3D SIMULATION IN THE PLEIADES SOFTWARE ENVIRONMENT FOR SODIUM FAST REACTOR FUEL PIN BEHAVIOR UNDER IRRADIATION

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Abstract

In the framework of the basic design of ASTRID (Advanced Sodium Technological Reactor for Industrial Demonstration), the GERMINAL fuel performance code is developed in the PLEIADES software environment. In order to improve one dimensional modelling of GERMINAL, a 3D simulation for the SFR fuel pin behavior under irradiation has been proposed.

The 3D model represents a single pellet fragment and its associated piece of cladding. The scale transfer between this single fragment model and the fuel pin scale is achieved through appropriate boundary conditions given by GERMINAL results. A preliminary 3D thermo-mechanical computation scheme has been implemented in the LICOS code of the PLEIADES platform. In this approach, chemo-physical state variables are pre-computed by the GERMINAL code and are introduced in the 3D computation scheme as some input data in a two-step procedure. First studies have been achieved in order to analyze pellet-to-cladding gap closure mechanisms at the beginning of irradiation. Two mechanisms of fuel relocation have been identified through the 3D simulation. The first one is linked to the hourglass shape of the fragmented fuel pellet under thermal gradient, and the second one is induced by the mass transfer due the central-hole formation and fuel restructuring. Thanks to our 3D results, the gap closure rate given by the fuel relocation displacement model of GERMINAL can be interpreted. The next step is now to propose a fully coupled formulation between fuel mass transfer model and the radial relocation displacement model. This new formulation will be used to improve the 1D computation scheme of GERMINAL and will prepare further developments to extend the GERMINAL fuel performance code to the 3D simulation.

Key Words: 3D simulation, fuel pin behavior under irradiation, PLEIADES, GERMINAL

1 Introduction

Sodium Fast Reactor (SFR) fuel pin behavior under irradiation is an important issue regarding the safety assessment of the first barrier. In France, experimental knowledge and fuel modelling have been capitalized for many years in the fuel performance code GERMINAL V2 [1] of the PLEIADES software environment [2]. This fuel performance code, used for the basic design of ASTRID (Advanced Sodium Technological Reactor for Industrial Demonstration), is still under development in order to improve the precision of the various models used to assess fuel behavior under irradiation. Among these improvements, one concerns the closure of the pellet-to-cladding gap which controls the fuel maximal temperature at the beginning of irradiation. In order to improve one dimensional modelling of GERMINAL, a 3D simulation for the SFR fuel pin behavior under irradiation is also under development. The 3D approach is based on a single pellet fragment model as it has been proposed for many years in the simulation of the Pressurized Water Reactor fuel rod behavior [2]. This 3D computation scheme, based on a nonlinear thermomechanical coupling formulation, has been implemented with the LICOS code of the PLEIADES plateform. First

studies have been achieved in order to analyse pellet-to-cladding gap closure mechanisms at the beginning of irradiation.

In this paper we first present the main features of the 3D fuel pin model. Then, two mechanisms of radial fuel relocation are detailed through the 3D simulation results. The first mechanism is linked to the pellet hourglass shape under thermal gradient, and the second one is induced by the mass transfer due the central hole formation and fuel restructuring.

2 3D fuel pin model

2.1 Finite element mesh and boundary conditions

The finite element model used in the 3D approach is presented in the Figure 1. The single fuel pellet fragment considered in the simulations is located at a given axial position in the pin. The size of the pellet fragment is consistent with post-irradiation examinations performed after the beginning of irradiation which show the existence of 4 to 8 pellet fragments in the circumferential direction. The pellet fragment angle (22.5°) can be chosen in order to maximize the magnitude of the fragment "hourglass" shape during nominal loading conditions.

The boundary conditions considered in the 3D calculations take into account the geometrical symmetries of the problem and for the pellet-to-cladding and pellet-to-pellet interactions. At the inter-pellet plane (plane $0, x_0, y_0$ in Figure 1), a unilateral contact condition $u_z \geq 0$ is used. The mechanical reaction of the fissile column above and under the meshed fragment is represented by a kinematics relation between the pellet and the cladding mid-planes (plane P, x_1, y_1 in Figure 1). This mid-plane locking condition is applied only when the pellet cladding gap is closed at least at one point.

Several force loading boundary conditions are defined. The internal pressure (gas pressure) is applied to the cladding inner surface and to the pellet fragment outer surface. The external pressure (sodium pressure) is applied to the cladding outer surface. Resultant of the axial pressure due to the «end-effects» on the fuel pin is applied to the cladding mid-plane.

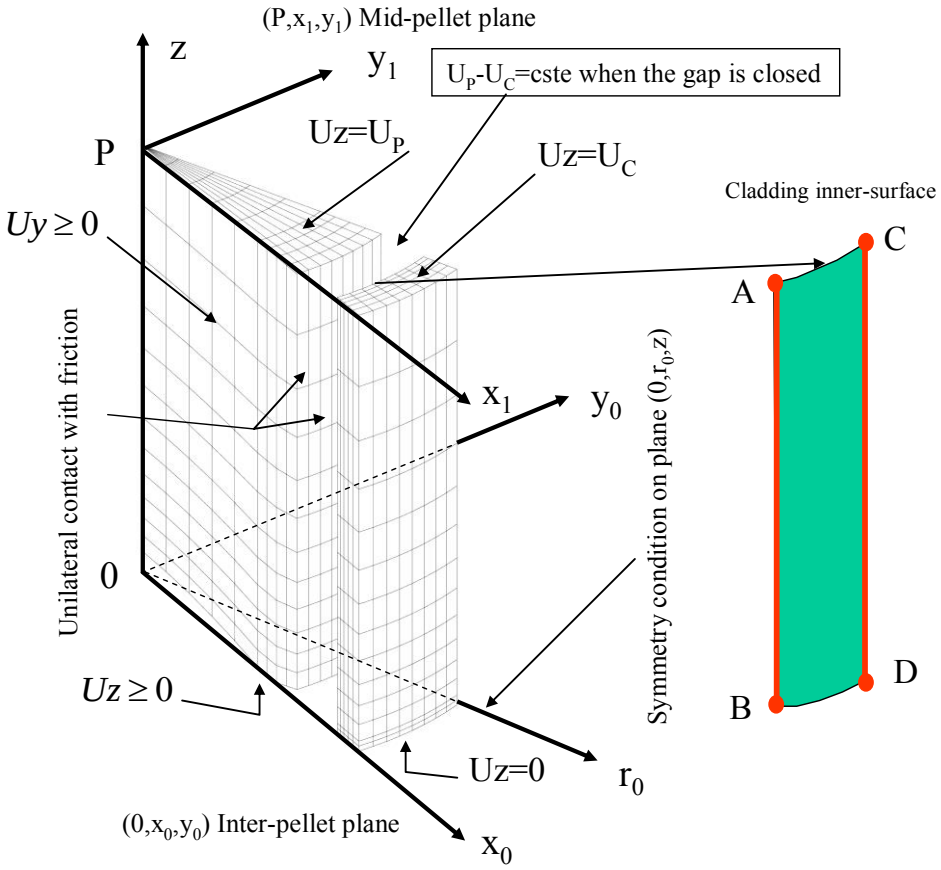


Figure 1: 3D finite element mesh for SFR fuel pin model

2.2 Thermo-mechanical coupling formulation

2.2.1 Thermal model

Temperatures of the fuel element are computed with the energy conservation equation (1) based on the Fourier's law for the thermal flux due to conduction.

(1) $div(\lambda . gradT) + p_v = 0$

With T the temperature, λ the conductivity and $p_v$the local nuclear power density source.

The thermal flux through the pellet cladding gap is computed with equation (2) where T_{clad} is the cladding internal wall temperature, T_{pellet} is the pellet external temperature and $h(T)$ a nonlinear heat exchange coefficient.

(2) $\Phi = h(T).(T_{clad} - T_{pellet})$

2.2.2 Mechanical model

Mechanical state of the fuel element is computed with the static equilibrium equation (3) integrated according to a weak formulation with the Finite Element method.

(3) $div\bar{\bar{\sigma}} = 0$

Where $\bar{\bar{\sigma}}$ is the Cauchy stress tensor.

In addition to this equilibrium principle, the non-linear behaviors of the pellet and the cladding are taken into account through several mechanical models with an elastoviscoplastic formulation based on the Hooke law (4) and an uncompressible formulation for plasticity and

creep (see equation (5) and (6)).

$$\dot{\bar{\sigma}} = \underline{\underline{E}} : (\dot{\bar{\varepsilon}}^{tot} - \dot{\bar{\varepsilon}}^{th} - \dot{\bar{\varepsilon}}^{ir} - \dot{\bar{\varepsilon}}^{plast} - \dot{\bar{\varepsilon}}^{creep}) \quad (4)$$

$$\dot{\bar{\varepsilon}}^{plast} = \mathrm{g}\left(\bar{\bar{\sigma}}, \mathrm{T}\right) . \frac{\partial \sigma_{eq}}{\partial \bar{\bar{\sigma}}} \quad (5)$$

$$\dot{\bar{\varepsilon}}^{creep} = \left(f_{ir}\left(\bar{\bar{\sigma}}, \dot{\phi}, \mathrm{T}\right) + f_{th}\left(\bar{\bar{\sigma}}, \dot{\phi}, \mathrm{T}\right)\right) . \frac{\partial \sigma_{eq}}{\partial \bar{\bar{\sigma}}} \quad (6)$$

Where $\underline{\underline{E}}$ is the Hooke fourth order tensor, $\dot{\bar{\varepsilon}}^{tot}$ the total strain rate according to a small strain assumption, $\dot{\bar{\varepsilon}}^{th}$ the thermal expansion strain rate, $\dot{\bar{\varepsilon}}^{ir}$ the irradiation volumetric strain rate, $g(\,)$ the equivalent plastic strain rate, $f_{ir}(\,)$ the equivalent irradiation creep strain rate, $f_{th}(\,)$ the equivalent thermal creep strain rate, $\dot{\phi}$ the fission density rate or the fast neutron flux damage rate and σ_{eq} the von Mises equivalent stress.

Unilateral contact condition used for the pellet cladding interface, the inter pellet plane and the pellet fragment surface crack, is derived from a contact status algorithm proposed in the Cast3M Finite Element solver [4].

2.3 Multi physic computation scheme

In the calculation process, chemo-chemical state variables and fuel rod scale global variables are still computed with the 1D models of GERMINAL V2, and are then considered as input loading data for the 3D thermo-mechanical coupling formulation. The list of these input data is the following:

- gas content and pressure in the pellet-to-cladding gap
- cladding external temperature
- mean power density and burnup in the pellet
- mean pellet porosity
- fast neutron damage level in the cladding
- internal pellet hole size and associated fuel mass transfer
- oxygen to metal ratio
- fuel shrinkage and swelling under irradiation

All these input data are time dependent and some of them depend also on the radius. In the latter case the 3D input field is built with an interpolation method based on the kriging technique according to an axisymmetric cylindrical geometrical assumption.

The coupling formulation for each time step has been implemented in the LICOS application as following:

- Input loading data initialization at the end of the time step
- Iterative computation of the thermomechanical solution
  - thermal computation
  - nonlinear mechanical computation
  - thermomechanical convergence test
- Solution update for the next time step

3 Radial fuel relocation process and 3D results

A first study has been achieved for SFR fuel pins extracted from the GERMINAL validation data base. This simulation is devoted to a phenomenological analysis of the pellet-to-cladding gap closure mechanism at the beginning of irradiation and cannot already be used for the validation. The results presented in sections 3.1 and 3.2 are respectively for an ASTRID annular pellet and a PHENIX full pellet. Nominal irradiation conditions are considered in both cases.

3.1 Pellet hour glass shape under thermal gradient

Thermal stresses induced by the temperature gradient under the first power increase will lead to the pellet fragmentation as it is assumed in the single pellet fragment model presented in section 2.1. The pellet fragment hourglass shape resulting of the mechanical equilibrium is shown in Figure 2. This hourglass shape leads to a first gap closure at the inter-pellet plane with lower temperatures in the pellet as shown in Figure 2. When comparing to the un-fragmented pellet, we can define radial relocation displacements at inter and mid pellet planes (see Figure 2). At the mid pellet plane, the radial relocation displacement is mainly due to the circumferential thermal expansion in the central zone of the pellet. For the inter pellet plane the axial curvature of the pellet fragment increases significantly the radial relocation displacement. The radial relocation displacement at the mid pellet plane can be compared to a uniform radial and circumferential strain field which can be in the range [0.5-0.8%] under nominal conditions and can lead to a pellet cladding gap thickness reduction between 15 and 25%

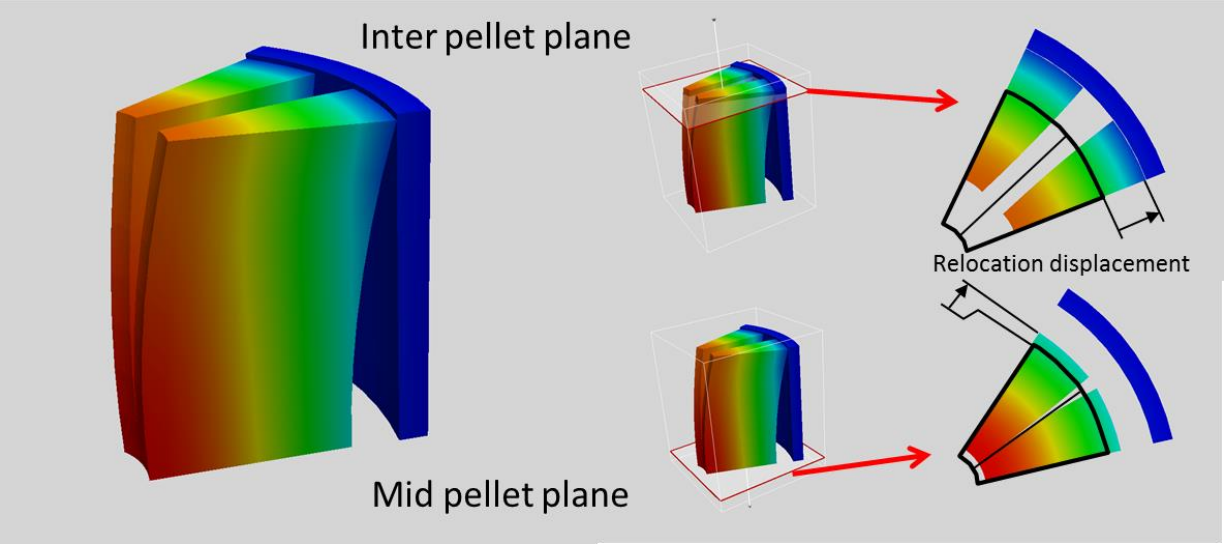


Figure 2 : Pellet fragment hourglass shape and temperature at the end of the first power increase.

3.2 Central hole formation and associated fuel mass transfer

At the beginning of irradiation under SFR nominal power loading conditions, high temperatures lead to a fuel restructuring in the pellet central part, resulting in the formation of a central hole [1]. The main mechanism involved in this restructuring phenomenon is a fuel mass transfer due the diffusion of a vapour phase through material porosities (see references [5] and [6]). A porosity diffusion model has been implemented in GERMINAL [1] in order to compute the fuel mass transfer and the size of the central hole under irradiation. In this paper

a coupling mechanism between mass transfer and fuel relocation has been proposed according to a kinematic assumption illustrated in Figure 3. This assumption consist in considering that the fuel volume leaving the pellet centre is inserted between fragments in the columnar grain zone where the fuel has been restructured. This assumption is consistent with the idea that crack surfaces act as source of lenticular porosities needed for the mass transfer [6].

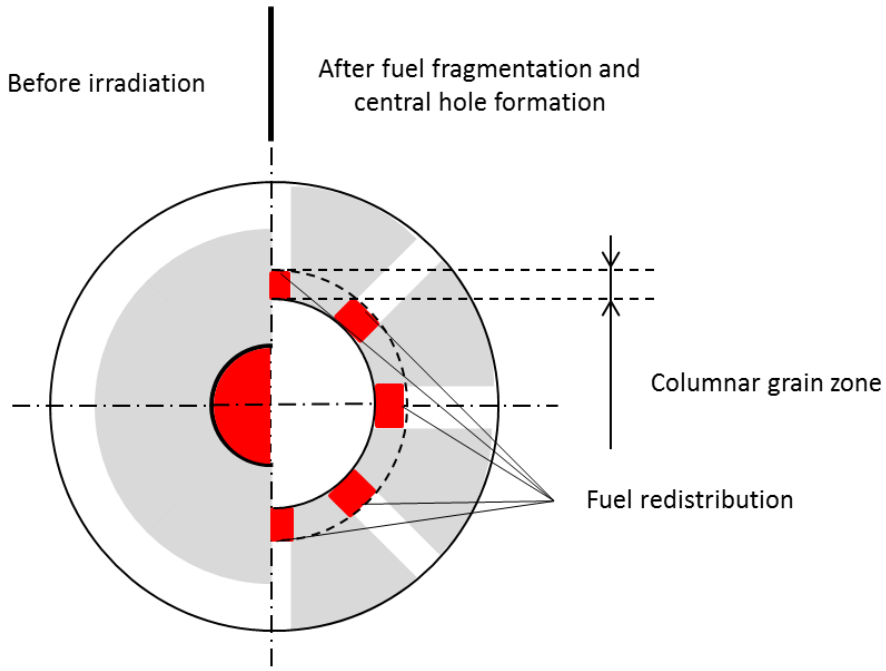


Figure 3 : Fuel mass redistribution and pellet fragment relocation during the central hole formation.

In the 3D fuel pin simulation, a first simple modelling has been proposed in order to compute the radial relocation displacement due to fuel mass transfer according to the kinematic assumption proposed in Figure 3.

First, GERMINAL results are post processed in order to compute the fuel volume transferred during the central hole formation (red surfaces in Figure 3). For each time step the fuel equivalent filling density can be derived from the porosity diffusion model of GERMINAL (see Figure 4). During the central hole formation, this equivalent filling density will decrease in the centre of the pellet, and, according to the mass balance equation, will increase for intermediate radii up to the maximal radius of the columnar grain zone. A radial integration of the negative part of the equivalent filling density variation between $t = 0$ and the current time step gives the fuel volume leaving the central part (blue hatched area in Figure 4).

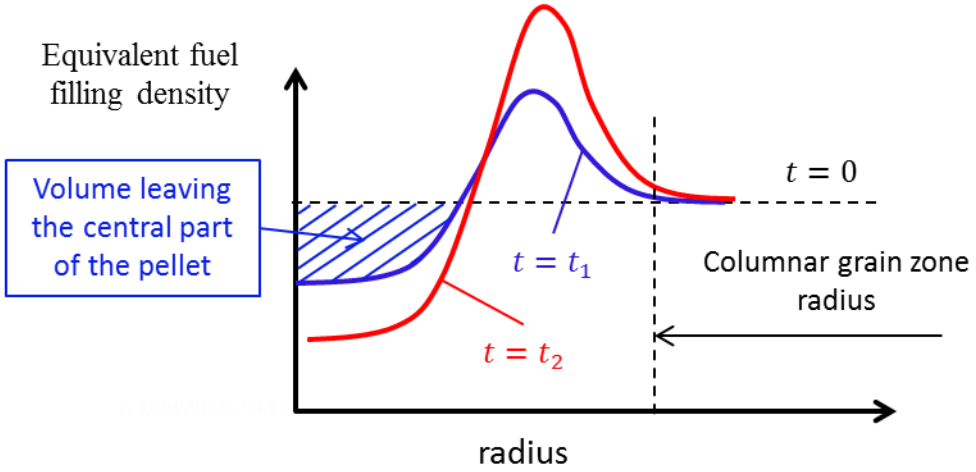


Figure 4 : Computation of the fuel volume transferred according to 1D results of GERMINAL.

Secondly, a displacement boundary condition is added in the 3D single fragment Finite Element model to compute the radial relocation displacement induced by the mass transfer. This boundary condition (see Figure 5) is defined on the free surface of the pellet fragment for the columnar grain zone (blue line in Figure 5) with a unilateral condition where $e(t)$ is the half thickness of the transferred volume between two pellet fragments at time t.

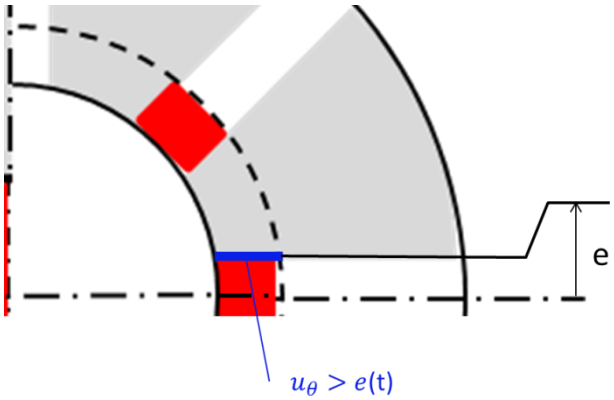
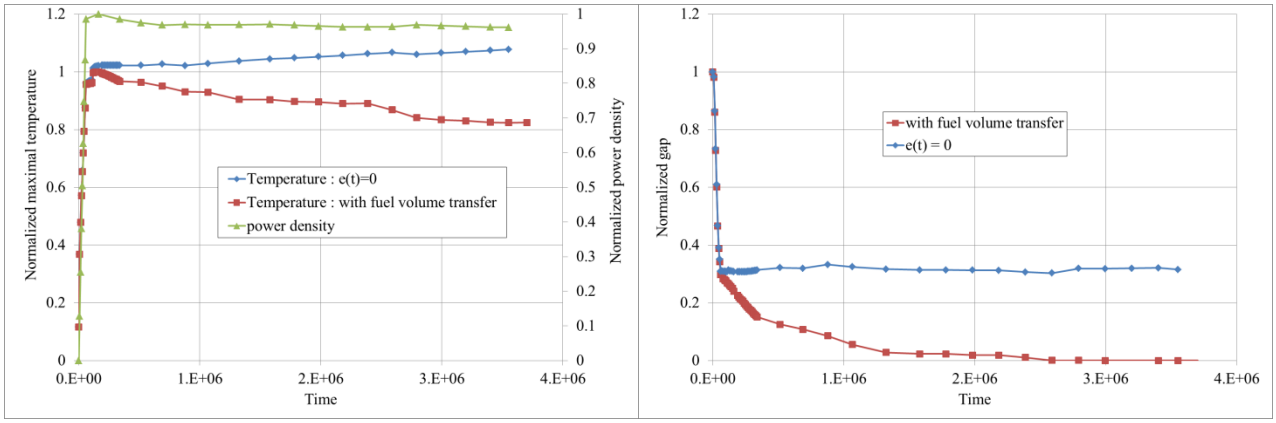


Figure 5 : Displacement boundary condition for the computation of the radial relocation displacement.

The results obtained in the 3D simulation are presented in Figure 6 a) for the maximal fuel temperature and Figure 6 b) for pellet cladding gap closure. To illustrate the impact of the mass transfer, a first computation has been achieved with a parameter $e(t)$ equal to zero. As expected, fuel volume transfer has a significant impact on the gap closure through the radial relocation displacement, we can see in Figure 6 b) that the pellet cladding gap is closed at the end of irradiation, compare to the case $e(t) = 0$. Consequently, a smaller gap leads to reduce the maximal fuel temperature of approximately 25% after an irradiation period of 45 days.



a) Maximal fuel temperature b) Pellet- cladding gap

Figure 6 : 3D simulation results: impact of the mass transfer on pellet- cladding gap closure.

4 Conclusions

In this work, a 3D Finite Element model of the SFR fuel pin is proposed to study pellet-to-cladding gap closure mechanism at the beginning of irradiation. The 3D model represents a single pellet fragment and its associated piece of cladding. A preliminary nonlinear thermo-mechanical computation scheme has been developed and implemented in the LICOS code of the PLEIADES platform. Chemo-physical state variables are pre-computed with the GERMINAL code and are introduced in the 3D computation scheme as some input data through the irradiation loading and interpolation techniques.

Pellet-to-cladding gap closure mechanism has been studied under nominal irradiation conditions and the fuel radial relocation displacement, computed through an empirical approach in the 1D model, can be explicitly defined with 3D results. Two mechanisms have been identified to explain the radial relocation displacement. The first one, due to the hourglass shape of the pellet fragments under thermal strains, is linked to the magnitude of the thermal gradient in the pellet and can lead to a significant relocation displacement at the mid pellet plane under an increasing power level. The second mechanism is based on a coupling phenomenon with the fuel mass transfer occurring during the central hole formation. The kinematic assumption, proposed to compute the relocation displacement, considers that the central hole volume in inserted between pellet fragments in the columnar grain zone where the fuel has been restructured. A first computation, with a simplified description of the coupling phenomenon, shows that this mechanism can explain a complete closure of the gap at the beginning of irradiation during the central hole formation.

New developments are now in progress in order to propose a fully coupled formulation between the porosity diffusion model and the radial relocation displacement model. This new formulation will be used to improve the 1D computation scheme of GERMINAL and will prepare further developments to extend the GERMINAL fuel performance code to the 3D simulation.

5 References

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