Current status and progression of GERMINAL fuel performance code for SFR oxide fuel pins

Marc Lainet[1], Bruno Michel[1], Jean-Christophe Dumas[1], Karl Samuelsson[2], Michel Pelletier[1]

[1] CEA Cadarache, DEN/DEC – Saint-Paul-lez-Durance, France

[2] KTH Royal Institute of Technology – Department of Physics – Stockholm, Sweden

E-mail contact of main author: marc.lainet@cea.fr

Abstract. A fuel performance code for SFR oxide fuel pins, GERMINAL, is developed by CEA within the PLEIADES simulation framework. The present main goal of GERMINAL is to meet the needs of the design studies of ASTRID, the future Advanced Sodium Technological Reactor for Industrial Demonstration in France. Recent works have been conducted to improve the modelling of different physical mechanisms having a strong influence on the design criteria evaluation. Thus, the formulation of the fuel pellet fragments relocation model has been revisited, by introducing a dependency to the thermal gradient inside the pellet. The description of this mechanism represents a key point to evaluate the pellet-to-cladding gap closure and the margin to melting at beginning of life. Another evolution concerns the pellet-clad mechanical interaction. The ability to simulate a stronger interaction for fuel pins with a higher filling fraction has been acquired with a focused work on fuel mechanical behavior. A stronger mechanical interaction may also happen with lower power operating conditions and a cladding material remaining stable under irradiation. Moreover, the description of the thermochemistry of oxide fuel is currently being improved by coupling GERMINAL with the OpenCalphad thermodynamic calculation software. In doing this, the goal is to obtain a better prediction of the amount of volatile fission products being transported outside the fuel pellet, and then contributing to the "Joint Oxyde-Gaine" formation. With refined estimations of JOG volume and composition, we expect further to improve the evaluation of heat transfer through pellet-to-cladding gap at high burn-up, and also a more mechanistic description of cladding corrosion due to released fission products. These works are based on a systematic comparison of calculation results to post-irradiation measures, by integrating progressively additional objects to our validation base. This process leads to a wider validity range targeting ASTRID design, and brings out new working perspectives.

Key Words: Fuel performance code, modelling, numerical simulation.

1. Introduction

To support the design studies of ASTRID, the future technological Sodium Fast Reactor demonstrator in France, the modelling of uranium-plutonium oxide fuel pins is constantly being improved by developing GERMINAL [1] fuel performance code within PLEIADES [2] simulation platform. PLEIADES is a unified framework for fuel simulation, co-developed by CEA, Électricité de France and Areva. The development of GERMINAL within PLEIADES started about ten years ago, among many activities supporting ASTRID project. By the end of 2013, a renewed version 2 was delivered for use to all partners contributing to ASTRID fuel elements design. Since, works have been pursued to improve the modelling of different physical mechanisms having a strong influence on the design criteria evaluation.

The article gives a quick overview of GERMINAL V2 and then details some recent modelling evolutions, concerning fuel fragments relocation, pellet-clad mechanical interaction and the coupling with OpenCalphad thermodynamic calculation software.

2. Overview of GERMINAL V2

2.1. Fuel pin representation

GERMINAL V2 uses a 1D½ axisymmetric representation of the fuel pin geometry. The fuel pin is decomposed into axial slices, whose thermal evolutions are linked by the heat transport by the coolant. Practically, the axial discretization may use from 10 to 40 slices. The slicing definition is correlated first to the fuel column composition: heterogeneous columns usually require more meshes to represent the different parts in a proper way. The fuel pin slicing can also be adapted according to the core axial power shape, by using a non regular slicing when it is appropriate to catch the power peak. In each axial slice, the resolution of the physical processes uses a radial meshing representing the fuel pellets, the fuel-to-cladding gap and the cladding. The radial meshing of the fuel is more refined near the centre, in order to describe with a satisfactory precision the central hole formation or evolution in case of annular fabricated pellets. The adopted meshing topology represents a compromise between reasonable calculation times and results precision. It includes 25 radial meshes, whose size is growing in geometric progression from 50 µm near the centre to 200 µm at the periphery. For the cladding, a regular meshing with 10 elements in the thickness is usually used; the mesh size is about 50 µm.

The use of a 1D½ calculation scheme leads to an average model size of about 1000 degrees of freedom, estimated with 25 axial slices. This little model size allows short calculation times and is thus appropriate for study processes, such as uncertainty analyses, which require thousands of simulations. This type of application is now currently taking part in ASTRID fuel elements design [3].

2.2. Calculation sequence

The evolution of the fuel pin all along irradiation is determined step by step. The resolution of one time step is performed according to the sequence defined by the following *FIG. 1*. In this description, global resolutions refer to physical processes affecting the fuel pin in its whole height; whereas local resolutions refer to processes evaluated in one considered axial slice. As the physical mechanisms occurring along irradiation are strongly coupled, a convergence loop is executed for each axial slice of the fuel pin. Finite Elements computations are implemented for thermal analysis and mechanics, using CAST3M [4] solver.

Global resolutions needed by the local resolutions to come

☞ Simplified thermal-hydraulics of coolant channel
Determines the boundary conditions for the local thermal analyses to come: cladding outer temperature in each axial slice
N.B. Preliminary resolution *for a stationary analysis only*.
For a transient analysis, coupled resolution with fuel pin thermal analysis.

Local resolutions ⇔ Loop on axial slices

☞ Neutronics

☞ Calculation of average (O/M) (burn-up dependent)

☞ Local convergence loop
⇒ Thermal analysis of fuel and cladding
Coupled with coolant thermal-hydraulics for a transient analysis.

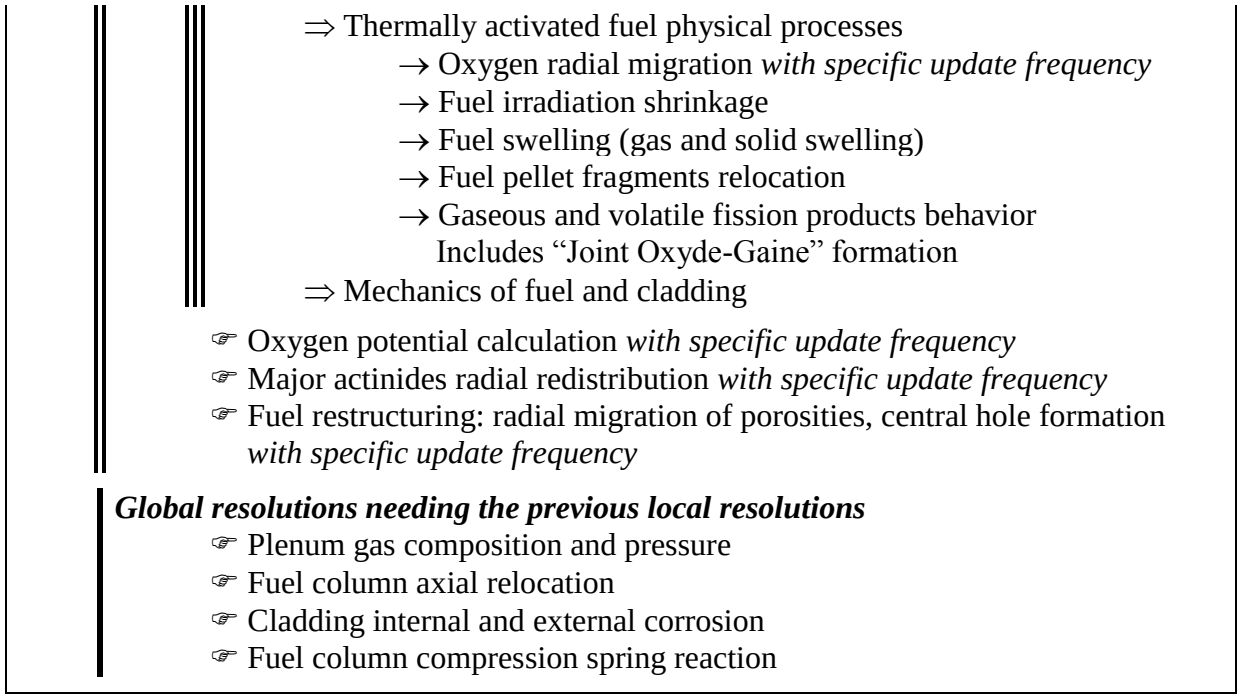

FIG. 1. One time step resolution by GERMINAL V2.

2.3. Code validation

The validation of GERMINAL V2 was carried out by using a selection of 100 SFR fuel pins. PHÉNIX standard geometry represents the major part of the validation base, with 45 fuel pins of internal core and 10 pins of external core. In addition, 15 SUPER-PHÉNIX 1 fuel pins with annular pellets of larger diameter and 3 PHÉNIX heterogeneous pins are of special importance considering the current design of ASTRID. The validation base also includes 8 transient tests operated in CABRI reactor, reproducing off-normal conditions such as power ramps, with different increase rates and peak levels, or Reactivity Insertion Accidents.

3. Latest evolutions of mechanical modelling

3.1. Fuel fragments relocation model

The goal of the fuel fragments relocation model is to describe the evolution of the free volumes opened by the pellet cracking at beginning-of-life. Practically, the fuel pellet cracks in many fragments very early during the first power increase, with a linear power around 30 W/cm according to PHÉNIX operation feedback. The opening of the free volumes between the fragments contributes significantly to the fuel-to-cladding gap closure, as illustrated by the following *FIG. 2*, leading to an important increase of the heat transfer through the gap. Consequently, this mechanism strongly influences the temperature evolution inside fuel at beginning-of-life. The evaluation of the margin to melting as a design criterion is thus closely linked to the ability to describe as well as possible the relocation of the fuel fragments.

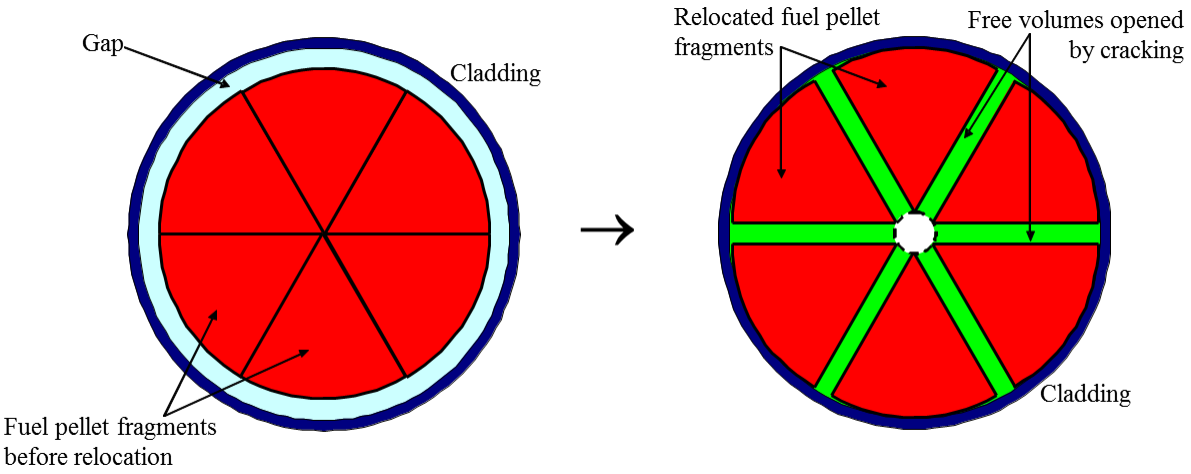

FIG. 2. Fuel pellet fragments relocation.

A first empirical formulation of the relocation model was elaborated and validated for GERMINAL V2 [1]. This formulation was using power density as a driving parameter to evaluate the fragment relocation rate. One drawback of this parameter choice was its lack of generality, regarding different fuel pin types and their corresponding operating conditions. Thus, the model formulation has been revisited by introducing a dependency to the thermal gradient inside the pellet. The model determines an ***homogeneous stress free strain*** to be imposed to the fuel pellet. The relocation rate is evaluated by:

$$\dot{\varepsilon}_{reloc}(t) = \frac{u_r^{\max}(t) - u_r(t)}{R_{pellet}^{ext}(0)} \Big/ \tilde{t}_0$$

$u_r^{\max}(t)$ is the radial displacement upper bound. $u_r(t) = R_{pellet}^{ext}(t) - R_{pellet}^{ext}(0)$ is the radial displacement of fuel pellet external bound. $R_{pellet}^{ext}(0)$ and $R_{pellet}^{ext}(t)$ are the fuel pellet external radius at initial and current time. $\tilde{t}_0$ is a time constant.

The average thermal gradient inside fuel pellet at *z* axial position along fuel pin and at current time *t* is defined as follows:

$$gradT(z,t) = \frac{T_{pellet}^{\text{int}}(z,t) - T_{pellet}^{\text{ext}}(z,t)}{R_{pellet}^{\text{ext}}(z,t) - R_{pellet}^{\text{int}}(z,t)}$$

$T_{pellet}^{\text{int}}(z,t)$ and $T_{pellet}^{\text{ext}}(z,t)$ are respectively the inner and outer fuel pellet temperatures. The corresponding radial positions are $R_{pellet}^{\text{int}}(z,t)$ and $R_{pellet}^{\text{ext}}(z,t)$.

The average thermal gradient is newly introduced in the evaluation of the radial displacement upper bound through a dimensionless variable *x*:

$$x = \frac{gradT(z,t)}{gradT_{ref}}$$

$gradT_{ref}$ is the first model parameter, representing a ***reference thermal gradient leading to a complete gap closure*** by fuel fragments relocation.

The radial displacement upper bound is evaluated by weighting the current gap size by a function depending on the dimensionless variable *x*:

$$u_r^{\max}(t) = Min\left(1, \omega(x)\right) \times \left(R_{clad}^{\text{int}}(t) - e_{JOG}(t) - R_{pellet}^{ext}(0)\right)$$

$\omega(x)$ is the dimensionless weighting function, further described.
$R_{clad}^{int}(t)$ and $e_{JOG}(t)$ are the cladding inner radius and the « Joint Oxyde-Gaine » thickness, to be taken into account at high burn-up when the precipitate has formed.

The new formulation keeps some basic principles of the original one. The relocation rate tends to zero when the radial displacement tends to its upper bound; this avoids strong mechanical interaction when reaching contact. The relocation rate is forced to zero when the power is decreasing during time step; the evaluation of fuel fragments relocation is thus disabled during reactor shut-down, when thermal contraction leads to re-open the gap.

The dimensionless weighting function $\omega(x)$ draws a non linear evolution with a zero-crossing not placed at the origin. It is expressed as follows:

$$\text{If } x_0 \le x \le x_1 \quad \omega(x) = x_1 \times \left(1 - \left(\frac{x - x_1}{x_0 - x_1}\right)^n\right) + (1 - x_1) \times x \times \left(\frac{x - x_0}{1 - x_0}\right)$$

$$\text{Else if } x \le 1 \quad \omega(x) = x_1 + (1 - x_1) \times x \times \left(\frac{x - x_0}{1 - x_0}\right)$$

$\omega(x)$ is varying in the range $[x_0 ; 1]$, with $x_0 > 0$. The lower bound x_0 represents the ratio of a ***thermal gradient threshold for pellet cracking*** (second model parameter), divided by the reference thermal gradient leading to complete gap closure. With a zero-crossing not placed at the origin, the formulation intends to reproduce a threshold effect for the fuel fragments relocation, which requires a minimum thermal gradient to provoke pellet cracking. The non linearity of the evolution induces a fast enabling phase, expressed by the first term:

$$x_1 \times \left(1 - \left(\frac{x - x_1}{x_0 - x_1}\right)^n\right)$$

This enabling term tends to an asymptotic weighting x_1 when the dimensionless gradient tends itself to x_1, which thus represents the ***enabling phase upper bound*** – third model parameter. The fourth model parameter is the ***exponent*** n of the enabling term, which drives the initial increase of $\omega(x)$. The following *FIG. 3* shows the evolution of $\omega(x)$.

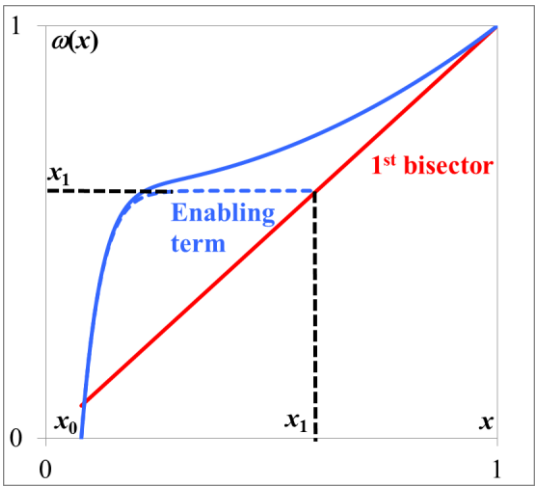

FIG. 3. Evolution of the dimensionless weighting function $\omega(x)$.

The time constant determining the relocation rate is adjusted by taking into account the thermal gradient rate during the time step. This sensitivity is introduced in order to accelerate relocation for off-normal transient conditions, when the power and consequently the thermal

gradient inside the fuel pellets are evolving faster than in normal operating conditions. The time constant adjustment is expressed as follows:

$$\tilde{t}_0 = t_0 \times Max\left(10^{-3},\ Min\left(1\ ,\ \frac{\dot{gradT}_{ref}}{\dot{gradT}(z,t)}\right)\right)$$

t_0 represents a ***characteristic time constant for fuel fragments relocation in normal operating conditions*** – fifth model parameter.

$\dot{gradT}_{ref}$ is a ***reference thermal gradient rate*** – sixth model parameter; its value fixes a bound between normal transient evolutions and off-normal ones.

$\dot{gradT}(z,t)$ is the thermal gradient rate inside fuel pellet at z axial position along fuel pin and at current time t.

The new formulation of the fuel fragments relocation model has been adopted by the latest revision of GERMINAL V2, observing the benefits brought for the simulation of the fuel pins of the validation base. The choice of the thermal gradient as a driving parameter for fragments relocation leads to a better agreement with post-irradiation measurements, when considering quantities closely linked to the thermal regime undergone by the fuel pin, such as the columnar grains expansion diameter or the central hole diameter. The main benefits are observed at intermediate power level, i.e. at the fuel pin extremities or for objects which have operated at lower conditions than normal ones – PHÉNIX cycles at two third of nominal power. These results are obtained with a model calibration not depending anymore on the fuel pin type; the new formulation is thus more general than the original one.

However, further improvements are still expected, concerning particularly the kinetics of the mechanism, and consequently this of fuel-to-cladding gap closure at beginning-of-life. Current works are in progress, based on tridimensional simulations of the fuel fragments, to study the link of gap closure with fuel restructuring: thermal-induced material redistribution, leading to the central hole formation or expansion in the fuel pellets. The current status of these works is presented by [5].

3.2. Pellet-clad mechanical interaction

A strong mechanical interaction between pellet and cladding may happen with lower power operating conditions, i.e. with a colder fuel having a higher mechanical resistance and a majored swelling due to a higher retention of fission gases. It may also happen at high burn-up, with a cladding material remaining stable under irradiation, and consequently not following the fuel volume increase induced by the fission products. The ability to simulate a pellet-clad mechanical interaction as representative as possible is thus interesting the design studies, for which both normal and off-normal conditions have to be taken into account.

To improve GERMINAL capabilities on this subject, we have used an experimental irradiation realized in PHÉNIX reactor. The considered POUSSIX capsule was carrying 12 fuel pins having different fuel surface fractions[1]. The main goals of POUSSIX irradiation were first to study experimentally the sensitivity of pellet-clad mechanical interaction to fuel filling fraction, and also to determine a pin filling threshold leading to a strong interaction.

---

[1] The fuel surface fraction is defined by the ratio of the fuel section area, including central hole, divided by the clad inner section area.

The four POUSSIX fuel pins that we have selected are the following:

Pin number	2	7	5	10
Fuel surface fraction	91,8%	94,5%	96,2%	97,1%

TABLE II: POUSSIX FUEL PINS SELECTION.

As explained in reference [1], the fuel mechanical behavior is described by a formulation combining creep with perfect plasticity. This choice was made since it appeared that the using of a cracking model was not adapted beyond the complete rupture of the material, leading to an indetermination – stiffness matrix singularity – when all elements are broken. Moreover, the behavior's description with perfect plasticity is more representative for compression state. In case of a maintained contact with cladding and after the complete closure of the pellet cracks, the compression stresses inside pellet are bounded by the yield strength of the fuel material, and this produces a representative loading on cladding. When using comparatively a fuel mechanical behavior model combining creep with cracking, the compression stresses inside pellet may only be relaxed by creep. By simulating the fast transient tests of GERMINAL validation base with this behavior modelling, we have observed that the stresses relaxation by creep is not quick enough, and this leads to an over-estimation of the loading induced on the cladding. These calculations determine sometimes a residual cladding deformation due to instantaneous plasticity that has not been observed experimentally. For this reason, the choice of the fuel mechanical behavior model combining creep and plasticity has been kept.

The first simulations of POUSSIX fuel pins performed with GERMINAL were not predicting the increase of end-of-life cladding residual deformation observed for pins N°5 and 10 having the highest filling fractions. This was explained by a too low estimation of the fuel yield strength. Thus, the first part of the work consisted in reconsidering the description of yield strength evolution with temperature. To do this, we made use of available characterizations of fuel plastic flow threshold stress. Taking into account the average characteristics of as-fabricated French oxide fuel for SFR – particularly in terms of porosity and grain size, a new temperature dependent correlation for yield strength was adopted:

$$\sigma_y(\theta) = 917{,}41.10^{6} \times \exp\left(-1{,}8.10^{-3}(\theta + 273{,}15)\right)$$

σ_y is the yield strength in Pa and θ is the temperature in Celsius. This evaluation is defined for low temperature range: $600°C \leq \theta \leq 1300°C$. For higher temperatures, the estimation at 1300°C is retained, to keep a minimum mechanical resistance of the material.

This correlation was then used to perform new simulations of POUSSIX fuel pins, and further to quantify its effect on the simulation of all objects of GERMINAL validation base. The updated predictions of end-of-life residual deformations for POUSSIX fuel pins are now in good agreement with observation, as shown by *FIG. 4*. When considering the whole validation base, the calculations stay consistent with measurements, especially in case of the fast transient tests: no artefact of cladding plastic deformation. Consequently, this evolution was adopted by the latest revision of GERMINAL V2, as a benefit to simulate fuel-clad mechanical interaction.

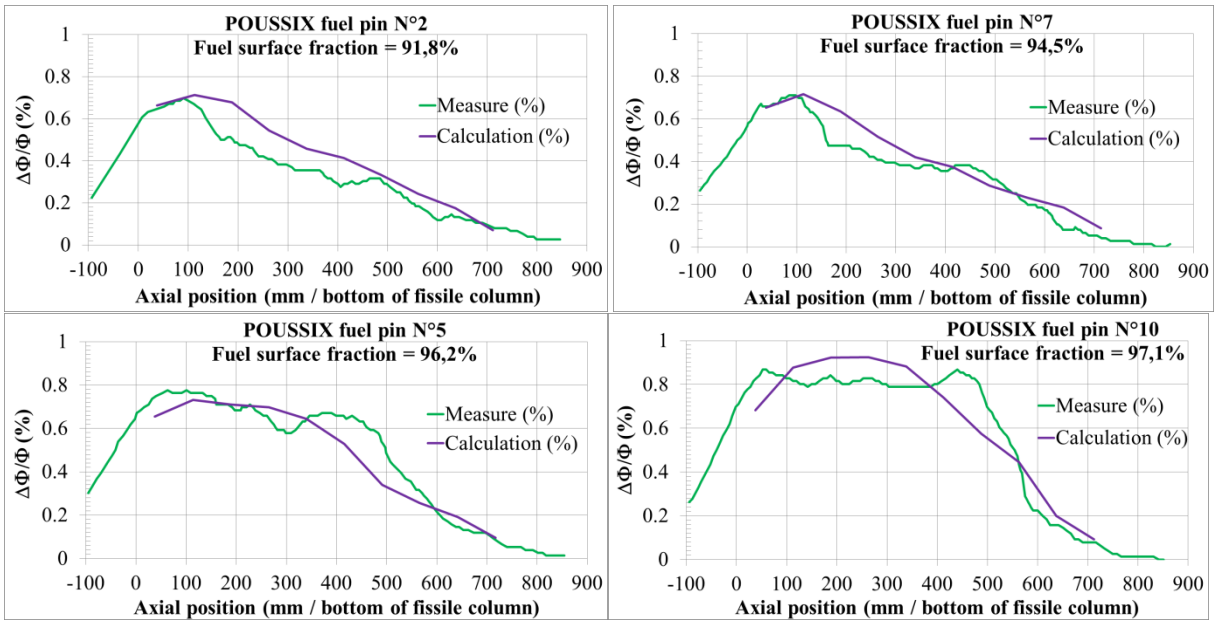

FIG. 4. End-of-life diametrical deformations: measures and calculations.

4. Coupling with OpenCalphad thermodynamic calculation software

4.1. Context – Motivation

The main specificity of FBR fuel compared to PWR fuel is to be submitted to both high temperature and large temperature gradients during operation. These extreme conditions are the cause of many thermal, mechanical and chemical transformations in the fuel. Moreover, the behavior of the fission products (FP) generated by the irradiation strongly depends on their chemical nature as well as conditions in the fuel (temperature, oxygen potential, …). Experimental observations show the formation of a layer located between the fuel and the cladding material for a burn-up of 6 to 8 ha%. This layer, called JOG for *"Joint Oxyde-Gaine"* [6], is due to the release, migration and association of caesium, iodine, and tellurium mainly with oxygen and molybdenum created in the fuel pellet. The apparition of the JOG has an impact on the thermal transfer between the fuel and the cladding. At high burn ups, these FP compounds can react with the cladding components (Fe, Cr, Ni) corroding the inner part of the cladding material, which can impact the integrity and the lifetime of pins in the SFR [7]. The prediction of these chemico-physical evolutions are thus of first importance to support ASTRID fuel pin design studies.

Present modelling of these phenomena in GERMINAL remains rather crude and is mainly based on empirical correlations, coming from experimental results obtained on PHÉNIX fuel pins thirty years ago. Thus, a more mechanistic description is planned, based on thermodynamic and diffusion aspects. Recent trends for modelling and simulation are moving towards comprehensive coupling of various phenomena to enhance predictive capabilities of multi-physics codes. In particular, there is a big interest in coupling thermodynamic computations with nuclear fuel performance and safety codes [8]. For these reasons, integrating a thermodynamic software appears to be particularly relevant in order to predict the amount of the volatile FPs being transported towards the JOG, and ultimately, the total quantity of elements available for FCCI (*Fuel Cladding Chemical Interaction*) that can occur in the future ASTRID fuel element.

4.2. The OpenCalphad software and the TAFID database

OpenCalphad (OC) is a free general thermodynamic software [9]. It can calculate the equilibrium in a system for various types of conditions as well as various properties like chemical potentials, heat capacities and so on... Particularly, for a given composition, the code evaluates, in isothermal conditions, the thermodynamic equilibria between the different chemical constituents which take place in the different solid, liquid and gaseous phases of a multi-component system. The principle of the calculation is based on the minimization of the Free enthalpy (or Gibbs free energy). The advantage of choosing OpenCalphad [9] is both the fact it is "open source" and also its ability to use efficient models/descriptions by its compatibility with the TAFID database [10]: *Thermodynamic Advanced Fuels International Database,* developed within the frame of the OECD/NEA. The goal of this project, which started in 2013, is to merge the different databases on nuclear materials and in the same time to promote exchanges on thermodynamic data and models for the nuclear fuel systems. For that purpose, it has been decided to choose a full CALPHAD modelling [11] in order to provide both phase diagram and thermodynamic data calculations. Also for the oxide phases, the two sub-lattice ionic model and the Compound Energy Formalism with ionic species were chosen for the liquid and the mixed oxides, respectively [10]. The current working database contains approximately 40 chemical elements with more than 200 binary systems and more than 60 ternary systems.

4.3. Outlook for an extended calculation scheme

The general idea consists in the following: at each time step, and for each node considered by the GERMINAL code, OC will take the local temperature, the hydrostatic pressure and the local isotopic concentrations (evaluated by the neutronic module) of all the chemical elements considered by the thermochemical modelling as input data for its calculations. For each radial mesh, a first thermochemical calculation will be performed in order to assess the local fuel chemical composition. Then, the migration of the volatile fission products will be done by assuming the associated chemical species are transferred towards the fuel to clad gap under gaseous phase with the same release rate than the fission gas one. After that, a second thermochemical calculation by using the chemical inventory determined in the fuel to gap of the corresponding axial slice will allow us to evaluate the chemical composition of both JOG and FCCI (which kind of phases, their quantities and their composition). Then, the width of the JOG and of the corroded inner cladding layer will be calculated from the corresponding molar volumes. This description will also have to be completed by taking into account kinetics aspects, especially by describing precisely the diffusion of the main fission products species, and as well as taking into account the phenomenological aspects associated to the FCCI process. However, thermodynamic computations are complex and can significantly have an impact in computational performance, which is generally not a major concern in constructing phase diagrams. But it is a requirement for a fuel performance code like GERMINAL. Calculation time will consequently be checked when integrating OpenCalphad within GERMINAL calculation process.

5. Conclusions – Perspectives

The works related in this article illustrate the constant effort to improve the modelling used in the GERMINAL fuel performance code, in order to make simulations always closer to observations. The current works based on tridimensional simulations of the fuel fragment [5]

will result in the future in a new revision of the fuel fragments relocation model, to be used by the 1D½ calculation scheme. The study of pellet-clad mechanical interaction also revealed the need of updated characterizations of the fuel material. Concerning the couplings with fuel physics, the use of OpenCalphad thermochemistry component represents the starting point leading to new evolutions to evaluate heat removal at high burn-up, in presence of a "Joint Oxyde-Gaine", and also to evaluate cladding integrity with a refined estimation of corrosion. In addition, a new major version of GERMINAL is now being developed within PLEIADES simulation framework, with the main goal to improve computation performance through parallel implementation. This future version 3 of GERMINAL will naturally integrate all modelling evolutions actually in progress.

The authors want to thank Électricité de France and Areva for their support to the development of GERMINAL. We also thank Dr. Bo Sundman for his precious help to perform calculations involving OpenCalphad software, as well as all the users of GERMINAL at CEA, Électricité de France and Areva for their useful feedback on the code.

References

[1] M. Lainet, V. Bouineau, T. Helfer, M. Pelletier, "Recent modelling improvements in fuel performance code GERMINAL for SFR oxide fuel pins", IAEA-CN-199/241, FR13, March 2013, Paris, France.

[2] D. Plancq and al., "A unified environment for multi-dimensional fuel performance modelling", International Meeting on LWR Fuel Performance, Orlando, USA, 2004.

[3] V. Blanc et al., "Fuel Melting Margin Assessment of Fast Reactor Oxide Fuel Pin Using a Statistical Approach", IAEA-CN-245-333, FR17, June 2017, Yekaterinburg, Russia.

[4] P. Verpeaux, T. Charras and A. Millard, "CASTEM 2000: une approche moderne du calcul des structures", Calcul des structures et intelligence artificielle, Editions Pluralis, France, 1988.
http://www-cast3m.cea.fr/

[5] B. Michel et al., "3D simulation in the PLEIADES software environment for Sodium Fast Reactor fuel pin behavior under irradiation", IAEA-CN-245-223, FR17, June 2017, Yekaterinburg, Russia.

[6] M. Tourasse, M. Boidron and B. Pasquet, "Fission product behaviour in Phénix fuel pins at high burnup", Journal of Nuclear Materials, Volume 188, 49-54, 1992.

[7] K. Maeda, "Ceramic Fuel-Cladding Interaction", Comprehensive Nuclear Materials, Section 3.16, Elsevier Ltd , 2012.

[8] D.R. Olander, "Fundamental Aspects of Nuclear Reactor Fuel Elements", U.S. Department of Commerce, 1976.

[9] B. Sundman, X-G. Lu and H. Ohtani, "The implementation of an algorithm to calculate thermodynamic equilibria for multi-component systems with non-ideal phases in a free software", Computational Materials Science, Volume 101, 2015.

[10] C. Guéneau et al., "Thermodynamic modelling of advanced oxide and carbide nuclear fuels: Description of the U-Pu-O-C system", Journal of Nuclear Materials, Volume 419, 145-167, 2011.

[11] N. Saunders, P. Miodownik, "CALPHAD: Calculation of Phase Diagrams", Pergamon Materials Series, 1998.