# Results of First Step in the Development of PIN2FRAS Computer Code Coupling

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## 1. Objective of the Work and Brief History

- 1997: Work started by innovation of RIA related part of the FRAS code – help of Mr. Volkov during his stay in NRI;
- 1999: Innovation of HiBu models of the PIN code, v.99 available from NEA – help of Mr. Strijov during his stay in NRI;
- 1999-2002: Developed, programmed and optimized mechanistic FGR diffusion model (stand alone and included into PIN2001);



Figure 1. Cumulative FGR at ramp and isothermal annealing temperature of 1500°C on a stepwise depressurization from 100 to 10 MPa



Figure 2. Cumulative FGR at ramp and isothermal annealing temperature of 1500°C

- 2000-2001: Definition and development of PIN2FRAS interface – draft presented in Park City ANS Top Fuel Meeting 2000;
- 2003: First version of interface finalized and tested at the NRI Rez – cooperation of Mr. Volkov, Mr. Strijov.

#### 1.1. PIN Innovations

- Authorized (RRC KI) cladding creep correlation for Zr1%Nb is fixed in the code;
- Mechanistic fission gas release (FGR) model for steady-state and transient modes included as input option;
- The FGR model was extended for high burnup UO<sub>2</sub> and for MOX fuel types (plutonium heterogeneity modeling);
- Models for local power and burnup radial distributions were added;
- Models for local fuel porosity at high burnup and the thermal conductivity correlation were chosen;
- Athermal FGR model for high burnup was fitted.
- 1.2. Mechanistic Fission Gas Release (FGR) Model (Valach, Strijov, Zymák)
- Diffusion of gas atoms to the grain boundary, trapping of gas atoms by intragranular and intergranular bubbles,
- Resolution of gas atoms from these bubbles,
- Sweeping of gas atoms by grain growth,
- Fission gas release due to the intergranular bubble interconnection,
- Micro-cracking models FGR during ramp conditions.

### 1.3. Verification of FGR Model (1)

The data from annealing experiments, carried out with irradiated fuel (burnup – 37 MWd/kgU) in a high temperature and high pressure furnace, were used to study the influence of the external restraint pressure on bubble interlinkage at the grain boundaries during very fast transients, Figure 1, [1].

#### 1.4. Verification of FGR Model (2)

Isothermal irradiation test was used for validation of the model, Figure 2, [2].

#### 1.5. Power and Burnup Radial Distributions

At average pellet burnup higher than 40 MWd/kgU there is a steep increase of the local power density and local burnup in the pellet surface layer, which is caused by neutron resonance capture by <sup>238</sup>U transforming to <sup>239</sup>Pu, Figure 3, [3].

#### 1.6. Review of the Code FRAS – Transient Modelling

- Computer code FRAS was originally developed at the NRI Řež (Czech Republic);
- The code verification, application and modernization was based on the co-operation with the RRC Kurchatov Institute IRTM (Russia) as well as the new versions of this code for LOCA and RIA;
- Structure of the programme, main physical models and several examples of RIA simulations are described.

#### 1.7. FRAS Code Characterization

Set of partial differential equations describing main physical phenomena observed in nuclear fuel during postulated design accidents is solved by the finite differences method, using implicit, explicit or Crank-Nicholson approach in various loops and modules as it was proven by practice. The code comprises following modules and models:

- Channel thermal-hydraulics;
- Heat transfer and time-space temperature distribution in all regimes;
- Stress-strain field in all fuel rod components up to the loss of geometry;
- Inner gases mixing and axial transient flow;
- Cladding high temperature oxidation and hydrogen release;
- Cladding ballooning and rupture using the theory of large deformations and mechanical state equations;
- Thermal and physical properties library of water, steam, gaseous fission products and technological gases;
- Mechanical properties libraries relevant for the WWER fuel and PWR type of fuel rods.

#### 1.8. Simulations Using PIN2FRAS

The burnup-dependent fuel characteristics, received from PIN through the newly developed interface, allowed the analysis of WWER fuel transient (RIA like) behaviour at different burnups. The calculations were performed at level of energy deposition which allows us to analyse fuel degradation effects for different burnups without a substantial influence of cladding overheating.

The accident begins at hot zero power conditions. The axial power distributions correspond to the axial burnup profiles at the time of an accident. The computations were performed with rod 7 from FA-222 of the Kola-3 NPP.

# 1.9. Calculation of NPP Kola Fuel Rod FA-222 (5-Year Cycle), Corrected Data

The calculation of NPP Kola fuel rod FA-222 (5-year cycle), corrected data, is shown on Figure 4.

#### 1.10. Stored Energy and Temperature Response vs. Time

The stored energy vs. time is shown on Figure 5 and the temperature response vs. time is shown on Figure 6.

#### 1.11. Inner Gas Pressure and Cladding Stresses (Axial, Hoop) vs. Time

The inner gas pressure vs. time is shown on Figure 7 and cladding stresses (axial, hoop) vs. time is shown on Figure 8.



Figure 3. Comparison between predicted and measured Nd concentrations



Figure 4. Power history for fuel rod 007 in FA-222



Figure 5. Stored energy vs. time



Figure 7. Inner gas pressure vs. time

# 2. Closing Comments

In frame of Project sponsored by MTI of CR and in first phase of our engagement in FUMEXII Project following results were achieved:

- Innovation of PIN code for HiBu domain;
- Innovation of FRAS code for burnt fuel transient simulation;
- Development and optimization of mechanistic FGR model;

Design of PIN to FRAS (PIN2FRAS) interface;

- Testing and validation runs of PIN2FRAS coupling on tentative RIA like accident superposed to the KOLA (FA 222, pin 007) irradiation history;
- Testing of PIN with built in diffusion FGR model;
- Testing of PIN2FRAS with/without diffusion FGR model.

Further engagement in FUMEXII is under discussion in view:

· How to find capacity to simulate all cases and



Figure 6. Temperature response vs. time



Figure 8. Cladding stresses (axial, hoop) vs. time

to innovate main models to achieve reasonable agreement with experiments?

 What is more effective - to use in-house PIN2FRAS or the newest TRANSURANUS version in synergy with ITU development team?

# References

- [1] S. Kashibe, K. Une. Effect of External Restrain on Density Change and Fission Gas Release in  $UO_2$  Fuels. Enlarged Halden Programme Group Meeting, Lillehammer, March, 1988.
- [2] H. Zimmermann. Investigations on Swelling and Fission Gas Behaviour in Uranium Dioxide. J. Nuclear Materials, 75, 154-161, 1978.
- [3] T. Matsumura, T. Kameyama. Burnup and Plutonium Distribution Near the Surface of High Burnup LWR Fuel. IAEA, IWGFPT/32.