

## Problems of Calculation Modelling of Nitride Fuel Performance: DRAKON Code

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### Abstract

The DRAKON code is designed for numerical simulation of temperature and stress-strain state of fast reactors nitride fuel pins. Code verification is based on the PIE data obtained after irradiation of standard FAs of BR-10 reactor (uranium mononitride) and experimental FA of BORA-BORA program in BOR-60 reactor (mixed nitride fuel). The calculation results are in good agreement with the experimental data. Code verification is planned to be continued using the results of PIE of experimental FAs with nitride fuel, which are under irradiation in BOR-60 and BN-600 reactors.

DRAKON code is currently used to study performance of the experimental nitride fuel pins of BN-600 reactor and to analyze the PIE results for such pins. As an example, the calculation results of experimental fuel pins with low-swelling FM steel cladding are given in the paper. It is shown that there are two major limiting factors: 1) FCMI stress in the lower cladding sections with the "cold" fuel where cladding creep rate is negligible; 2) cladding damage due to FCMI and fission gas pressure in the upper "hot" sections where high-temperature strength of FM cladding is low (CDF – criterion). The fuel rod performance is limited by one of these factors depending on actual irradiation parameters.

**Key Words:** uranium-plutonium mixed nitride fuel, experimental fuel pins, stress-strain state, DRAKON code.

### 1. Introduction

The Federal Target Program "Nuclear Power Technologies of the New Generation in 2010-2015 and until 2020" provides for development of sodium-cooled BN-1200 fast reactor design and commissioning of lead-cooled BREST-OD-300 fast reactor. Mixed uranium-plutonium nitride fuel is planned to be used in these reactors. The DRAKON code is applied for calculation justification of performance of fuel pins with nitride fuel.

One of the main factors limiting the life of the nitride fuel pins at high burn-up is fuel cladding mechanical interaction (FCMI) leading to strong deformation or even cladding failure. The consequences of FCMI are determined by fuel and cladding swelling rates, cladding thermal and radiation creep rates, cladding long-term stress rupture, cladding strain capacity, cladding corrosion, fuel creep rate, as well as the level of fuel pellet cracking and fragmentation. The main calculation modelling problems arise from not enough data on nitride out-of-pile properties and in-pile behavior depending on plutonium content, fuel density, irradiation temperature, as well as shortage of reliable data on irradiated steel cladding properties, thermal creep and long-term stress rupture.

Within the framework of the PRORYV project, a comprehensive program for calculation and experimental studies of mixed nitride fuel for BN-1200 and BREST-OD-300 reactors has been designed to provide the required data. The program aims at studying performance of fuel

pins with mixed nitride fuel at the main operating characteristics of BREST-OD-300 and BN-1200 reactor cores [1]. The program is to provide additional data on out-of-pile properties of mixed nitride fuel, to develop methods and criteria for fuel pin performance substantiation, and to test the experimental fuel pins with mixed nitride fuel in BOR-60 and BN-600 reactors.

The results of the reactor testing and post-irradiation examination of experimental fuel pins will provide the data on the stress-strain and temperature states of fuel pins, fission gas release, distribution of fission products in the nitride fuel, as well as additional information on the mechanisms and characteristics of nitride swelling, on fuel and cladding microstructure.

## 2. Updated version of DRAKON code

The thermomechanical code DRAKON is designed for quasi-stationary numerical simulation of temperature and stress-strain behavior of the fuel pins with uranium nitride and mixed uranium-plutonium nitride fuel in liquid metal-cooled fast reactors [2]. The calculation of temperature fields and stress-strain state of fuel pins in the DRAKON code is based on the self-consistent solution of thermal-physical and mechanical boundary value problems describing the nonlinear propagation of heat, deformation of the fuel core and the cladding with allowance for materials creeping and swelling.

The DRAKON code was developed in 2004 to calculate the stress-strain state of cylindrical fuel pins. The first code version was developed for the fuel pins of thermal reactors with  $\text{UO}_2$  fuel. In 2004-2006, a code version for fuel pins of fast reactors with  $\text{UPuN}$  fuel was developed. In 2013-2016, the nitride version of DRAKON code was modernized: computational scheme was improved to allow automatic transition from non-contact loading scheme to the contact one and to account for variable loading regimes; fuel swelling module and fission gas release module, as well as other nitride properties modules were improved on the basis of the available experimental data.

The mathematical modeling of stress-strain state (SSS) parameters of the fuel pin is based on the following assumptions:

- Operation mode is quasi-stationary (i.e. the loading factors change versus time slowly enough to neglect a dynamic loading component).
- The loading axial symmetry is considered.
- The following processes associated with transient loading of the fuel pins, such as thermal cracking of the fuel core, local thermo-mechanical interaction of fragmented fuel pieces with cladding at power increase (axial ratchet) are not modeled.
- Changes of radial fuel-cladding gap and free volume under cladding are influenced by cladding elastic and creep deformation under pressure, fuel swelling and temperature deformations of fuel and cladding at power rise. The fuel mass transfer on inner cladding surface is not taken into account.
- Mechanical contact between fuel and cladding results from fuel temperature or swelling expansion. In the contact area the fuel can slip along the cladding.
- The cladding wall is thick (thickness/radius  $< 0.1$ ), radial stresses are assumed to be small compared to circumferential and axial stresses. The deformation of cladding is viscoelastic, cladding swelling is isotropic.
- Calculation of gap conductivity accounts for the contribution of gas heat conductivity, contact and radiation components.

- The pin core is divided into Nz axial sections small enough to neglect axial gradients of temperature and other parameters. Each of Nz pin axial sections is considered in conditions of flat deformation.
- Each fuel section in radial direction is divided into thin coaxial layers. Temperature, swelling, creep and other fuel properties are assumed to be equal inside each layer.
- The elastic, creep components of deformations, temperature deformations and swelling are considered for cladding and fuel.

The following parameters are calculated for each radial and axial layer:

- Principal stress components and their rates for fuel and cladding
- Radial and circumferential deformation components and their rates for fuel and cladding
- Axial deformation component and its rate for fuel and cladding
- Irradiation-induced swelling and swelling rate for fuel and cladding
- Fuel porosity
- Fuel and cladding temperature and temperature variation rate
- Total volume of fission gas produced, volume and pressure of fission gas under the cladding
- Rates of linear heat generation, burnup, damage dose, solid swelling rate, rates of cladding outer radius change, of radial gap change
- Cladding cumulative damage factor (CDF)

The models of fuel swelling and release of fission gas under the cladding have a great influence on the computational results. For calculation of fuel swelling DRAGON-M uses the model of spherical gas pores [3] or the empirical function of fuel swelling rate, which depends on fuel temperature and burn-up. The major contributors to the swelling of the fissile fuel composition are the increase in the total amount of fission products with respect to the volume ("solid" swelling) and the increase in the pore volume due to pressure of the fission gas accumulated in these pores ("gas" swelling).

Hypotheses used in the mathematical model of fuel swelling:

- All pores are spherical, have the same dimensions and are evenly distributed in the fissile material
- The volume of fuel is conditionally divided into regular spherical cells with one pore in each.
- Accumulation of solid and gaseous fission products cause a uniform change in the volume of fissile composition in each unit cell.
- The produced gas fission products are distributed as follows: one part remains in the crystal lattice, another part goes into closed pores and the remaining part comes out of the fuel core under the cladding. The sum of these three components is equal to the one.
- The fission gas formed in the material unit cell diffuses only into its own pore. Accordingly, the same amount of gas is accumulated in every pore of the unit cell.
- The surface of the unit cell is loaded only by hydrostatic pressure.
- There are no forces of interaction between unit cells. All the unit cells are deformed equally in a homogeneous temperature field.

Under these assumptions, certain part of the fission gas builds up in the closed pores of fissile fuel composition. The accumulation of gas in the pores leads to pressure buildup which is constrained by the fuel and deforms it.

Thus, fuel deformation can be locally described as deformation of empty thick-walled sphere (unit cell) in view of viscous and isotropic deformations. So, the local fuel deformation is defined, i.e. swelling at micro-level, when the hypothesis about uniformity of temperature within the unit cell is valid (i.e. "micro-problem").

At the same time, the swelling (relative change of the fuel volume as the macro-object in non-uniform temperature field) should be defined from the solution of the independent "macro-problem": deformation of the elastic-creep cylinder made of fissile material (see FIG. 1).

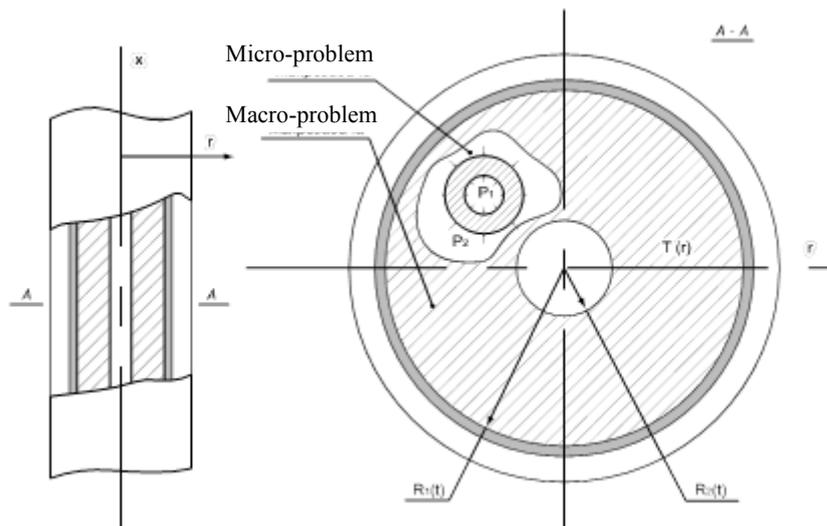


FIG. 1. Micro- and macro-problem areas for calculation of fuel material deformation.

To calculate the fission gas release, the DRAKON-M code uses empirical balance model of gas release from nitride fuel obtained from the analysis of experimental results. The model was fitted based on the results of post-irradiation examination of gas release from uranium mononitride fuel in three experimental and eight standard fuel subassemblies, irradiated in the fourth and fifth BR-10 reactor core loadings in the range of burnup from 3.4 at% to 8.4 at%. [4].

The model is based on the following assumptions:

- Fission gas releases under the cladding and into the closed pores are the functions of fission gas remained in the crystal lattice.
- The maximum fuel temperature at the current time point in the current cross-section is used to estimate gas release rate under the cladding.

The following correlation for fission gas release rate is used in the code:

$$F_{if} = \begin{cases} 4,3 \% / \text{at.}\%, & T_{\text{fuel\_max}} \leq 1050^{\circ} \text{C} \\ 8 \% / \text{at.}\%, & 1050^{\circ} \text{C} < T_{\text{fuel\_max}} \leq 1200^{\circ} \text{C} \\ 27 \% / \text{at.}\%, & 1200^{\circ} \text{C} < T_{\text{fuel\_max}} \leq 1550^{\circ} \text{C} \\ 30\% / \text{at.}\%, & T_{\text{fuel\_max}} \geq 1550^{\circ} \text{C} \end{cases} \quad (1)$$

where  $F_{if}$  – a ratio of the fission gas released under the cladding to the total fission gas produced.

The equation (1) is used when the burn-up is more than, so called, incubation burnup value, defined on the basis of experimental data:

$$\text{Bu\_inc} = 1.35 * \text{th}\left(\frac{1315 - T}{90}\right) + 1.35 \quad (2)$$

where  $\text{Bu\_inc}$  – burnup, at%,

$T$  – irradiation temperature, °C.

It is planned to adjust the models of fuel swelling and fission gas release basing on the results of post-irradiation examination of experimental fuel subassemblies irradiated in BOR-60 and BN-600 reactors within the framework of the Comprehensive program for calculation and experimental studies of mixed nitride fuel [1].

One of the aims of the ongoing code modernization is to consider cracking of the fuel pellets and modeling of the consequences of local thermomechanical interaction of fuel and cladding.

### 3. DRAKON code verification

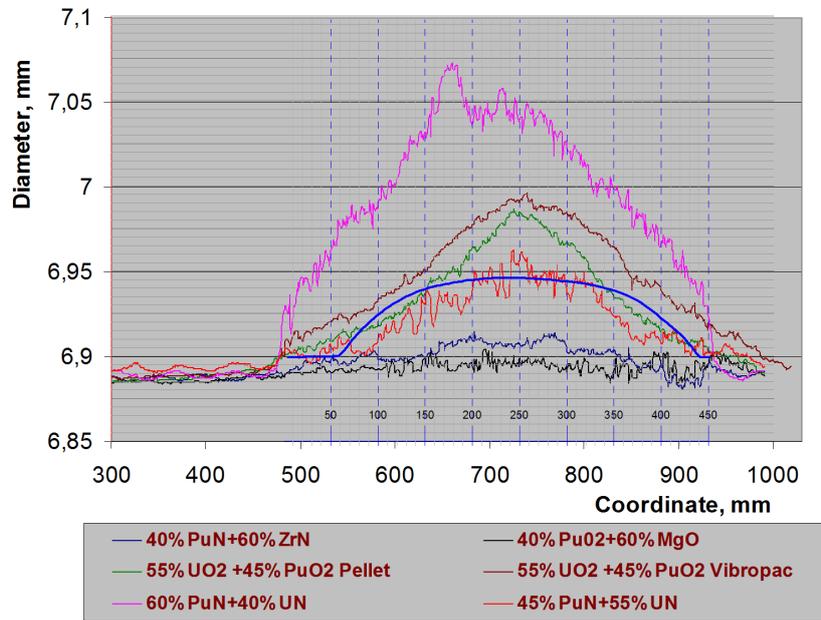
The code has been verified based on a comparison with the exact analytical solutions of the following problems:

- Elastic deformation of the hollow cylindrical shell under pressure or inhomogeneous temperature field
- Viscous deformation of the hollow cylindrical shell
- Contact deformation of two hollow cylinders under changing internal pressure conditions
- Contact deformation of two hollow cylinders caused by thermal expansion of the inner cylinder under alternating uniform volume heat degeneration density

The analytical testing results led to the conclusion that the errors introduced in the DRAKON code calculation by the algorithm and numerical methods are insignificant.

The results of the stress-strain state calculation of fuel pins of standard fuel subassemblies irradiated in the BR-10 reactor were compared against the post-irradiation examination data on fission gas release under the cladding and the gas pressure under the cladding [4] as well as a comparison of the calculation results with the experimentally measured values of irreversible cladding deformation, fuel swelling and gas release for the fuel pins with mixed nitride fuel UPuN (45% Pu) and UPuN (60% Pu), irradiated as part of BORA-BORA experiment in the BOR-60 reactor [5].

The experimental data on the axial distribution of the cladding outer diameter of the BORA-BORA fuel pins, including the fuel pin with UPuN (45% Pu), at the end of the second stage of irradiation [5], and the results of calculations by the DRAGON code for nitride fuel are presented in FIG. 2. As it can be seen from this figure, the calculation and experimental data on the cladding outer diameter are in rather good agreement.



— DRAGON code calculation for fuel pin with UPuN (45%Pu) (red line)

FIG. 2. Axial distribution of claddings diameters of BORA-BORA pins with different fuels at the end of the second stage of irradiation

It is planned to continue the code verification using the results of post-irradiation examination of experimental FAs with mixed uranium-plutonium nitride fuel, which are irradiated in BOR-60 and BN-600 reactors within the framework of the Comprehensive program for calculation and experimental studies of mixed nitride fuel.

#### 4. Calculation estimation of nitride fuel performance for experimental fuel subassemblies irradiated in BN-600 reactor

The DRAGON code is currently used for calculation study of fuel pin performance of the experimental fuel subassemblies with mixed nitride fuel irradiated in BN-600 reactor and for analysis of post-irradiation examination results for these fuel pins. The following figures show some calculation results: maximum fuel temperature as a function of time (FIG. 3.), axial distribution of maximum circumferential stresses in the cladding (FIG. 4.), axial distribution of cladding long-term damage (FIG. 5.) and axial distribution of maximum circumferential strain of the cladding (FIG. 6) of one of the BN-600 experimental subassemblies with the maximum lifetime of 11 intervals (about 40,000 eff. hours). The subassembly is installed in the radial blanket area in order to reproduce the operating conditions of the BREST fuel pins with cladding made of EP-823 steel.

The fuel temperature is determined by the conductivity of the gap between the fuel and cladding, which primarily depends on the gap size, as well as the composition of the gas mixture in the gap. At the initial stage, the fuel temperature decreases because the gap size

gets smaller due to fuel swelling. Then the fission gas goes under the cladding, which causes a decrease in the helium fraction in the gas under the cladding and reduction of the gap conductivity, which leads to a temperature increase. After that the gap size decreases due to increasing of the fuel swelling rate, and the gap conductivity increases.

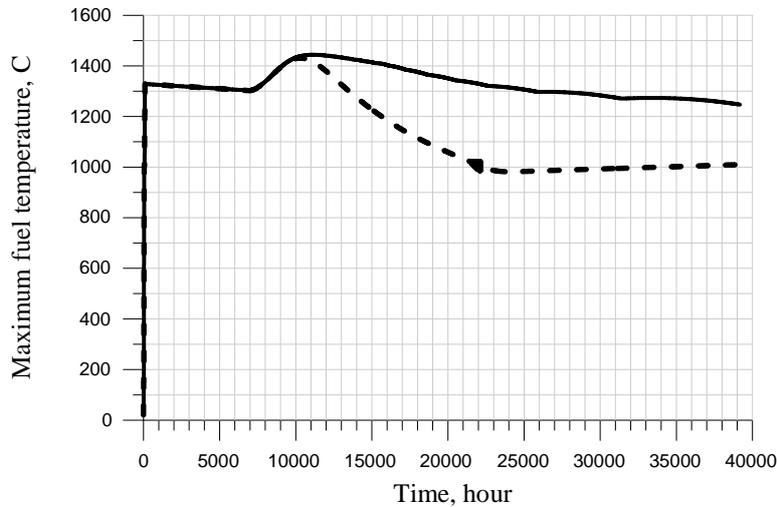


FIG. 3. Maximum fuel temperature for all sections (—) and maximum fuel temperature in the middle of the core (-----) in fuel pin of BN-600 experimental subassembly as a function of time.

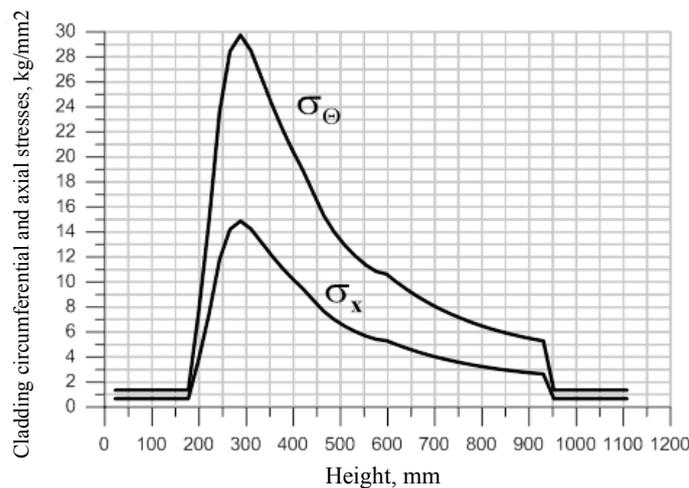


FIG. 4. Axial distribution of cladding maximum circumferential ( $\sigma_\theta$ ) and axial stresses ( $\sigma_x$ ) in BN-600 experimental subassembly at the end of life

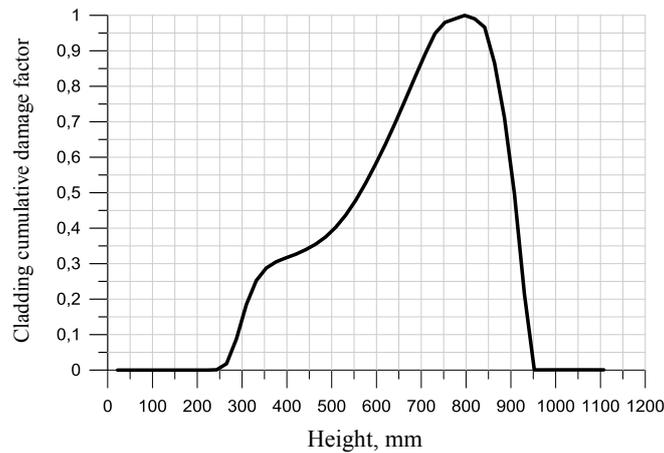


FIG. 5. Axial distribution of cladding cumulative damage factor (CDF) in BN-600 experimental subassembly at the end of life

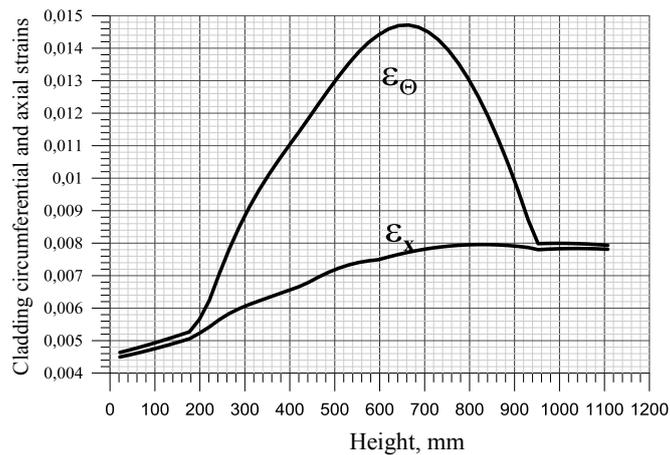


FIG. 6. Axial distribution of cladding circumferential ( $\epsilon_\theta$ ) and axial ( $\epsilon_x$ ) strains for BN-600 experimental subassembly at the end of life

The calculation results of experimental fuel pins with low-swelling FM steel cladding show that there are two major limiting factors: 1) high cladding stress due to mechanical interaction of "cold" fuel with cladding in the lower cladding sections, where cladding creep rate is negligible (FIG.4); 2) high CDF due to FCMI and fission gas pressure in the upper "hot" sections, where high-temperature strength of FM cladding is low (FIG. 5). The fuel pin performance is limited by one of these factors depending on the actual irradiation parameters (cladding and fuel temperatures, fuel burnup, and damage dose in cladding).

It should be noted that under the conditions of lengthy contact loading of the cladding, it is not the criterion of short-term strength, but the level of cladding residual deformation (i.e. cladding deformation capacity) that becomes more important. The deformation of low-swelling ferritic-martensitic cladding is primarily driven by the steel irradiation creep under the contact pressure from the nitride fuel. The ferritic-martensitic steel swelling can happen only at damage doses exceeding 100-110 dpa. To estimate the level of hazard of such deformation under rigid contact loading from the nitride is rather difficult because corresponding experimental data is virtually absent. One of the goals of the comprehensive program for calculation and experimental studies of mixed nitride fuel is to obtain necessary experimental data for this criterion.

## 5. Conclusion

The modernized version of the thermomechanical code DRAKON is designed for quasi-stationary numerical simulation of temperature and stress-strain behavior of the fuel pins with uranium nitride and mixed uranium-plutonium nitride fuel in liquid metal-cooled fast reactors.

The code verification was based on the comparison against the exact analytical solutions and PIE data obtained after irradiation of standard FAs of BR-10 reactor (uranium mononitride) and experimental FA of BORA-BORA experiment in BOR-60 reactor (mixed nitride fuel). The analytical testing results let us conclude that the errors introduced in the DRAKON code calculation by the algorithm and numerical methods are insignificant. The calculation results are in good agreement with the experimental BR-10 and BORA-BORA data. The code verification is to be continued using the results of PIE of experimental FAs with nitride fuel, which are being irradiated now in BOR-60 and BN-600 reactors.

The DRAKON code is currently used to study performance of the experimental nitride fuel pins of BN-600 reactor and to analyze the PIE results for such pins. The calculation results of experimental fuel pins with low-swelling FM steel cladding show that there are two major limiting factors: 1) FCMI stress in the lower cladding sections with the "cold" fuel, where cladding creep rate is negligible; 2) cladding damage due to FCMI and fission gas pressure in the upper "hot" sections, where high-temperature strength of FM cladding is low.

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