# Multi-scale approach to advanced fuel modelling for enhanced safety

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**Abstract:**
The activities on fuel behaviour modelling using the multi-scale approach, carried out at IRSN and PSI, are described. The perspective of the two organizations on already acquired and potential future advantages from mutual application of the micro-, meso- and macroscopic simulations for fuel reliability and safety is presented. Finally, the conclusion is put forward regarding the merit to further develop the multi-scale approach to fuel behaviour modelling at IRSN and PSI.

## 1. INTRODUCTION

Understanding the thermo-mechanical behaviour of complex systems such as nuclear fuels is more and more based on a detailed description of mechanisms that involve a hierarchy of spatial (from nm to microns) and temporal (from picoseconds to tens of years) scales. In this context, the multi-scale methodology is highly developed in material science. It aims to develop relevant models to describe the interaction between atomic scale, micro or nanostructure and macroscopic behaviour. This approach requires a good understanding of the theoretical methods (statistical physics, diffusion and rate theories for atomic-scale objects, as well as macroscopic thermo-mechanics of the continuum materials) and the experimental ones (X-ray diffraction or neutron, local or global mechanical and thermal measurements) used to characterize systems at different scales. The overall objective is to achieve, by building bridges between spatial and temporal scales, the understanding of the macroscopic behaviour of materials. For example, from the nanoscale interatomic interaction description, based on the electronic structure determination with a relevant and possibly adjustable precision, it is possible to identify the basic mechanisms involved in the phenomenon under study at scales less than a nanometer and nanosecond. Then, deducing effective mechanisms (e.g. diffusion), it is possible to move to higher scales (distance and time) and connect the microscopic approaches and continuous approaches (elastic, plastic and creep deformation, fuel material dimensional change, fission-gas release, etc). Finally, the events identified and their characteristics can be used to feed simulation software used to better understand the evolution of "realistic" materials at the macroscopic scale during their entire life. These programs are generally based on approaches of “continuum” type and are based on simplified behavioural models.

As part of study of complex materials, the use of multi-scale approaches became very promising if one wants to be predictive, with a consideration of finer material complexity and required accuracy in the characterization of their behaviour, while the full macroscopic tests are extremely expensive and therefore limited in numbers. If one wants to understand and explain the phenomena governing the behaviour of these materials at macroscopic scale or predict the evolution of their properties, it is essential to exploit data from the microscopic scale and provide feedback to mesoscopic and macroscopic ones. A study at the atomic

scale can not only identify the predominant mechanisms considered at the upper level, but also feed the model with parameters very difficult to obtain experimentally. Indeed, fuel behaviour codes are becoming more accurate and predictive as they are based on increasingly mechanistic models, but assume thereby more parameter to determine and validate. From a scientific point of view, the challenge is multifaceted: first of all, it is to be identified what the relevant phenomena for one macroscopic characteristic, and the scale at which this phenomena must be studied are. Then, the different scales of interest should be connected, making sure that the same physical phenomena are not taken into account several times (once effectively hidden in the mesoscopic approach, and a second by an additional term directly from atomistic approaches for example).

The aim of this document is to outline how this multi-scale approach to the nuclear fuel behaviour simulation has been utilized at IRSN and PSI to improve fuel behaviour modelling.

## 2. CONTEXT AND SCIENTIFIC METHOD

### 2.1 Macroscopic scale

The objective of the multi-scale approach applied to the study of pressurized water reactor fuel behaviour is to provide modelling tools to simulate the macroscopic behaviour of the fuel throughout its life cycle, i.e. in normal and accident conditions, and also during transport and storage. These tools are essential for the safety analysis and also help to interpret and analyze the full scale experiment results that are available (SCIP, CIP, FGD, Halden, NSRR, etc. ). These computer codes, called fuel performance codes, reproduce the global thermomechanical behaviour of one or more fuel rods. In particular, they calculate the time evolution of temperature, mechanical stresses, deformation and oxidation of the fuel cladding elements based on power levels and thermal-hydraulic conditions (temperature, nature and flow of the coolant), that they are subject to. In general, they also provide information on the behaviour of fission gases (fission gas release, bubble and pore formation and evolution, etc). Currently, most fuel codes, and in particular those used in the field of safety, work with correlations based on the burnup, adjusted on available experimental data. The validity ranges of these models are in fact limited to the experimental data used to define these relationships, and any extrapolation to new materials or new fuel loading schemes is prohibited. In addition, experimental data often present a relatively high dispersion for a given burnup. Indeed, the fuel micro-structure and therefore all its thermomechanical properties can be quite different depending on the irradiation history and the power and temperature to which it was submitted. For example, fuel cracking, fission gas distribution inside the fuel pellet are very closely related to the levels of temperature and neutron flux to which the fuel has been exposed to. Also, the correlations used did not allow for a very accurate modelling of fuel behaviour.

### 2.2 Mesoscopic scale

To meet the previous challenges and extend their validity domain, fuel codes tend to change, and the old correlations were replaced by physical models that explicitly take into account the evolution of the fuel microstructure. Given the very small size of the microstructural heterogeneities compared to the size of the modelled fuel rods, it seems inconceivable at present to simulate directly the microstructural evolution of a whole reactor

core. The difficulty is twofold. It is on the one hand to find equivalent behaviour laws for fuel, which allow – from a given microstructural distribution, – to determine the properties of the fuel, and on the other hand, to be able to determine the temporal evolution of the microstructure. On the first point, it is the objective of scaling methods in general and micromechanical homogenization in particular. On the second point, it is solved by the development of new computer codes, called mechanistic codes. These codes are designed to a comprehensive and accurate modelling of all the mechanisms occurring at the mesoscopic scale. They are focused on phenomena taking place at scales ranging from a few tens of microns (the size of a fuel grain) to a few millimeters (a fuel pellet ) and of the order of a millisecond up a few tens of seconds. Models are usually based on mean-field approaches. These new computer codes allow on the one hand to explore conditions of operation much broader than those of fuel codes, and on the other hand, they are valuable tools for interpretation and definition of experimental programs, particularly for analytical tests. Finally, they provide a scientific basis for the development and validation of simplified physical models used by macroscopic fuel codes. Another type of modelling approaches allows studying the evolution of the microstructure beyond the mean-field models: kinetic Monte Carlo approaches, accelerated molecular dynamics, phase field approaches, and dislocation dynamics, for example.

It is important to note that all these mesoscopic approaches requires coupling and that these approaches should not be separated. The mechanical properties, the microstructure, the fission products behaviour, the nature of the phases, all of these are intrinsically interrelated: the microstructural evolution explicitly depends on the temperature and stress which are obtained via the behaviour laws dependent on the microstructural state. Although it may seem tempting to link the microstructural and micromechanical approaches (coupling of a mean-field code and a thermomechanical code for example), such a coupling is complex to implement and could lead to prohibitive computation times. It is therefore appropriate at this time to estimate the relevance of any coupling with respect to a simple chaining or even the use of codes at the lower level to provide more relevant models to the next level as it is currently the case.

All these mesoscopic models are based on microstructural data (fission gas pressure, surface tension, characteristics of the populations involved, and diffusion coefficients). These data can be obtained by two different ways:

- by experimental microstructural characterization techniques such as adsorption microstructural analysis, scanning electron microscopy (SEM), transmission electron microscopy (TEM), wavelength dispersive X-ray spectroscopy (WDS), energy dispersive X-ray spectroscopy (EDS), micro-XRD, and more recently the secondary ion emission spectroscopy (SIMS), elastic recoil detection analysis (ERDA), micro-indentation or tomographic probe. Although more efficient, these approaches do not allow access to all parameters. In addition, the need for these studies on hot cells for nuclear materials greatly limits the amount of available data;

- by simulations at the atomic scale, those describe the interatomic interactions. This description includes the so-called *ab initio* approaches as well as the lighter but parameterized ones such as the tight-binding method which allows modulating the level of description necessary for the proper treatment of the problem discussed.

These are atomistic simulation approaches that are describe below.

## 2.3 Microscopic scale

### *2.3.1 Needs*

As part of the multi-scale approach, the calculations at the atomic level concern nanometric systems for periods of picoseconds to milliseconds. These approaches allow:

- To access the value of parameters needed for mesoscopic modelling (phases identification, solubility, stress calculations and local pressure, diffusion coefficients, microstructure thermomechanical properties);

- To identify and clarify the preponderant physical mechanisms at the mesoscopic scale and thus specify mechanistic models to be introduced in mesoscopic codes or even more simplified models used by macroscopic fuel codes (e.g. thermal or athermal fission gas bubble resolution);

To identify the stable phases of a system amounts to identify those with lower free energy at the considered temperature. Two variables appear fundamental: the internal energy of the system and its entropy, which formally allows taking into account the temperature effects.

### *2.3.2 Internal energy calculation*

The internal energy can be obtained in quantum mechanics by solving the Schrödinger equation $H \Phi = U \Phi$, where H is the Hamiltonian of the system, U its internal energy and $\Phi$ the wave function which characterizes the system state. Analytically, this equation can be solved only for two particles. Therefore, the internal energy determination of complex systems requires various approximations that lead to many more or less accurate methods. The first approximation is made on the nucleus and electron movement separation due to the difference in mass and hence speeds of both types of particles (Born-Oppenheimer approximation). The system is thus reduced to a system of movable nuclei in an electronic medium energy field if one is interested in the dynamics of the nuclei or to an electron system in the field of fixed nuclei if one is interested in electrons. In practice, it decouples the dynamics of nuclei and electrons. The second approximation concern the description level of the interaction that binds the nuclei together and for which there are three main methods:

- The first are methods of electronic structure called “first principle” (or *ab initio*), including in particular the density functional theory (DFT). They consist to solve the electronic Schrödinger equation with an approached Hamiltonian. These methods are accurate but very computational resource and time consuming;

- Then there are the methods of parameterized electronic structure, including in particular the Tight Binding method (TB). In this case, the parameters used are the atomic orbital energy levels, and the integrals describing the electron delocalization. These parameters are adjusted on experimental data or DFT calculations. This type of method allows a calculation of localized electronic structure calculations less accurate than " first principle” ones but much faster;

- Finally, the methods of semi-empirical potentials equate the nucleus with its electron cloud to one single particle. These particles interact with each other by means of a potential describing overall atomic interaction. The internal energy of the system is then expressed as an analytic function dependent on the distance and angle between the constituent particles. This expression is determined based on experimental results and / or results of "first principle" methods. These methods are much faster

than the methods of electronic structure and, therefore, allow a greater number of atoms to be considered. However, they are less precise and *a priori* non-transferable to other systems than those on which their parameters have been adjusted.

The minimization of the electronic energy allows to determine the stable phases, the energy of a chemical reaction (or creation of defects), the barriers to chemical or diffusion reaction and thus the migration mechanisms. It also calculates material thermal, optical and mechanical properties. However, these simple minimization methods do not allow to accurately reflecting entropic contributions and therefore the temperature effects. They are also expensive in computation time and therefore difficult to apply to large systems (greater than a few hundred atoms).

### *2.3.3 Temperature effect*

To access the physical parameters of a macroscopic system in temperature, it is necessary to take into account the entropic effects. For this, several methods exist, based on thermostatistical exploration of what is called the configuration space of a system, i.*e.* the space of different possible atomic configurations (position and velocity of each atom system). They enable to evaluate thermodynamic averages. Two kinds of thermostatistical methods are mainly used:

- Monte Carlo methods, also used in other fields of physics or science, where one draws lots of configurations and where the most relevant ones, *i.e.* the most probable ones are retained;

- Molecular Dynamics to simulate the evolution of the system over time and to explore areas of the phase space around the initial configuration.

In general, the thermostatistical study of the system requires the calculation of the internal energy for a very large number of configurations. It is therefore necessary to find a good compromise between a very accurate but expensive description of the electronic structure and the use of more analytical formulations, depending on the phenomena to be studied. In general, the system energy calculations in these approaches rely on the use of semi - empirical potential models, even if the calculation of direct electronic structure can sometimes also be used (Car Parrinello approach in particular). These simulation techniques at the atomic scale are used to deal with radiation, stress and temperature effects.

So, modelling materials can not be limited to “first principle" methods that are operational at the lowest level and reduced system complexity. The recommended approach is then to use the results of atomistic approaches to build the best possible interaction (semi-empirical) potential, realistic and tailored to the particular system studied. In this context a key protocol seems to be the following: *ab initio* electronic structure ➔ semi-empirical potential ➔ basic mechanisms (Molecular Dynamics) ➔ effective mechanisms ➔ large-scale processes (Kinetic Monte Carlo).

Figure 1 illustrates the global multi-scale approach applied to the case at the nuclear fuel rod. In the next section, we will develop some illustration of this approach IRSN and PSI in attempting to describe the initial results and to take a critical look at the developments at each of the scales.

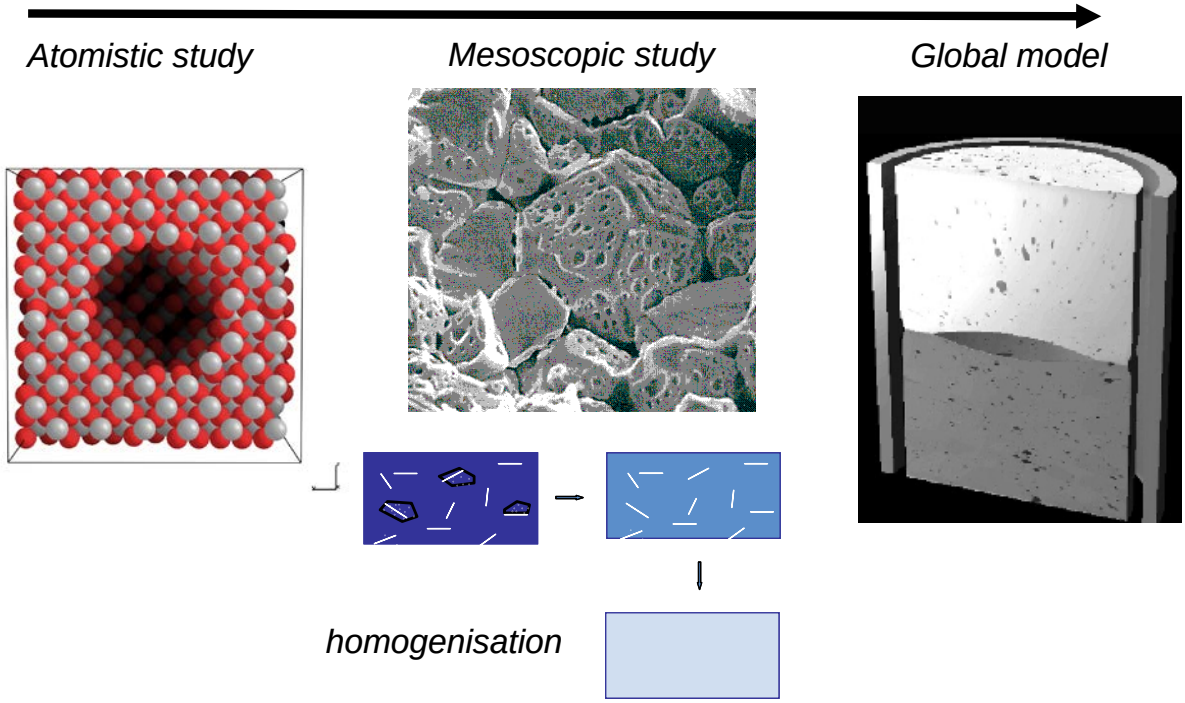


**Figure 1: Illustration of the fuel multi-scale modelling.**

## 3 MULTISCALE APPROACH DEVELOPPED IN IRSN AND PSI

### 3.1 Macroscopic models

We set up in the previous section the fuel codes in the multi-scale approach and, more generally, understressed their importance as support for safety expertise. They must allow:

- To be able to conduct a critical and technical analysis of the safety document offered by operators,
- To be able to study the behaviour of fuel under accidental conditions, particularly through the interpretation of experimental databases available,
- To maintain a strong scientific and technical competence in the field of nuclear fuel and physical mechanisms which it is registered,
- To capitalize the knowledge on the fuel behaviour;
- To have an operational chain of integrated computing codes (IRSN ESCORTE chain for example), if we consider the relationship between this code and the codes dedicated to the study of one type of accidental sequence (DRACCAR SCANAIR for example, as described below) .

*3.1.1 PSI experience: the FALCON fuel behaviour code*

3.1.1.1 Nominal conditions

From the PSI point of view, there are certain experimental data and modelling results showing a possibility of the considerable effects of the initial fuel rod state, particularly specific features of the fuel microstructure and characteristics of the retained fission gases, on the macroscopic rod behaviour during the transients. Sufficient knowledge of the initial conditions just mentioned, for the credible prediction of transient fuel behaviour, needs eventual detailed analysis of the base irradiation under nominal/normal conditions. This applies to fuel behaviour in both RIA and LOCA conditions [1][2].

Specifically, for the special experiments in the research reactors, using re-fabricated fuel samples, proper consideration should be taken of the effects of fuel pre-irradiation and re-fabrication. It seems to be particularly important because a lot of knowledge on the integral fuel behaviour during the RIA and LOCA, as well as verification and validation of the corresponding codes, have been acquired from the interpretation of the results of such experiments. Indeed, each individual case can be unique from the viewpoint of the radial distribution of the fission products and fuel structure, which therefore should be properly calculated and translated to transient calculation. Additionally, proper simulation of re-fabrication can be crucial for some results, e.g. for predicting the mutual fuel-stack and cladding elongation during the transient. To cope with this challenging issue of modelling, the new function has been recently developed for FALCON with the GRSW-A model, which writes the whole array of the integrated microscopic and macroscopic variables for each calculation node and time step of the base irradiation analysis into a binary file. When beginning the following calculation of the thermal transient, the variable arrays are ‘plugged out’ from the binary file in question for the predetermined life time – when the transient starts, – and a interpolation technique is applied to determine the array variables in the nodes of the new finite-element mesh, which now corresponds to the new rod re-fabricated from the mother rod after the simulated base irradiation (Fig.2).

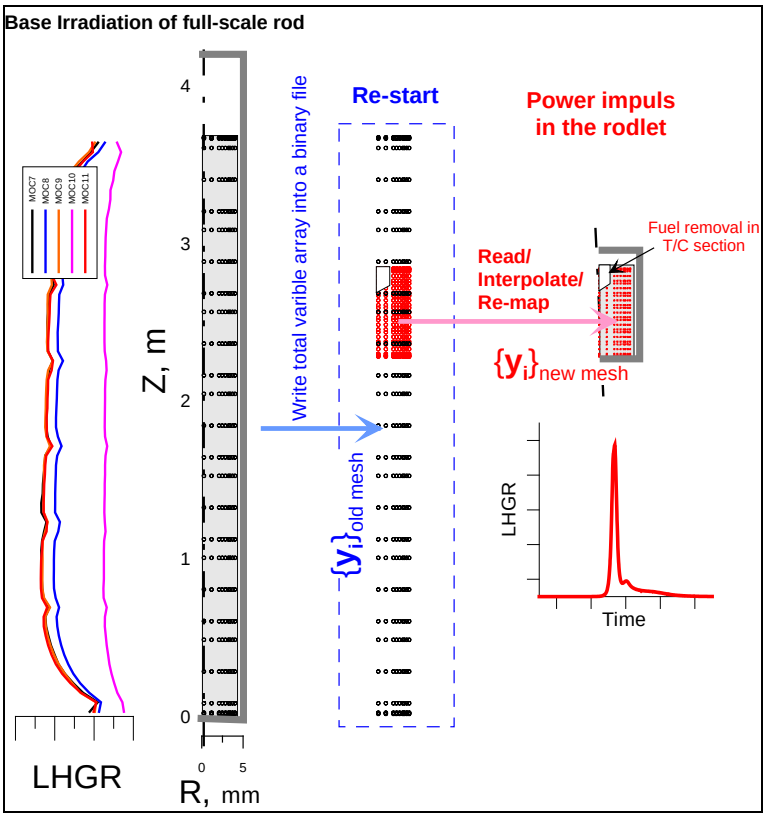


**Figure 2: Schematics of numerical simulation of the transient in a re-fabricated rod after the base irradiation using the new re-start function.**

### 3.1.1.2 Description of the FALCON fuel behaviour code

The FALCON code [3] is currently the main tool used in the Laboratory for Reactor Physics and System Behaviour of PSI for the fuel behaviour analysis. The FALCON code had been created by coupling of a code for steady-state analysis (ESCORE) and a fast transient code (FREY). The macroscopic analysis, namely the calculation of the thermo-mechanical characteristics of the integral fuel rod, constitutes the pillar element of the code. Other models have been developed and integrated into the code in line with the need of the main thermo-mechanical calculations, varying over the range of macro-, meso- and microscopic scales. Specifically, the FALCON code incorporates models for material properties, such as elasticity modules, thermal expansion coefficients, cladding anisotropy, heat capacity and thermal conductivity. The other group of models addresses prediction of physical processes, such as thermal expansion, fuel densification and swelling, porosity formation and migration, formation and development of the high-burnup structure (HBS), high-temperature fuel restructuring, the fission gas atoms kinetics, etc.

The solution processor of the FALCON code is based on the Finite Element Method (FEM), which allows for fully 2-D thermal and mechanical analysis. The cladding behaviour description covers a wide range of macroscopic effects, from elastic response to elastic-plastic-creep strain-rate dependent (viscoplastic) response in the high power and high temperature regimes. The models used in FALCON for Zircaloy cladding creep include dependencies on the time, temperature, stress, and fast-neutron flux, as well as the material metallurgical conditions. The 2-D finite-element analysis of the pellet-cladding contact in the FALCON code utilizes a special type of gap elements, characterized by a stiffness matrix that allow calculation of the normal and shear stresses as functions of geometric gap state

and intensity of PCMI. The variable stresses just mentioned are used for calculation of the parameters characterizing the current state of pellet-cladding interface, such as gap conductance, stick-slip condition, and friction forces. Fuel pellet cracking has been paid particular attention in the FALCON code, because this is an inherent behaviour of ceramic fuel pellets, which plays an important role in fuel relocation and fuel-cladding mechanical interaction. A thorough analysis of cracking, included in FALCON, considers the tension response curve with the phase of softening for the ceramic fuel material. Specifically, a smeared-cracking model is used in which the crack is viewed as a mechanism that changes the material behaviour from isotropic to orthotropic, where the material stiffness normal to the crack surface drops to zero while full stiffness parallel to the crack is maintained.

PSI has been using the FALCON MOD01 code as platform for its own method development. Specifically, a new model for fission gas release and gaseous swelling of uranium dioxide fuel has been developed and integrated into the FALCON code at PSI [4]. The GRSW-A model predicts macroscopic characteristics of fuel state by analyzing meso- and microscopic processes occurring in the elements of fuel material. Represented in the model are:

- The group of microscopic intra-granular processes, including the kinetics of point defects in the lattice and gas mono-atoms diffusion, as well as nucleation, migration, coalescence, trapping, irradiation-induced resolution and point-defect-diffusion-controlled growth of the gaseous bubbles;

- The group of microscopic and mesoscopic processes related to the grain boundaries of the fuel, viz., formation and growth of the large gaseous pores resulting in grain-boundary swelling and FGR into the free volume of the fuel rod.

The latter group of phenomena is described in the GRSW-A model using an original dynamic approach. Additionally, both intra- and inter-granular behaviour are considered as closely linked with the phenomena of intra-granular fuel restructuring (polygonization) and high-burnup structure (HBS) formation under low-temperature irradiation, as well as with the process of equiaxed grain growth under higher temperature. These phenomena have been simulated in the GRSW-A models using the phenomenological model based on mesoscopic approach. Furthermore, a special model is devoted specifically to describe the as-fabricated intra-granular pore behaviour, which is related to the macroscopic effects of low-temperature irradiation-induced densification and high-temperature sintering.

Finally, the calculated characteristics of the micro-structural state of the fuel are used to predict the macro-characteristics of the fuel pellets – directly used by the FALCON code analysis, – such as porosity, swelling and FGR. The general approach to coupling of the model with the integral fuel behaviour analysis is illustrated by the flowchart in Fig. 3. On the one hand, the GRSW-A analysis utilizes variables calculated by FALCON, viz., temperature, temperature gradient, external pressure and fission rate in the fuel material elements of interest. At the same time, there are a number of explicit and implicit feedback-effects of GRSW-A analysis on the results of the FALCON calculation through that the model returns a number of variables used by the fuel behaviour code, namely, distribution of fuel porosity over the pellets affecting fuel thermal conductivity, distribution of fuel swelling due to both solid and gaseous fission products (gas mono-atoms, gaseous bubbles and intergranular pores), fuel element volumetric strains caused by densification and/or sintering of the fuel, which are governed by the evolution of the as-fabricated pores, as well as the effects of FGR from the fuel into the free volume of the fuel rod entailing reduction of the fuel-cladding heat conductance and increase in the internal gas pressure. Consequently, new micro- and mesoscopic effects have been introduced into the FALCON code after coupling with GRSW-A, which influence the macroscopic variables, such as volumetric strains in the fuel caused by the fission products, and result in the evolution of fuel porosity.

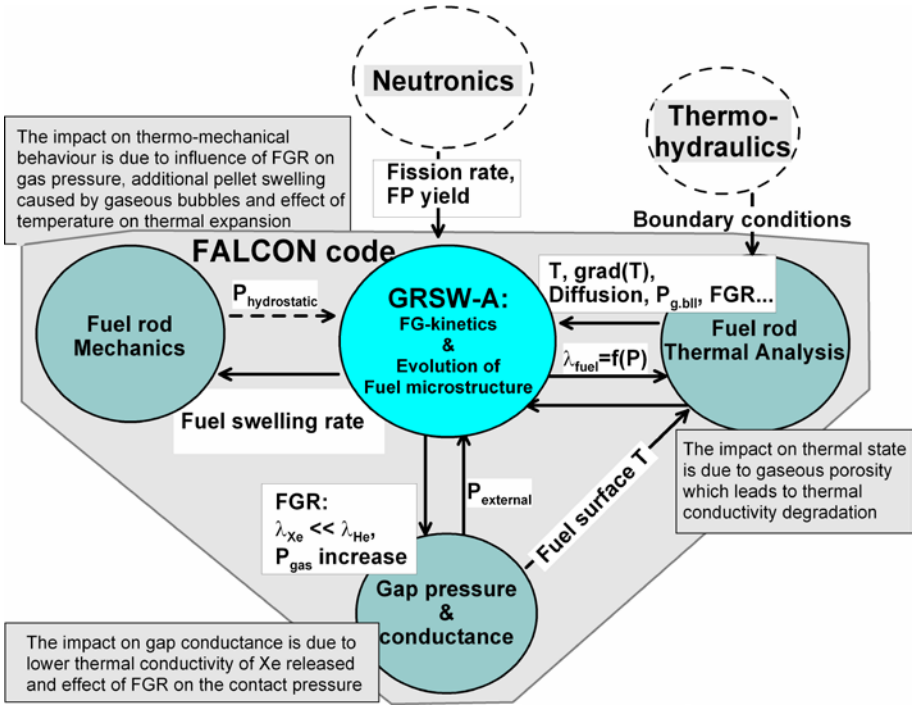


**Figure 3: Flowchart for FALCON and GRSW-A mutual feedback effects.**

### 3.1.1.3 Transient situation

As far as fuel rod behaviour modelling is concerned, so far the same code, FALCON version MOD01 coupled with the GRSW-A model, is used at PSI for the analysis of both base irradiation and the transients, such as power ramps, RIA and LOCA, which is based on the appropriate capabilities of FALCON and the GRSW-A model. At present, the verification and validation (V&V) matrix of the coupled FALCON/GRSW-A code, includes more than 30 single-effect experiments used for V&V of the GRSW-A model as a sand-alone code, and ca. 115 cases for validation of the integral analysis, as outlined in Table 1 [4].

However, the code prediction for fuel behaviour under the RIA and LOCA is, to very large degree, dependent on the adequacy of the boundary conditions assumed in the calculation, particularly the thermo-hydraulic ones. Except a limited number of types of nominal bundle conditions, or simple single rod experiments, – where the built-in thermo-hydraulic models of the FALCON code, or test-specific models [5][6] are applicable, a close coupling to large system codes would be necessary for application of FALCON to analysis of real LOCA and RIA. Yet, such integration is not available at PSI, and corresponding work has been currently planned.

**Table 1: Verification and Validation matrix for coupled FALCON/GRSW-A**

| Item No. | Description | Num. of data sets |
|---|---|---|
| **Stand-alone model verification** | | |
| 1. | Tests on algorithm robustness and numerical stability | - |
| 2. | Verification of the results against theoretical solutions, i.e. for:<br>- the concentration irradiation-induced point defects;<br>- the radius of gaseous bubbles;<br>- the total balance of the fission gas;<br>- grain-faces fractional cover after the saturation of the porosity-growth. | 4 |
| 3. | Intra-granular FGR after steady-state irradiation to medium burn-up in function of temperature | 1 |
| 4. | Intra-granular porosity in a pellet rim in function of local burn-up | 3 |
| 5. | Concentration of matrix Xe in pellet rim in function of burn-up | 1 |
| 6. | Total concentration of Xe in the pellet rim | 1 |
| 7. | Verification against the data of tests on post-irradiation annealing for:<br>- characteristics of intra-granular porosity;<br>- FGR;<br>- characteristics of inter-granular porosity. | <br>20<br>3<br>1 |
| **Integral experiments** | | |
| 8. | Selected cases of FUMEX-2 | 2 |
| 9. | Cases of FUMEX-3 | 53 |
| 10. | KKL/PSI data on FGR in high-burnup fuel rods (in progress) | 34 |
| 11. | Pellet swelling during base irradiation to high-burnup | 1 |
| 12. | Power ramps with high-burnup fuel-rod-segments within SCIP project | 10 |
| 13. | NSRR /RIA: LS-1,2,3, FK-1, VA-1 | **6** |
| 14. | CABRI/RIA: CIP0-1, CIP3-1 (blaind calculation) | **2** |
| 15. | HRP/LOCA: IFA-650.3/4/5/7/9/10/12/13/(14) | **8** |

*3.1.2 IRSN experience*

IRSN has chosen not to develop simulation code on the fuel behaviour under nominal situation, but to use the FRAPCON code and to participate in its future development. Concerning fuel behaviour modelling under LOCA or RIA accidental situations, IRSN develops its own tools that are SCANAIR and DRACCAR. All these codes will now be briefly presented.

3.1.2.1 FRAPCON

FRAPCON is fuel behaviour modelling code developed for the NRC (Nuclear Regulatory Commission) by the Idaho National Engineering Laboratory and the Pacific Northwest National Laboratory, on the basis of FRAP -S and GAPCON - THERMAL codes. It simulates the behaviour of the fuel during irradiation, during its operation at rated speed or during power ramps. It thus provides the temporal evolution of the characteristic of a fuel rod (temperature, rod and pellet geometry, fission gas release ...) . This code calculates the most important fuel rod thermomechanical quasi-steady state characteristics: temperature, pressure and rod strain, depending on the time, the linear power, and boundary conditions

(coolant flux). This code can also be used to determine the initial state of the fuel before it undergoes different power ramp or accidental situations such as LOCA or RIA.

The main physical phenomena modelled by the code are:

- as a thermal point of view, the conduction within the fuel and cladding and heat transfer between the fuel and the cladding and between the cladding and the refrigerant;
- as a mechanical point of view, the elastic and inelastic deformation of the cladding and the pellet-cladding mechanical interaction;
- as a physicochemical point of view, the fission gas releases, and the cladding oxidation, the internal rod pressure.

FRAPCON has become a tool of choice for the design and simulation of the behaviour of the fuel in nominal situation and to achieve the pre-calculations of accidental situations such as RIA or safety cases. It provided an opportunity to recalculate all father rods of CABRI REP Na tests and CIP campaigns. A SCANAIR FRAPCON interface has been completed and can be chained directly to the calculation of a pre and post accident state.

Finally, the use of FRAPCON could be extended to other issues as radiation at rated power: application to the study of safety interest in fuel transportation and storage, as well as the study of power ramps and extended intermediate power operation.

### 3.1.2.2 Transient codes

#### *3.1.2.2.1 SCANAIR*

The SCANAIR software is developed by the IRSN since 1990 in support of the expertise of the safety analysis of pressurized water reactors. It simulates the thermomechanical behaviour of fuel rod during transient accident and help evaluating their risk of rupture. In addition, the software is used to define, prepare and interpret transient experiments (especially those made in the Japanese reactor NSRR at ALPS programs ALPS2 and FGD and in the CABRI reactor for the REP-Na and CIP programs). Finally, the software should help to extrapolate these experimental results to the real reactor conditions. The kinetics of accidents can be considered to be fast (case of an accident caused by the ejection of a control rod for example - this is called RIA) or slow (if uncontrolled withdrawal of control rod for example when we talk about power ramp). Physical phenomena involved in these accidents have completely different characteristic times and adaptations are necessary so that the modelling is appropriate to the accident in question. Thus, until now, the software is suitable for the simulation of such RIA accident. However, versions which can handle other types of accidents (power ramp) are under development.

SCANAIR is used to:

• check the adequacy of safety criteria,

• make a consistent interpretation of all the experimental basis regards RIA and power ramp.

#### *3.1.2.2.2 DRACCAR*

The DRACCAR software (Déformation et Renoyage d'un Assemblage de Crayons Combustibles pendant un Accident de Refroidissement), is developed by IRSN to simulate the thermo-mechanical and thermo hydraulic behaviour of a PWR fuel rod assembly during a loss of primary coolant accident (LOCA). During such an accident, the vaporization of the cooling water leads to the drying of the fuel rods, the rod temperature increase, the cladding oxidation, the rod swelling and to the rupture of the cladding surrounding the fuel. Swelling of the claddings can cause a significant part of the core blockage and thus compromise the cooling ability. DRACCAR software aims to model a fuel rod assembly behaviour during an accident to assess the rate of closure due to the distorted rod and the impact on their cooling, taking into account the mechanical and thermal interactions between fuel rods. It allows a consistent interpretation of the entire experimental database whether geometry "single-rod" or "rod bundle" with real or simulated fuel. It also allows transposing to the reactor scale the phenomena involved with the validated results of these models.

#### *3.1.3 CONCLUSION*

In terms of radiation and transient codes we have seen that the necessary and relevant tools are available and the use of them (FRAPCON, SCANAIR, DRACCAR) is acquired. However, several deficiencies in FRAPCON modelling (creep model, gas model including HBS) must be filled so that the institute has a calculation chain performance, suitable for transient situations (SCC-PCI risk under PCC 2conditions, RIA) .

On the other hand, PSI has had considerable experience in application of the integral analysis of fuel behaviour covering the effects of base irradiation on the transient behaviour. As it seemed from the analysis of some experiments (e.g. RIA type transients with high enough inserted energy, and the recent Halden LOCA tests with high-burnup fuels), the detailed consideration of the fuel micro-structural state after the base irradiation may bring additional insights into the macroscopic fuel behaviour during the transients of interest. At the same time, the predictive analysis with the FALCON code for fuel behaviour in real RIA and LOCA needs close coupling with the integral system codes, which is currently not available, and is to be implemented in the future.

### 3.2 Mesoscopic models

#### *3.2.1 MESOSCOPIC APPROACH TO MODELING EFFECTS OF FUEL RE-STRUCTURING*

A treatment of the mutual effects of fuel restructuring during the base irradiation (e.g. formation of HBS) and slow power ramps (e.g. high-temperature assisted restructuring), integrated into the microscopic GRSW-A model for fission gas behaviour and fuel microstructural evolutions, represents an example of the use of a mesoscopic approach in the fuel behaviour simulation [4]. The two types of the fuel restructuring are considered in the GRSW-A model, namely: 1) equiaxed-grain growth (aggregation of grains) under high temperature and 2) intragranular polygonisation (subdivision of grains into sub-grains) taking place under a long enough irradiation at relatively low temperature. The equiaxed-grain growth generally takes place in the central region of the pellet, while the polygonisation is typical for the fuel at a pellet outer rim and known also as an appearance of the High Burnup Structure (HBS). These two models deal basically with the response of the grain structure to different regimes of irradiation temperature (e.g., base irradiation, power ramps and fast thermal transients in the pellet centre, mid-radius and periphery), and strongly influence other

parts of the GRSW-A model. The fuel grain and sub-grain dimensions as well as the fraction of the restructured fuel are the main output of the fuel restructuring model. The approach used by the GRSW-A model for description of the fuel grains and sub-grains is schematically shown in Fig. 4.

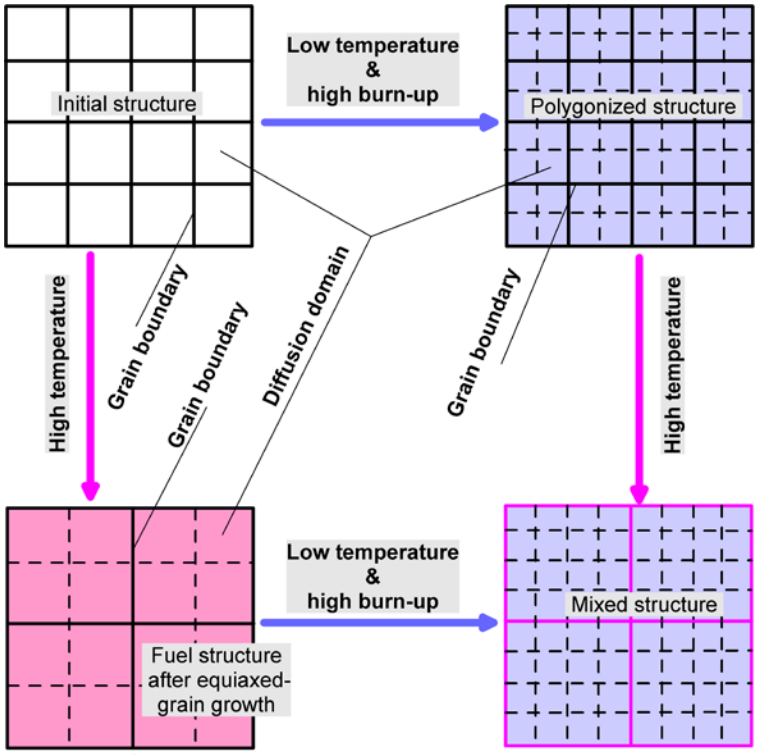


**Figure 4: Schematic topology used for modelling of fuel restructuring.**

To describe the mutual effects of the polygonisation and equiaxed-grain growth the two independent arrays of boundaries are introduced: boundaries of the grains and of the sub-grains. At the beginning of irradiation, these boundaries are geometrically the same. The intragranular polygonisation results in the formation of more and more sub-grains, i.e. small fuel domains where all the types of intragranular processes and objects occur. The boundaries of these domains serve as the perfect sinks for the fission gas, which is generated in the fuel bulk and, further, migrates by a number of mechanisms. GRSW-A employs also a strong simplification that the sub-grain boundaries, formed during the polygonisation, have no capacity to accumulate fission gas that arrives at them from the fuel bulk. Therefore, an assumption is accepted about instantaneous transition of the gas from the sub-grain boundaries (the dashed lines in Fig. 4) to the grain boundaries (the solid lines in Fig. 4). The grain polygonisation model, which is utilized in GRSW-A, impacts mainly the intragranular processes (in particular, intragranular gas loss), through the decrease in the average sub-grain size. The fraction of the polygonised fuel, $\varepsilon_{s\text{-}gr}$, is calculated using an expression based on the generic equation by Kolmogorov [7]:

$$\varepsilon_{s-gr}(t) = 1 - \exp\left(-k_d\left(\frac{b_x(t)}{b_0}\right)^3\right) \qquad (1)$$

Conventionally, the formulation by Kolmogorov (1937) just mentioned is applicable to any restructuring phenomenon, and was already used by other researchers to describe the polygonization process in the $UO_2$ fuels [8].

The value of $\varepsilon_{s\text{-}gr}(t)$ is used in GRSW-A to evaluate the effective sub-grain size $d_{s\text{-}gr}$.

The equiaxed-grain growth at high temperature is interpreted in the GRSW-A model as the aggregation of the fuel grains, which results in the additional FGR solely due to the assumed release of the gas from the disappearing grain boundaries (the dashed lines in Fig. 1). The dynamics of the equiaxed-grain growth is analysed using the classical approach [9][10], with a modification to account for the blockage of the grain-merging on the open surfaces:

$$\dot{R}_g = k_0 \exp\left(-\frac{E_{g.growth}}{kT}\right)\left(\frac{1}{R_g}-\frac{1}{R_{g.\max}}\right)\left(1-\left(\frac{S_F}{V}\right)_{open}\left(\frac{S_F}{V}\right)_{tot}^{-1}\right) \quad (2)$$

$$R_{g.\max} = k_1 \exp\left(-\frac{k_2}{T}\right) \quad (3)$$

where $R_g$ is the grain radius; $k_0$, $k_1$, $k_2$ are the empirical coefficients; $E_{g.growth}$ is the activation energy for the equiaxed-grain growth; $R_{g.max}$ is the maximum grain radius for the current temperature (i.e. the grain radius rate is set equal to zero if $R_g > R_{g.max}$); $k$ is the Boltzmann constant; $(S_F/V)_{open}$ and $(S_F/V)_{tot}$ are the open and total specific areas of the grain boundaries, respectively.

The expression used for the fractional volume of the fuel affected by the high-temperature equiaxed-grain growth, $\varepsilon_{g.growth}$, is as follows:

$$\varepsilon_{g.growth} = \frac{\Delta V_g}{V_g} \quad (4)$$

where $\Delta V_g$ is the increase in the grain volume due to the equiaxed-grain growth calculated using Eqs. 2 and 3 for the grain radius growth rate; $V_g$ is the current grain volume.

Both the equiaxed-grain growth and polygonisation are supposed to entail transformation of the intergranular pores from the lenticular-shaped to spherical ones [4].

It is important that the model takes into account the mutual effect of the two types of restructuring, after they have affected the same material element. For example, a fuel element at the mid-radius of the pellet can build up a considerable amount of the polygonised fuel during base irradiation and then be subjected to high temperature during a power ramp. The GRSW-A model copes with such situations by using a variable volumetric fraction, $\varepsilon$, to characterize an overall degree of fuel restructuring [10].

$$1-\varepsilon = \prod_i (1-\varepsilon_i) = (1-\varepsilon_{s-gr})(1-\varepsilon_{g.growth}) \quad (5)$$

where $i$ is the index determining the fuel restructuring type, which currently can be either the low-temperature polygonisation ($\varepsilon_1 \equiv \varepsilon_{s\text{-}gr}$), or the high-temperature equiaxed-grain growth ($\varepsilon_2 \equiv \varepsilon_{g.\,growth}$).

*3.2.2 TOOLS DEVELOPED BY IRSN WITHIN THE MIST*

Fuel rod mesoscopic scale studies achieved so far at the IRSN concern mainly mechanical aspects and are largely based on the work carried out under the joint CNRS / IRSN laboratory “Micromechanique et Intégrité des Structures” (MIST) [11]. Three main axes are developed in the MIST:

- Scaling methods, which aim to provide equivalent homogeneous material behaviour based on its microstructure and eventually its evolution over time. To fix ideas, these methods yield the apparent property "P" of a medium as a function of "p" in each of the phases that constitute their spatial arrangement and properties "a" : P = f (p, a);

- Crack and fragmentation method. Indeed, being able to predict the integrity of structures comes down to being able to predict when they break. According to the variety of materials present in a reactor (ceramics to metals ), this break may be covered by ductile damage by growth - coalescence of pores, multicracking of brittle fracture or fragmentation. This is the subject of studies on crack – fragmentation;

- Granular flow. Reactor safety is based in particular on the integrity of the barriers interposed between the radioactive products and the environment, including that of the first barrier, the fuel cladding. The loss of tightness of the cladding, particularly by breaking, could lead to a loss of containment of radionuclides, but also, by interactions between fragments of fuel and coolant to a loss of core coolability, and eventually to a steam explosion. The knowledge of fragments behaviour is then very important.

The main outstanding achievements of the MIST are briefly summarized in the following sections. Regarding the contribution to the theme RIA, we can note :

- The provision for SCANAIR code of micromechanical behaviour laws for UO2 and Zircaloy-4 cladding (thermal conductivity, elastic properties, creep, plasticity, damage, depending on the case considered) at any burnup. Micromechanical laws allow consideration of microstructural changes that materials undergo during their lifetime in the reactor. The provision of such constitutive equations allows calculation codes to increase their relevance, predictability and field validation;

- The optimal representative elementary volumes determination for cracking of quasi-brittle heterogeneous materials, and application to hydride Zircaloy. The search for energy fracture properties of hydrided Zircaloy at any burnup is a major issue of support for the analysis of safety requirements. However, the experimental determination of this property is a particularly difficult problem. The MIST results are used to estimate these quantities with a controlled precision from a micrograph of hydrided Zircaloy and optimised numerical simulations.

- The reverse identification of the plastic anisotropy degree of the irradiated Zircaloy matrix for any burnup. In particular, this analysis showed that beyond 40-50 GWd / tU, the Zircaloy matrix lost its initial plastic anisotropy. This is a result expected by the community of cladding materials and it clarifies the relevance of the modelling assumptions made in the SCANAIR framework.

Regarding the LOCA theme, the main achievements are:

- Contribution to the validation of DRACCAR code: expertise for the validation of modelling 1.5D large deformation assumptions and first results regarding the role of frictional contact between deformed cladding (balloons);

- Evaluation of the rate of relocation of ballooning fuel at any burnup. This assessment contributes to safety analysis and study.

Regarding the thermomechanical modelling of fuel and the development of homogenization methods in mechanics of heterogeneous media by IRSN / CNRS MIST mixed team, this works leads to have laws for the mechanical behaviour of fuel including the porosity presence. This is a real highlight of the institute. However, these models are based on microstructural data (pressure in the bubbles, surface tension, size and orientation of zirconium hydride precipitates , ... ) not available *a priori*.

### *3.2.3 OXIDATION MODELING*

#### 3.2.3.1 MECOX

A code of oxidation mechanical modelling (MECOX2D) was developed [12] to assess stress and / or strain levels in the oxide and in the cladding under oxidation. The main contribution of the model lies in the formulation of strain induced by oxidation, which is the sum of three contributions: the geometric contribution, the only one mentioned in the literature, the indirect contributions of inelastic behaviour and especially the metal creep, which helps to explain quantitatively many experimental observations.

Deflection tests were used to evaluate the geometric deformation term by an analytical method. MECOX2D is based on solving the equations of compatibility of strain and mechanical equilibrium. The results were validated by comparison with experimental literature and strain measurements on oxidized sections. MECOX2D confirms the presence of high compressive stresses at the interface, and the presence of a large stress gradient in the oxide layer. An accurate prediction of the depth of the radial cracks, the main factor of non-representativeness of the morphology of the oxide layer formed under the experimental conditions used, is possible using this model.

MECOX2D is a particularly useful tool for analyzing both the oxide layer created in the laboratory but also to compare it with that obtained by irradiation in a reactor. However, this tool needs to be fed up by a kinetic oxidation law, which depends *a priori* on irradiation conditions suffered by the cladding (temperature, radiation...) and is obtained experimentally.

#### 3.2.2.2 DIFFOX

During a loss of coolant accident, the distribution of oxygen in the cladding, and in particular, the concentration of oxygen in phase $\beta$ plays a vital role regarding the mechanical properties of the post-quench cladding material. Analytical solutions of the diffusion equations in complex multilayer and multiphase systems describing the cladding material during high temperature oxidation are limited to stationary isothermal conditions. To solve the problem of non-stationary transient situations of LOCA type, DIFFOX [13] numerical tool was developed. In parallel to the development of the code, an experimental program was initiated to provide a database validation and improve models of the code.

Samples of Zircaloy-4 cladding were pre-oxidized at low temperature, then vacuum annealed or oxidized in high temperature steam. The distribution profiles of oxygen were

studied by EPMA. The results were used to validate the code DIFFOX regarding the depletion of the pre-oxidation and diffusion of oxygen into the metal during high temperature annealing. Regarding the oxidation under high temperature steam, a good agreement between the experimental results and DIFFOX is obtained when the pre-oxidized layer retains its protective properties. By cons, when oxide layer develops in the pre-oxidized layer, the DIFFOX code fails to reproduce the experimental data. The effect of hydrogen was also studied by performing oxidation tests on cladding loaded to 600 ppm hydrogen. The main purpose of these experiments is to provide quantitative data on the change induced by the presence of $\alpha/\alpha+\beta$ and $\alpha+\beta/\beta$ □ hydrogen transitions in the binary Zy4 -O phase diagram.

Although DIFFOX code in the latest version already incorporates the effect of hydrogen on the basis of literature data, this experimental study has shown that improvements can be made. In the future, tests on pre-oxidized and pre-hydrided cladding will continue to broaden the base of IRSN data. Furthermore, experiments with controlled cooling rates before quenching are planned to provide "off-balance" data on the oxygen concentrations at the interphase $\alpha/\beta$ □ and to expand the database of representative oxygen profiles for transient situations.

3.2.2.3 REVIEW

The MECOX and DIFFOX tools are very efficient to analyze cladding oxides and their behaviour in steady state or not. However, taking into account the presence of hydrogen in the cladding and its impact on the diffusion oxide remains inadequate. Experimental work is underway to improve the models used. Moreover, simulation studies on the atomic scale behaviour of hydrogen in zirconium and zirconia should lead to a better understanding and therefore modelling of these interaction mechanisms Zr / H / O.

## 3.3 MICROSCOPIC MODELS

Atomistic modelling has been an integral part of the fuel behaviour analysis both at PSI and IRSN.

For example, at PSI, so far considerable expertise has been acquired in the application and development of the CP2K code [14] as applied to study the diffusion behaviour of selected elements in uranium-dioxide fuel [15], and the evolution of atomic displacement cascades caused by fission fragments. However, the macroscopic models have not managed to benefit from these capabilities yet. Currently, the intention is to start changing the ‘philosophy’ towards a closer link of the atomistic modelling within the fuel modelling group activities, dealing with the applied aspects of reliability justification and safety analysis of the fuel in the Swiss LWRs. As, at least, the existing external experience shows [16], the possible outcomes of the future microscopic modelling at PSI might be as follows: (1) the study and review of the details of already existing and published models [17][18]; (2) considering alternative models for the same physical phenomena with a view to forming recommendations on which of them are better consistent with the results obtained by atomistic simulations; (3) estimation of the parameter values for the existing meso- and macroscopic models.

At IRSN, extensive works in the microscopic modelling area have focusing on a number of aspects, as described in the subsections below.

3.3.1 UO2 FUEL

The work in this area was initiated by studying the properties of fission gas intragranular bubbles and their impact on the thermoelastic properties of the fuel. This work started with the use of molecular dynamics and Monte Carlo approaches. In both cases the GULP (General Utility Program) and LAMMPS software are used and work is conducted in collaboration with the Centre for Interdisciplinary NAnoscience of Marseille (CINAM) .The studies are based on the use of semi-empirical potentials interatomic interaction [19].

3.3.1.1 Thermomechanical properties

On this basis, molecular dynamics calculations were used to quantify the impact of the presence of pores on the thermoelastic properties (bulk modulus, shear modulus, thermal expansion) of the UO2 matrix at different temperatures. These calculations in excellent agreement with experimental results available in the literature as well as with conventional micromechanics (homogenization) approaches demonstrated on the one hand the ability of molecular dynamics to establish relationship between atomic and mesoscopic scales and on the other hand identified the importance of surface phenomena previously neglected in micromechanical approaches [19][20].

Work is in progress to take into account these surface effects in ad hoc micromechanical models. All of these works establish that the porosity distribution is a factor to be taken into account as well as the total pore fraction if you want to accurately model the effects of bubble on macroscopic thermomechanical fuel properties.

The porosity impact on the thermal conductivity of UO2 was also established, again in perfect agreement with the classical homogenization approaches, but with the presence of an additional term due the interface effects. Once again, the total porosity is not the only factor to consider, but the distribution of it (bubble size and density) is at least as important . An original analytical model of thermal conductivity developed takes into account this parameter very simply.

3.3.1.3 Adsorption isotherms of intragranular bubbles

A Monte Carlo simulation code was used to study the isothermal filling of intragranular bubbles by Xe and therefore to access not only to the evolution of the pressure in the fuel and in the bubble depending on the temperature, but also to study the physical state of the fission gas inside the bubbles and to better understand and characterize phenomena such as thermal resolution of fission gas. In view of the results obtained, it appears that the assumed resolution of intragranular bubbles is not relevant and only radiative resolution is to be considered at meso- and macroscopic scales. These results, which need to be confirmed by further studies, should help to simplify the models used to describe the behaviour of noble gases in the fuel.

3.3.1.4 Pressure in intragranular bubbles

Work is also underway [21] to quantify the pressure within the gas bubble and its evolution during rapid temperature transient. This work has highlighted a very important effect of pressurization of rare gas bubbles due to the presence of the interface with the fuel matrix, and identifies a condensed phase in the bubble, in agreement with the available experimental data.

## 4. CONCLUSIONS AND PROSPECTS

We presented in this paper the multi-scale use for the study of nuclear fuel, applying to highlight at each step the strengths or locking points of the used approaches. The objective of the multi-scale studies is, using a better understanding and modeling of basic phenomena at the atomic scale and linking microstructure and thermomechanical properties, to extend the predictive capabilities of macroscopic computer codes on one hand, and to allow better interpretation and use of analytical and integral tests on the other hand.

IRSN has a global vision on multi-scale approaches, difficult issues have been identified, the advantages and disadvantages of the main approaches at different scales are well established. Efforts are underway to address the major challenges, including the establishment of collaborations with academic labs to benefit from their experience. Regarding fuel codes, i.e. the macroscopic scale, very strong skills exist. Similarly, with regard to mesoscopic and microscopic scales IRSN now has solid skills, even if they are not complete yet. Finally, with respect to the atomic scale, the work done focused on thermostatistical approaches for now. Indeed, the physical domains investigated (high temperature, irradiation) limit the use of electronic structure calculations to very specific uses, such as parameterization and validation. However, these promising approaches will be fully utilized if the following points are addressed with great care:

- Regarding the microscopic approaches, different tools are still based on know-how and relatively complex methodologies. It is important to include these activities in collaboration with academic laboratories and specialists in these approaches to include our studies as much as possible within the network or research group, to ensure their quality;

- At the mesoscopic scale, elements of the multi -scale approach are still missing in the institute. It will be necessary to make an assessment on the potential contributions of approaches such as dislocation dynamics and phase field;

- All models must be validated at each scale with experimental approaches to equivalent scales. Access to experimental characterization of fuels and nuclear data remains remains fundamental;

- Finally, a very special care should be focused on how the different scales can exchange data and parameters, and a communication effort will be carried out by specialists of each scale in order to exchange more effectively with the other scales.

PSI has built up experience in application of the integral analysis of fuel behaviour covering the effects of base irradiation on the transient behaviour. As it seemed from the analysis of some experiments (e.g. RIA type transients with high enough inserted energy, and the recent Halden LOCA tests with high-burnup fuels), the detailed consideration of the fuel micro-structural state after the base irradiation may bring additional insights into the macroscopic fuel behaviour during the transients of interest. At the same time, the predictive analysis with the FALCON code for fuel behaviour in real RIA and LOCA needs close coupling with the integral system codes, which is currently not available, and is to be implemented in the future. As far as atomistic modelling is concerned, for the time being the macroscopic models have not managed to significantly benefit from the atomistic simulation capabilities available at PSI. However, the intention is to start changing the ‘philosophy’ towards a closer link of the atomistic modelling within the fuel modelling group activities, dealing with the applied aspects of reliability justification and safety analysis.

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