 (to the left) and HS1 (to the right) of experiment INTERRAMP.
Figures 7, 8 show a comparison of the calculated and experimental dynamics of the change in HR2 fuel rod diameter and length at the stage of preliminary irradiation and at the end of the experiment. The change in the fuel rod geometrical parameters at the preliminary irradiation stage is caused by pressure exerted by coolant and radiation creep of the cladding. A good agreement between the computations by the code and the measurements is observed.

The time taken by the calculations on GPU for the considered 3D problems was typically reduced by 5-7 times as compared with the calculations on the central processor. For the comparison Intel Core2Duo E8500 processor and Nvidia GTX 260 video card were used.

The increased tensile stress in cladding could lead to fuel rod failure. One of the mainly considered failure mechanisms is iodine-induced stress corrosion cracking (ISCC). Concentration of the iodine released from the fuel matrix into the rod free volume depends on fuel burnup and linear heat rate. Calculation of birth and release of I-129 were carried out using the developed modules of the RTOP code. As an example, concentration of released I-129 is shown in Fig. 9 for the fuel rod HS1 in INTERRAMP experiment. The HS1 rod failed during the hold at increased power level of 47.8 kW/m. To estimate the magnitude of tensile stress required for ISCC the model [11] is used. For the HS1 fuel rod the model yields the threshold value of 750 MPa for circumferential stress in cladding while thermomechanical 3D calculations give the values about 700-800 MPa depending on friction coefficient and quantity of cracks in fuel pellet. Therefore calculations confirm the possibility of cladding failure in transient regimes by a mechanism of iodine-induced stress corrosion cracking.
CONCLUSION

The present paper concerns the simulation of fuel rod thermomechanical behavior under transient power regimes with the RTOP code. A comprehensive approach is implemented in the RTOP code that incorporates 1.5 D computation of the dynamics of the plastic deformation of fuel and cladding for the conditions of standard operation and the 3D computation of the stress-strain state under the conditions of peak loads of the fuel rod. The program implementation of the module for 3D calculations uses the finite element method and the software-hardware CUDA technology. At present the application of CUDA technology using the current possibilities of available video cards for personal computers made it possible to increase by 5-7 times the performance of 3D module computations.

The models of the mutual effect of the fuel rod thermomechanics and fission gas atom behavior are implemented in the RTOP code, in particular, the models of fuel microcracking, effect of stresses in the fuel on the percolation threshold of the intergranular bubbles and gas blockage in large pores and macrocracks under radial fuel pellet deformation. Increase of mechanical stress in cladding resulting from gas swelling of the fuel is also considered. The application of complex approach makes it possible to describe the fuel rod behavior in a self-consistent manner including thermoelastic state, dynamics of plastic deformations, pressure of stable fission gases, changes in thermophysical properties and geometrical parameters. At present the self-consistent models of the mechanical behavior of the fuel rod and fission gas release described in the paper are additionally verified.

Modeling of pellet-cladding mechanical interaction in 3D geometry for the conditions of experiments INTERRAMP and Risø3 is carried out using the RTOP code. It is shown that consideration of gas swelling and 3D calculations is necessary to model the PCMI for the conditions with a fast power increase. The possibility of iodine-induced stress corrosion cracked is also concerned. The results of analysis show that the RTOP code can correctly describe thermomechanical behavior of fuel rod under transient conditions.

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