BERKUT – Best Estimate Code for Modelling of Fast Reactor Fuel Rod Behaviour under Normal and Accidental Conditions

A.V.Boldyrev[1], S.Yu.Chernov[1], A.P.Dolgodvorov[1], I.O.Dolinsky[1], V.D.Ozrin[1], V.I.Tarasov[1]

[1]Nuclear Safety Institute of the Russian Academy of Sciences (IBRAE RAN), Moscow, Russia

E-mail contact of main author: bav@ibrae.ac.ru

Abstract. A short description is presented of code BERKUT designed in Nuclear Safety Institute (IBRAE RAS) in frame of "The new generation codes" branch of “BREAKTHROUGH” (or “PRORYV”) project for mechanistic modelling of oxide and nitride single fuel rod behavior under normal and accidental conditions of liquid metal cooled fast reactor operation. The code models are grounded on the contemporary understanding of mechanisms governing the basic processes in fuel rods under irradiation, which substantially enhances the predictive ability of the code in comparison with the engineering analogs. Simulations of the nitride fuel rod behavior in BN-600 and BOR-60 reactors have demonstrated good agreement with the data of the post-reactor fuel rod examination on fuel and cladding geometry changes, fission gas release and fuel porosity profiles. Further validation is foreseen as the corresponding data are available.

Key Words: Fast Reactor, Fuel Rod Code, Nitride Fuel.

1. Introduction

At present the new generation integral code "EUCLID" [1] is under development in IBRAE RAS in the framework of the Russian federal target program "The new generation nuclear energy technologies" and “BREAKTHROUGH” (or “PRORYV”) project for comprehensive computer modelling of the next-generation fast reactors with the closed fuel cycle. Similar approaches are widely used over the world for modelling of thermochemical, mass transfer, radiative, thermo-mechanical and other processes in nuclear reactors under normal, transient and accidental conditions, which promote justification of the safety of existing and the newly designed nuclear power plants.

The integral code EUCLID has the module architecture, one of its constituents being the fuel rod module BERKUT designed for prediction of thermo-mechanical and physico-chemical behaviour of a single rod with oxide or nitride fuel in liquid cooled fast reactors (FR). The module was first designed as the homonymous stand-alone code, which can be used to solve specific tasks beyond the integral code.

In its turn, the code BERKUT was designed basing on the prototype, the fuel rod code SFPR [2], [3], elaborated earlier in IBRAE RAS for simulations of a single rod behaviour in thermal reactors. The models of SFPR code initially designed for accident conditions (and for this reason, were rather mechanistic grounded on the contemporary knowledge of the mechanisms governing basic physico-chemical processes in fuel rods under irradiation) and later extended to normal operation conditions were comprehensively validated against extended set of data of analytical and in-pile tests, in which the normal and off-normal conditions were simulated including severe accidents [2]. The validation, in combination with multiscale modelling basing on quantum mechanics, atomistic Monte Carlo and molecular dynamics, allowed

specifying the microscopic parameters of the code specific models describing the fuel behaviour under irradiation. In addition, the careful finite element 3D-simulations of the stress fields in the rod under irradiation were used to validate the key thermo-mechanical models.

The most processes in oxide fuel are of similar physical nature for both thermal and fast reactors while there is significant difference in the temperature and irradiation conditions of the processes. So the corresponding specific models developed earlier for thermal neutron reactors can be used in FR calculations. Moreover the functional forms of the modes are generally applicable to simulate the processes in nitride fuels as they generally have the close physics with the oxide fuels. However the microscopic parameters of the models for the oxide and nitride fuels often significantly differ from each other, and, as a rule, the "nitride" parameters are ill-defined or not defined at all. Their specification requires careful code validation as the corresponding experimental data become available. The first results in this direction are presented in this paper.

In Section 2 the brief description of basic principles and physical models of BERKUT code is given. In Section 3 the code performance is illustrated by example of simulation of fuel rods with nitride fuel under irradiation in FR. In these calculations one of the model parameters, resolution constant, was first fitted to describe correctly the measured gas release from the fuel irradiated in reactor BOR-60 in the framework of project BORA-BORA [4]. The code so tuned was further applied to simulate behavior of the nitride rods of the KETVS-1 assembly irradiated in reactor BN-600 [5]. In these calculations, the BORA-BORA data can be therefore considered as the training set for the code tuning whereas the KETVS-1 data serve as the test set, which essentially differs from the former by fuel composition and irradiation conditions.

2. Description of the code BERKUT

BERKUT is the multiscale code, the simulated processes being characterized by the range varying from 1 nm to 1 m.

For the microscale, the code describes evolution of fuel microstructure within the range of order of fuel grain size: concentration profiles of point defects, formation and development of dislocation network, nucleation and growth of intra- and intergranular gas-filled porosity, fission product (FP) generation and radioactive transformations, FP transport in grains and release to the intergranular position, formation of chemical compounds and their distribution over condensed phases.

For the mesoscale, the code simulates the processes in the scale of the fuel pellet: intergranular transport of FPs, oxygen or nitrogen, evolution of the as-fabricated porosity and columnar grain formation, FP release due to recoil and knockout mechanisms.

For the macroscale, the code describes thermomechanical behaviour of the rod as the whole: heat transfer within the rod and heat exchange with the coolant, temperature distribution in the fuel, fuel-cladding gap and cladding, evolution of fuel and cladding deformation mode, gas pressure within the cladding.

For modeling of the rod geometry and specifying the boundary conditions, an axial grid is generated with the arbitrary cell heights. Generally the upper and lower plenums, breeding blankets and fuel column are taken into consideration. Each cell includes the fuel column (absent in the plenums), gas filled gap and cladding, the different radial grids being introduced for the fuel and cladding.

The code BERKUT has module architecture and contains three basic modules: thermal, deformation and fuel.

Thermal module simulates evolution of temperature field taking into account dependence of thermophysical properties of materials on temperature, burnup and damage dose, change of the gap thickness, gas pressure within the rod due to release of gaseous FPs, formation of solid precipitates on the fuel surface, contact heat transfer when the gap closes.

Deformation module simulates fuel straining, cracking and crack healing, evolution of the cladding mechanical state, damage accumulation including cladding destruction taking into account gas pressure within the rod, coolant pressure, mechanical fuel-cladding interaction, temperature and swelling radial variation, local fuel melting, elastic deformations (thermal, elastic, thermal and irradiation-induced creep, related to fuel sintering and swelling), dependence of physico-mechanical properties of the rod materials on external conditions and their degradation under irradiation.

Fuel module was elaborated generalizing the fuel code MFPR [6], [7] for simulation of oxide or nitride fuel behaviour in FR. The code includes five macro-models: (1) FP generation and radioactive transformations, (2) evolution of fuel microstructure and intragranular FP transport, (3) formation of intergranular porosity, intergranular FP transport and release from fuel, (4) thermodynamics of irradiated fuel, formation of chemical compounds and their distribution on condensed phased and (5) transport processes in the pellet scale in the external gradients (oxygen/nitrogen diffusion, intergranular pore migration resulting in porosity redistribution, formation of columnar structures, evolution of the central void, etc.). The module describes changes in fuel microstructure including swelling, formation of FP-bearing gaseous and condensed phases, FP transport including their release to open porosity. This allows predicting dependence of fuel thermophysical properties on burnup, pressure and thermal conductivity changes of the fuel-to-cladding gap as well as FP release to the coolant after cladding failure. Near 500 isotopes are taken into consideration in BERKUT code, all of them being distributed over 25 chemical classes (He, Xe, Cs, I, Mo, Ru, Rh, Pd, Tc, Ba, Sr, Zr, La, Ce, Eu, Nd, Nb, Sb, Te, U, Pu, N, O, C, Na). Each class includes elements with the similar chemical properties. For instance class Xe includes all Xe and Kr isotopes. The same thermodynamic and transport properties (and therefore the same parameters of the code particular models) are prescribed to all members of the class.

3. Simulation of rod behaviour under irradiation in FR

As noted in Section 1 parameters of most of the particular models are poorly defined for nitride fuel. Therefore the calculations were performed with the "oxide" parameters. The exceptions were the FP solid state diffusion coefficients and the helium solid solubility.

In the literature there are a few evaluations of FP diffusivity in nitrides [8]–[10]. All of them are relate to Xe and demonstrate considerable scattering. Matzke [8] suggested that the Xe diffusivity in nitride fuel is somewhat lesser than in carbide fuel, the latter being an order of magnitude greater than in oxides. In this paper we choose the parameterization recommended in [9] for Xe, which is characterized by intermediate activation energy among the other papers. This diffusivity was assigned to all other FP classes. In addition the irradiation-induced a-thermal diffusivity was taken into account for Xe class; following Matzke's recommendation [8] it was set and order of magnitude less than that in oxide fuel.

Solubility of He in uranium dioxide was measured by Rufeh et. al [11] to be of $(3.8 - 7.9)\times10^{-6}$ mol He/mol UO_2 for the temperatures 1473–1573 K. Therefore, in the model,

for the helium activity coefficient (that is inverse solubility) in both oxide and nitride fuel, an intermediate value of 2.5×10^5 was chosen.

To get agreement between calculated Xe release and that measured in BORA-BORA test [4] we varied parameter b_0 characterizing strength of irradiation-induced resolution of gas atoms from gas-filled bubbles (the thorough description of the resolution model see in[12]). Then this parameter value was used for rod simulation in KETVS-1 assembly [5].

Note that irradiation induced resolution is one of the critical mechanisms, which governs development of intra- and intergranular porosity. In turn, the bubbles serve as the traps for the gas migrating in fuel resulting in suppression of gas release into the fuel-to-cladding gap. Therefore correct simultaneous description of gas release and fuel swelling by variation of a single parameter would be considered as additional argument in favor of the suggested validation procedure.

3.1. BORA-BORA test

Two rod types, below referred to as Pu45 and Pu60, were irradiated in reactor BOR-60 in the framework of BORA-BORA project [4]. The fuel was prepared from the weapon-grade plutonium and dump uranium with the composition of $U_{0.55}Pu_{0.45}N$ and $U_{0.4}Pu_{0.6}N$ referenced to as Pu45 and Pu60, respectively. In both cases the initial porosity was of about 15%. The rods were irradiated during 900 days at maximum linear heat rate varied from 37.3 to 54.5 kW/m up to burnup of 9.4% for Pu45 and 12.1% for Pu60. The thorough description of the rod characteristics and irradiation conditions is given in [4]. The post-reactor examination was performed upon completion of the irradiation. In particular He, Kr and Xe releases to the fuel-to-cladding gap were measured as well as swelling profiles.

In BERKUT calculations the rod geometry and time dependence of the heat rate were chosen to be close to the experimental ones. The fuel grain size was set equal to 30 μm and the pellet diameter (not specified in [4]) was supposed to be of 5.9 mm.

As explained above, the value of parameter b_0 was first found to fit the calculated Xe release to the experimental one. The found value 7.52×10^{-24} m^3 is a half order of magnitude less than that for the oxide fuel. This result is in qualitative agreement with theoretical estimates resulted from Monte Carlo and molecular dynamics simulations predicting lower resolution rate in nitrides in comparison with oxides (e.g. see [13], [14]), whereas the relevant experimental information is absent.

The calculated kinetics of Xe and He accumulation in fuel-to-cladding gap are compared with the experiment in *FIG. I*.

It is seen a good description of the kinetics for Pu45 rod and final release for Pu60. Essential difference in the releases between Pu45 and Pu60 at the first stage of irradiation is supposed in [4] to be due to higher portion of intergranular pores in Pu45, which contribute to the gas release and reduce the swelling rate. However the available data are insufficient for the further thorough analysis.

As for He, its volumes are somewhat underestimated due to underestimation of the release rate by a factor 2–3. However this discrepancy can be easily eliminated, for example, by increase of He diffusivity by a factor of ~5, which would be reasonable correction as He mobility is supposed to be higher than that for other nobble gases. However there might be other reasons related to, for instance, uncertainty in initial actinide composition in the fuel.

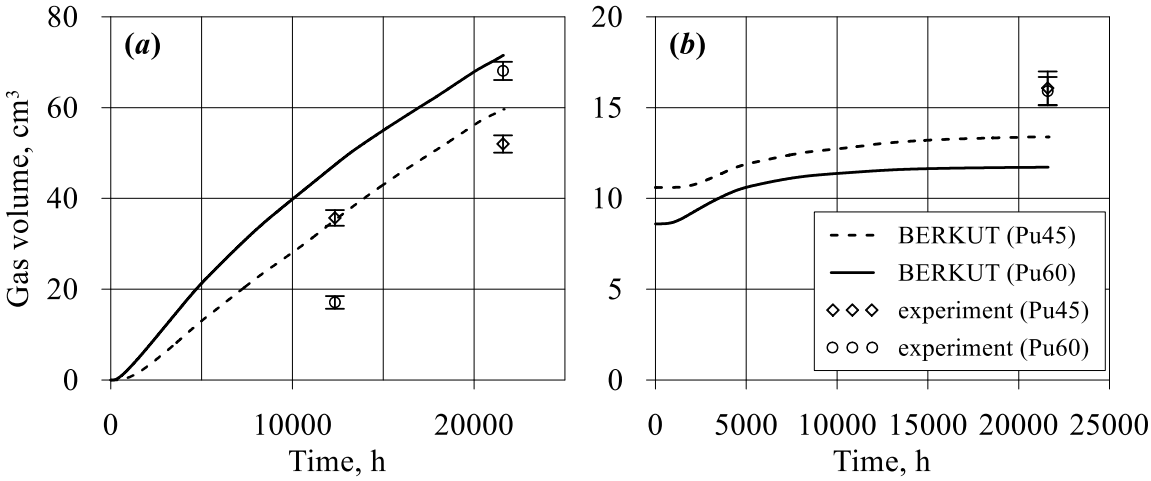

FIG. I. Nobble gas accumulation kinetics. (a) Xe + Kr, (b) He

The calculated axial profiles of fuel swelling are compared with the experimental data in *FIG. II*.

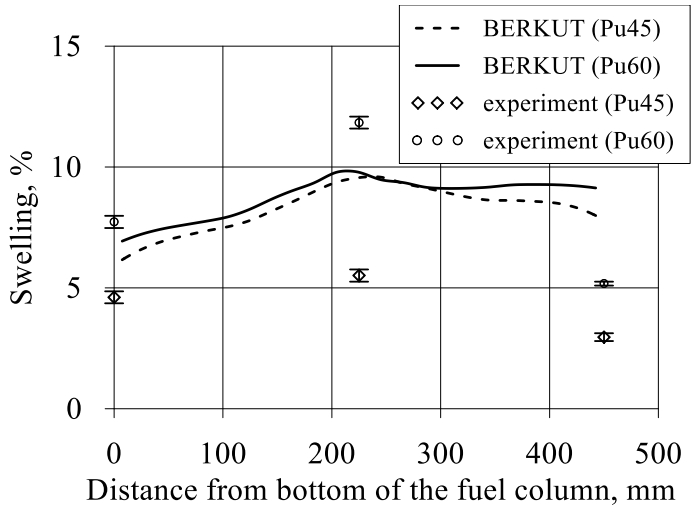

FIG. II. Final axial swelling profiles

It is seen, that BERKUT reasonably describes some average axial profiles, but the difference in swelling for Pu45 and Pu690 is underestimated. A possible reason may be the different character of the initial porosity in the two kinds of fuel; however this analysis is out of scope of the present paper. The same comments refer equally to simulation of porosity distribution along the pellets, see *FIG. III*.

The calculated Xe and Cs fractional contents in fuel were found to increase from pellet center to the periphery (from 74% to 84% for Xe and from 84% to 99% for Cs), in agreement with the observations.

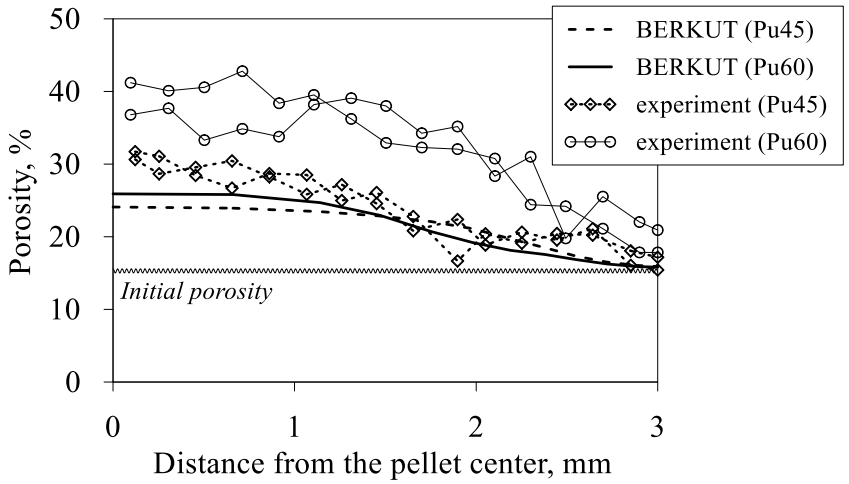

FIG. III. Final radial porosity profiles in the central section of the rods

3.2. KETVS-1 test

Simulation of the nitride rod behavior in KETVS-1 assembly in BN-600 is illustrated in this section. The assembly included four rods with the fuel composition $U_{0.86}Pu_{0.14}N$ and initial porosity of 15% was irradiated during 433 days at peak linear heat rate of 39.5 kW/m, the maximum burnup and irradiation damage doze being 5.46%FIMA and 55 dpi, respectively. Descriptions of the assembly and irradiation conditions are given in [5].

The calculations were performed with the value of parameter b_0 found in simulations of BORA-BORA test (see the previous subsection), the rod geometry and time dependence of the heat rate were close to the experimental ones. Due to uncertainty for the pellet size within the tolerance limit comparative calculations were performed with the lesser pellet diameter by 0.1 mm in comparison with the nominal one; below this calculation variant will be referred to as CT-variant (contrary to NM-variant for the nominal pellet size). Below comparisons of the calculated and measured values are given in the dimensionless form.

In *FIG. IV* dependences of pellet dimeters, d_{pel} on distance, Z, from the fuel column bottom are plotted. It is seen that both calculation variants are in a good agreement with the experiment; however the NM-variant seems to be more preferable. Near the same agreement has been found comparing calculated and measured values of fuel swelling.

The calculated and measured final values of the fuel-to-cladding gap are compared in *FIG. V*. Similarly to the pellet size calculations, the basic variant NM better agrees with the experiment than the CT-variant.

In *FIG. IV* the calculated kinetics of gas volume in the fuel-to-cladding gap is shown. It is seen that BERKUT provides good overall description of the gas release; however the release variation for different rods is somewhat underestimated.
Radial profile of intragranular porosity calculated for the maximum burnup section of rod 64 (the central rod in the assembly) is shown in *FIG. VII*. A good agreement with the measurements is demonstrated. Note that this result was attained without any additional code tuning as the only varied code parameter, b_0, was fitted to the gas release in another test (BORA–BORA).

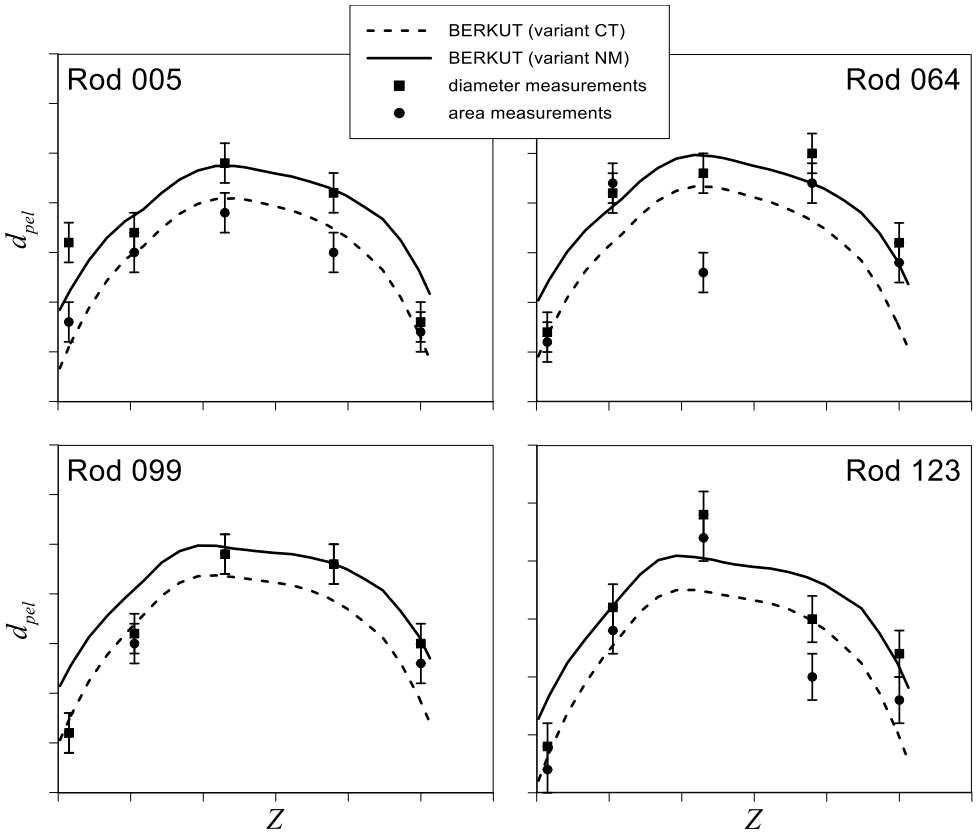

FIG. IV. Axial profile of the pellet diameter

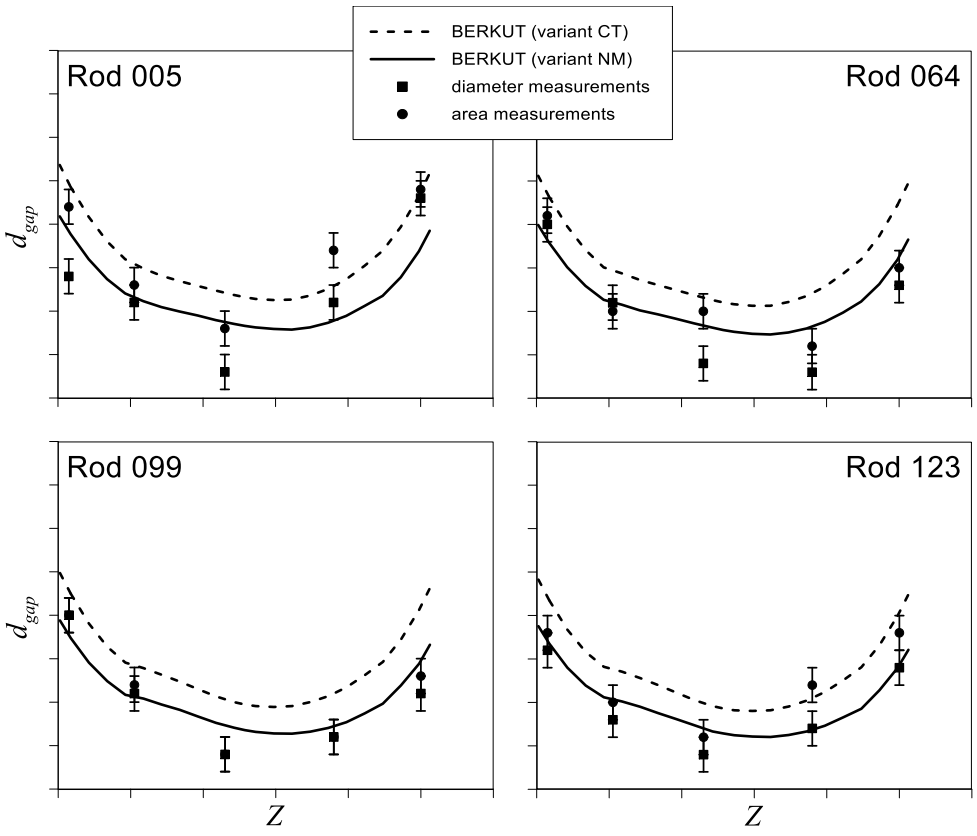

FIG. V. Axial profile of the fuel-to-pellet gap

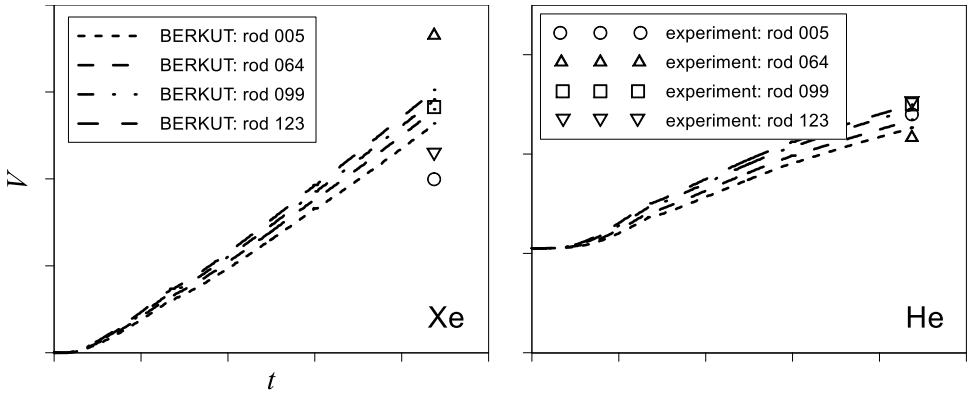

FIG. VI. Kinetics of gas volume in the fuel-to-cladding gap (NM-variant)

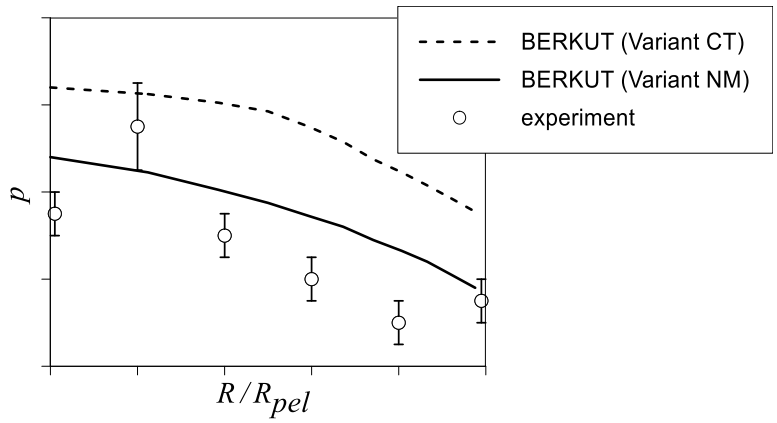

FIG. VII. Radial profile of intragranular porosity in the maximum burnup section of rod 64

4. Conclusion

The new best-estimate single rod code BERKUT is presented in this paper. The code was elaborated on the base of mechanistic code SFPR and inherited its particular models extensively validated against analytical and in-pile tests, in which the normal and off-normal conditions were simulated including severe accidents in thermal reactors. The models incorporated in BERKUT were extended to irradiation conditions in FR and to nitride fuels. The mechanistic approach bases on contemporary theoretical description of mechanisms governing basic physico-chemical processes in fuel rods under irradiation allows increased predictive ability of the code in comparison with the engineering analogs based on empirical correlations, especially in simulations of accidental conditions.

The thorough validation of BERKUT models is presently initiated, especially concerning to nitride fuels. The first example of this activity on the base of available observations is presented in this paper illustrating advantages of the theory based approaches. Further activity in this direction is in prospect; the validation is foreseen to be essentially extended as the new experimental data are available.

References

[1] AVVAKUMOV, A.V., et al., Coupled calculations for the fast reactors safety justification with the EUCLID/V1 integrated computer code, (Proc. Int. Conf. FR-17, Ekaterinburg, 2017), Contributed Papers.

[2] VESHCHUNOV, M.S., et al., A New Mechanistic Code SFPR for Modeling of Single Fuel Rod Performance under Various Regimes of LWR Operation, Nucl. Eng. Design **241** (2011) 2822.

[3] VESHCHUNOV, M.S., et al., Development of the advanced mechanistic fuel performance and safety code using the multi-scale approach, Nucl. Eng. Design **295** (2015) 116.

[4] ROGOZKIN, B.D., et al. Results of irradiation of $(U_{0.55}Pu_{0.45})N$ and $(U_{0.4}Pu_{0.6})N$ fuels in BOR-60 up to ~12 at.% burn-up, J. Nucl. Mater. **440** (2013) 445–456.

[5] VASIL'EV, B.A., et al. Support of the irradiation conditions of the nitride fuels in the experimental assembly of BN-600 reactor. (Proc. IV Int. Conf. "Innovative projects and technologies of nuclear energetics", Moscow, September 27–30, 2016) 274–280; TROYANOV, V. M., et al., Program and results of reactor tests of mixed nitride fuel for fast reactors, Atomic Energy **118** (2015) 96–100.

[6] VESHCHUNOV, M.S., et al., Development of mechanistic code MFPR for modelling fission product release from irradiated UO_2 fuel. Nucl. Eng. Design **236** (2006) 179.

[7] VESHCHUNOV, M.S., et al., Mechanistic modelling of urania fuel evolution and fission product migration during irradiation and heating. J. Nucl. Mater. **362** (2007) 327.

[8] MATZKE Hj., Fundamental aspects of inert gas behaviour in nuclear fuels: oxides, carbides and nitrides, NATO ASI Series **279** (1991), 401.

[9] THETFORD R., MIGNANELLI, M., The chemistry and physics of modelling nitride fuels for transmutation, J. Nucl. Mater. **320** (2003) 44.

[10] WEINSTEIN, M.B., DAVISON, H.W., A fission gas release correlation for uranium nitride fuel pins, NASA TN D-7401 (1973) 6

[11] RUFEH, F., OLANDER, D. R., PIGFORD, T. H., The Solubility of Helium in Uranium Dioxide, Nucl. Sci. Eng. 23 (1965) 335.

[12] VESHCHUNOV, M.S., TARASOV, V.I., Modelling of irradiated UO2 fuel behaviour under transient conditions, J. Nucl. Mater. **437** (2013) 250.

[13] RONCHI, C., ELTON, P.T., Radiation re-solution of fission gas in uranium dioxide and carbide, J. Nucl. Mater. **140** (1986) 228.

[14] MATTHEWS, C., SCHWEN D., KLEIN, A.C., Radiation re-solution of fission gas in non-oxide nuclear fuel, J. Nucl. Mater. **457** (2015) 273.