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Development of the advanced mechanistic fuel performance and safety code using the multi-scale approach

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ABSTRACT

The SFPR code designed for mechanistic modeling of single fuel rod behavior under various regimes of LWR reactor operation (normal and off-normal, including severe accidents), is under development at IBRAE during the last two decades and currently, being extended to Fast Reactors, serves as a prototype for a new mechanistic fuel performance code BERKUT. The SFPR meso-scale models include an extended set of microscopic parameters, characterizing the crystal defect structure, thermo-physical and thermo-chemical properties of irradiated fuel. Increasing computational capabilities and rapid development of effective interatomic potentials allow micro-scale representations of the materials and physics to inform – via meso-scale code – the macro-level simulation. The first examples of atomistic calculations (by molecular dynamics and Monte-Carlo methods) of the key microscopic parameters for input in SFPR and BERKUT, validation of the modified code and application of the 3D finite element method for improvement and verification of the 1D thermo-mechanical model, are presented.

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1. Introduction

Nuclear fuel materials are exposed to complex thermo-mechanical and physico-chemical processes during manufacturing, operation and storage. The physics, chemistry and materials science of nuclear fuel materials are tremendously complicated by irradiation effects. That is why many commercial fuel performance codes

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incorporate empirical correlations to describe materials properties. The applicability of such correlations is limited to a regime where experimental data are available. Past attempts to extrapolate outside this regime have sometimes led to faulty predictions and costly engineering decisions.

To address these issues, a large number of models and codes have been developed all over the world to assess the properties of nuclear fuel materials. However, most assessments involve fitting of known data followed by extrapolations or interpolations into new temperature, pressure or irradiation regimes. There is an obvious need for a more theory based approach to develop a fundamental understanding of properties of nuclear fuel materials, leading to improved tools for predicting phenomena such as phase stability, heat transfer, species diffusion, and fission products (FP) retention.

The SFPR code (Veshchunov et al., 2011) for mechanistic modeling of single fuel rod behavior under various regimes of LWR reactor operation (normal and off-normal, including severe accidents) is under development at IBRAE. The code is designed by coupling of the two stand-alone mechanistic codes MFPR (for *meso*-scale modeling of irradiated UO_2 fuel behavior and fission products release, in collaboration with IRSN, Cadarache, Veshchunov et al., 2006, 2007) and SVECHA/QUENCH, or S/Q (for *macro*-scale modeling of fuel rod thermo-mechanical and physico-chemical behavior, in collaboration with FZK (Karlsruhe) experimentalists, Hofmann et al., 1997, 1999), intensively developed during the last two decades.

SFPR is currently under extension to Fast Reactors (FRs) and serves as a prototype for a new mechanistic fuel performance code BERKUT (Veshchunov et al., 2012), the constituent part of the multi-physics integrated code EUCLIDE (Alipchenkov et al., 2014) developed for safety justification of Gen-IV NPP within the Russian Federal Targeted Program "Nuclear Power Technologies of the New Generation for 2010–2015 and until 2020".

The MFPR *meso*-scale models include an extended set of *microscopic* parameters, characterizing the crystal defect structure, thermo-physical and thermo-chemical properties of irradiated fuel. Up to now, these parameters, which are grounded in the physics and chemistry of the materials (the main advantage of the mechanistic, theory-based approach), were tuned offering the extensive calibration of the code and then fixed without additional tuning in further applications of the code. However, the high sensitivity of the code predictions to values of the sometimes poorly known parameters was regarded as a serious disadvantage of the mechanistic approach, often criticized for this reason. This critical assessment has significantly impeded the development of mechanistic fuel codes all over the world.

An alternative approach is to get these parameters from supporting lower-length-scale simulations of microscopic phenomena (Stoller and Greenwood, 1998; Bacon et al., 2004; Stan et al., 2007). Increasing computational capabilities allow *micro*-scale representations of the materials and physics to inform – via *meso*-scale code – the *macro*-level simulation. Such multi-scale simulations of the key microscopic parameters for input in SFPR are based upon accurate atomic scale physics. Accordingly, the development of first principles informed mechanistic models will be significantly improved by advanced computing capabilities. The first examples of atomistic calculations, e.g. description of the damage formation in the fission tracks from molecular dynamics (MD) and Monte-Carlo (MC) models, estimates of the diffusion and recombination parameters by *ab initio* and molecular dynamics approaches, etc., resulting in the improvement of SFPR predictions for UO_2 fuel behavior under irradiation, are presented.

Consequently, the improved predictions of the meso-scale code MFPR for the fuel swelling and fission gas release, determining the pellet-cladding gap thickness and gas pressure, specify the boundary conditions for the thermomechanical module, which simulates the temperature distribution, local stresses and their evolution with time under irradiation and temperature conditions at the continuum (*macro*) scale (for real times of hours or longer). Some examples of the self-consistent operation of MFPR with the thermomechanical module SVECHA within the fuel performance code SFPR were presented in the previous publication (Veshchunov et al., 2011).

Further improvement of the key 1D thermomechanical models of SFPR and BERKUT can be attained using capabilities of the 3D finite element method (FEM) techniques. Once in the reactor, the fuel pins are subjected to severe radiation environments that continuously alter their thermo-mechanical properties. Mapping the local stresses and simulating their evolution with time under irradiation and temperature conditions at the continuum (*macro*) scale (for real times of hours or longer), using capabilities of the 3D finite element method (FEM) techniques, would help in improvement and verification of the key thermomechanical models of SFPR and BERKUT, as demonstrated by presented calculation results.

2. Meso-scale code MFPR

Any model that attempts a realistic description of fission-gas release and fuel swelling as a function of fuel-fabrication variables and in a wide range of reactor operating conditions must treat them as coupled phenomena and must include various microscopic mechanisms influencing fission gas behavior under irradiation and/or thermal treatment conditions. MFPR gives the common advantages of mechanistic modeling, first of all, concerning the realistic consideration of fission product (FP) behavior based on physically-grounded parameters (Veshchunov et al., 2006, 2007). The main outputs of the code are gas-bubble size and concentration (including intra- and intergranular bubbles and pores), chemical speciation of solid-phase FPs, point- and extended-defect characteristics, fuel oxygen potential, densification, swelling and FP release.

For steady irradiation conditions MFPR overcomes simplifications, accepted in the traditional Booth-Speight approach and resulting in an inadequate treatment of the gas atom transport at high temperatures (cf. a critical analysis of the traditional approach in Veshchunov and Tarasov, 2013), by a more consistent mechanistic modeling, taking into consideration the non-linear character of the gas atom transport equation associated with the gas atom trapping by intragranular bubbles. For adequate treatment of the mass transport in grains, MFPR self-consistently describes evolution of fuel micro-structure (point defects, such as vacancies and interstitials, and extended defects, such as gas bubbles, sintering pores and dislocations, their nucleation, evolution and interactions) (Veshchunov and Shestak, 2009), up to very high burnups, where the dislocation density significantly increases and evolves in the so-called High Burnup Structure (HBS) in the rim zone of fuel pellets. The additional analysis of the fuel porosity evolution under various regimes of UO_2 irradiation and further development of the key MFPR models was recently presented in (Tarasov and Veshchunov, 2014).

In accordance with the general approach to consideration of FP release from irradiated UO_2 fuel, it is shown in MFPR that the gas arriving at grain boundaries saturates the grain boundaries through a network of interconnected bubbles, as observed at elevated temperatures (usually, above $\approx$1400 °C) under in-pile irradiation. However, on the basis of self-consistent consideration of the effects of atom diffusion over the grain surface, their trapping by and irradiation-induced re-solution from intergranular bubbles, the MFPR predicts a noticeable gas release from UO_2 fuel without visible interlinkage of grain face bubbles, i.e. at a very low grain-face coverage, below the saturation threshold (Veshchunov and