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A SIMPLE MULTIPHYSICS COUPLING FOR HIGH-FIDELITY NEUTRONIC MODELLING IN FUEL PERFORMANCE CODES

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ABSTRACT

This work focuses on the development of a coupling scheme between the fuel performance code ALCYONE and the neutron code APOLLO3® in order to provide the most accurate simulation environment of a fuel rod. Steady state calculations are considered with fuel depletion along exposure. The coupling scheme is demonstrated on a UO2 fuel pin. Fuel performance codes generally use simplified neutronic models to calculate fast approximations of the thermal power distribution produced by nuclear reactions. A short review of the simplified models is here provided with a discussion on their limitations. The results with the new coupling scheme are compared with those obtained using the recommended neutronic model PRODHEL in stand-alone ALCYONE calculations in order to verify the implementation in its own domain of validity.

KEYWORDS: Multi-physics, fuel performance code, neutronics, water reactors

1. INTRODUCTION

The most accurate physical modelling is necessary to reproduce computationally the real behavior of a fuel rod under long exposures in a nuclear water reactor. Different physical phenomena concur at the same time, providing a strongly coupled problem whose implementation is technically very challenging. Thermal energy produced by fission and by deposition of gamma radiation accumulates as enthalpy in the solid fuel, and it is transferred by heat convection to the coolant. The high neutron flux creates structural damages by inducing atom displacements and dislocations in structural materials. It causes severe build-up of gaseous fission products which migrate towards the free space within the cladding as a consequence of fuel cracking and porosity change. Pressurization of the clad works against external compression operated by the primary coolant. The closure of the gap between the fuel pellet and the cladding due to mechanical stresses on the clad, swelling, thermal dilatation and other deformations of the pellet, imposes a complex modelling especially when both normal operation and transient accidental conditions are requested [1,2]. Further, clad oxidation and possible deposit on its outer surface (CRUD) are now demanded in safety studies. All these physical phenomena can be reproduced by fuel performance computer codes, like ALCYONE.

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Fuel pin simulations cover various applications and case scenarios to estimate the performances of the fuel and to study the pellet-cladding interaction (PCI) during operational exposure, load following and accidental transients [3–5]. Because of the physical complexity, approximations and simplified physical models may be used to achieve affordable calculations. This is generally the case for the simplified neutronic models integrated in the fuel performance codes in order to reproduce the energy deposition in the fuel pellet, whose radial function is almost flat at the center and very steep towards the outer surface because of cross section self-shielding and the RIM effect. Furthermore, plutonium production, mainly ^{239}Pu from ^{238}U capture, makes the gradients even steeper with exposure.

Traditionally, fuel performance codes take input axial rod power distributions and coolant channel temperatures computed by coupled thermo-hydraulic and neutron codes for PCMI investigations and screening purposes [6,7]. This stand-alone use is one-way, and requires own neutronic modules in the fuel performance codes to recompute radially the power profile in the fuel. On the other hand, the coupled core codes use uniform temperature in the fuel materials, with the need of defining additional equivalent data, like the effective fuel temperature [8].

The goal of this work is to provide, in a unique simulation environment, the most appropriate models and computer codes, by means of a loose coupling between the thermo-mechanical code ALCYONE [9,4] and the neutron code APOLLO3® [10,11]. Specifically, APOLLO3® is providing realistic power distributions within the pellet and the isotopic concentrations all along the irradiation history inside the reactor. Iteratively, APOLLO3® performs the self-shielding in the pellet rings using the latest temperature profile computed by ALCYONE. On the other hand, ALCYONE provides accurate modelling of the fuel pin thermal-mechanics and chemistry, feeding APOLLO3® with new estimates of local temperature values. Thermal expansions are currently disregarded because of additional development work needed in APOLLO3®; size and porosity changes are deferred as future improvements. Steady state calculations with isotopic depletion are considered here to model fuel rods under exposure. The solution of coupled problems in fast transients are left for future development programs.

This work represents the first realization of a close coupling at the fuel pin level applied to LWR lattices that has been accomplished at CEA, which enables to validate the simplifying assumptions about the temperature distribution in a stand-alone neutronic calculations on one hand, and the approximate neutronic models in ALCYONE on the other. The latter question is addressed in this paper.

Previous efforts in coupling high fidelity neutron codes to the fuel thermo-mechanics are shown by Clarno et al. [12] with AMPFuel and the radiation transport code Denovo. The analysis was extended to a full PWR assembly, using Zernike polynomials to smooth the power computed on a coarse mesh by Denovo. Finer meshes for the resolution of the neutron transport problem with the method of characteristics were used instead in the code DeCART, coupled to BISON on the MOOSE framework [13,14]. In this work, the method of characteristics is also used, and cross sections are self-shielded according to the fine structure Livolant-Jeanpierre formalism [15]. Mesh refinement towards the outer pellet surface is adopted with a trade-off between minimal mesh size to represent the rim region and the computational effort, thus following tight tracking of the neutron trajectories.

Sec. 2 presents the computer codes used in this work. A short review of the simplified neutronic models available in literature follows in Sec. 3, with a discussion on their limitations. As a complement, the problem of the RIM effect is introduced in sec. 4. The numerical scheme of the new proposed coupling is shown in Sec. 5. The implementation of the coupling scheme is demonstrated in Sec. 6 on the example of a regular UO2 pin typical of a PWR along fuel exposure. A second stage of validation on complete fuel rods and on other fuel types is postponed to future works.

2. CODES OVERVIEW

2.1. APOLLO3

APOLLO3® is the CEA general purpose deterministic transport and diffusion code developed under a collaborative program with AREVA and EDF. It replaces the previous generation of codes comprising APOLLO2/CRONOS2 and ECCO/ERANOS system of codes. It treats thus both thermal and fast neutron spectra and performs the calculation on the scale of a lattice (assembly) and the whole reactor. Different 2D and 3D solvers are adapted for the specific problems of reactor physics studies. The method of characteristic is implemented for the principal flux solver used for detailed transport at the fuel pin level and also for the 3D motifs or small cores in direct calculation without homogenization. The short (IDT) and long (TDT) characteristics approximations are available. The other two methods used mainly for 3D reactor calculations are based on SPN or diffusion approximation (MINOS), based on Raviart-Thomas finite elements and on discrete ordinate method with discontinuous Galerkin finite elements.

Three different approaches are implemented in the self-shielding module. The first is the APOLLO2 classics, that is the Livolant-Jeanpierre method or "fine structure" based on equivalence theory and mainly used for thermal reactors. The second is the subgroup method, whose development is inspired by ECCO formalism and intended to fast spectra applications; the third is the recently implemented Tone's method. All three are based on extensive use of probability tables. The depletion calculation is performed using the MENDEL solver [16], which is an independent project linked to APOLLO3®. The algorithm is based on the predictor-corrector scheme assuming a linear or a parabolic dependency of reaction rates on burnup variables. The Bateman equations are solved numerically using the fourth order Runge-Kutta scheme.

2.2. ALCYONE

ALCYONE is a fuel performance code developed under a collaborative program by CEA, EDF and AREVA [17]. ALCYONE is distributed with the platform PLEIADES and it is dedicated to pressurized water reactors (PWR). PLEIADES is a code system for the simulation of different kinds of nuclear fuel with data management based on SALOME [18].

ALCYONE offers multi-dimensional accurate physical modelling of fuel rods in quasi-static applications along base irradiation and in transient conditions. In particular, both fast transient and programmed power ramps can be reproduced. The solution of the thermal and of the mechanical problems are delegated to the FEM code Cast3M [19].

The fuel rod is represented with multiple slices along the axial dimension, which are coupled by the

gas release in the gap, the fuel pellet cracking and the mechanical stresses in the clad. Azimuthal description of the rod slices is also possible with 2D calculations.

Two simplified neutronic models are available in ALCYONE [20]. The first is an extended version of the original Palmer's model RADAR, whereas the second, called PRODHEL, computes in addition also the helium concentration in the fuel. PRODHEL is the recommended model in ALCYONE. These models are explained in detail in sec. 3.

3. SIMPLIFIED NEUTRONIC MODELS

A neutronic model is necessary in fuel performance computer codes to provide the power profile in the fuel elements. Simplified models are used in all existing codes for the high computational efforts required by the neutron transport codes. These models may solve on-line simplified physics or call precalculated lookup tables.

The thermal power P is calculated as the reaction rate of deposited thermal energy, mainly produced by fission. By the volume-specific power density P_V (W/cm^3), the power is generally factored as $P = P_V(t)q(r)$, where q is the dimensionless spatial power profile. The power density is determined through the linear heat rate P_{lin} (W/cm), given in time as input data, as $P_V = P_{lin}(t)/S_q$, where S_q (cm^2) is the heating surface of the fuel region. The following normalization must then apply to q, provided azimuthal symmetry around the rod axis:

$$\frac{1}{S_q}\int_{r_0}^{r_s} 2\pi r q(r) dr = 1, \tag{1}$$

with r_0 and r_s respectively as inner and outer surface radius of the fuel region, so that $S_q = \pi(r_s^2 - r_0^2)$.

RADAR (RAting Depression Analysis Routine) by I. Palmer is probably the first model occurring in literature [21]. Originally developed for uranium fuel with the only tracking of ^{235}U and ^{239}Pu, it was extended in later versions with more actinides to cover the MOx fuel type and high burnup exposure [22]. The explicit Euler scheme in time is used to solve the Bateman equations. It requires however reactor specific input data, like the fast leakage factor and the resonance escape probability, to estimate the total amount of plutonium produced at a given burnup step. A steep exponential function is added to the balance equation of ^{239}Pu in order to reproduce the increased production near the surface of the pellet:

$$\Delta f_P = 1 + 3\exp\left(-9.7\sqrt{r_s - r}\right), \tag{2}$$

subject to a condition of volume normalization to the total amount of plutonium generated.

The resolution of the Helmholtz equation in cylindrical coordinates yields the thermal neutron flux as combination of modified Bessel functions of the first kind. This assumption is common to the most of the simplified models. The isotope concentrations computed in discrete points along the radius draw the spatial distribution of the macroscopic cross sections, since only constant values are available for the microscopic cross sections.

RADAR was also used by the code TRANSURANUS developed at JRC-KIT by Lassmann et al., who evolved it into a new model called TUBRNP [23]. TUBRNP uses a modified Palmer's

function to radially distribute ^{238}U, thus avoiding the original normalization that requires reactor specific data [24]. This model covers both LWR and HWR applications [25].

Although ALCYONE v1.4 has its own customized version of RADAR, its recommended model is PRODHEL [26]. As suggested by its name, it can also calculate the helium production in the rod, which is of particular interest for MOx fuel. PRODHEL uses one-group burnup-dependent cross section data produced by the code APOLLO2 and JEFF3.1.1. The tracked actinides are $^{235-239}$U, $^{237-239}$Np, $^{238-243}$Pu, $^{241-243}$Am, ^{242M}Am and $^{242-244}$Cm. The depletion solver can use a Chebyshev algorithm from EXPOKIT or the Runge-Kutta method by SLATEC. Fuel-type dependent Palmer's functions are used to distribute radially the capture reaction rates of ^{238}U and $^{239-241}$Pu.

Eventually, the simplified models often use one-group cross sections, spatially constant and possibly burnup-dependent, stored in separate lookup tables. Their validity range is generally limited to the only simulated modelling conditions. Reduced chains of actinides are employed, with the only thermal flux for calculating the reaction rates and empirical corrections to account for fast fissions. Only a short list of fuel types are allowed, demanding ad-hoc developments for new ones. It must also be noted that the Helmholtz equation with constant coefficients gives a poor approximation of the neutron transport, and mostly, it is not suitable to reproduce heterogeneity in fuel poisoned by burnable absorbers.

4. THE RIM EFFECT AND THE SPATIAL MESH

In water reactors, neutron fission increases at the outer layer of the fuel pellets because of thermal moderation in the coolant, spectrum hardening in the fuel and the consequent self-shielding effects in the pellet edge, also called RIM [27,28]. This means as well a decreasing neutron flux in the central region of the fuel. Hence, ^{235}U depletes radially inwards in the pellet with ^{239}Pu produced mostly outwards by epithermal resonance capture of ^{238}U after two beta decays.

The radial power distribution is higher in the pellet RIM yet with fresh fuel, becoming more peaked along exposure for the occurrence of further heavier fissile actinides, see Fig. 1. Due to favoured reaction rates, an excess of fission products in the RIM is verified with increasing porosity in the burnup for diffusion and migration of the gaseous terms, mainly xenon and krypton, to the gap of the fuel rod. A degradation of the thermal conductivity in the outer fuel layer with the concomitant modification of the power profile (Fig. 1) redistributes the temperature profile, so that, provided the same surface temperature and linear power, its center maximum value may decrease slightly. At burnup higher than about 50 GWd/t, the fuel undergoes a restructuring process known as HBS (High Burnup Structure). The RIM zone extends radially for a few tenths of μm.

It follows that the isotopic content of the fuel changes all along the exposure with stronger gradients in the rim region and in its neighborhood, demanding for a very fine mesh indeed. Reliable power profiles need accurate local temperatures and isotopic concentrations, thus enforcing the tight coupling between neutron transport, heat transfer and material science. However, the neutron flux calculation with a mesh size of O(10-100) μm in radial pin problems can be from 10 to 100 times longer than its ALCYONE counter-part depending on the use case (1D or 2D), with limiting acceptance in feasibility for the modelling of a full rod. Hence, a trade-off between local accuracy and the computational effort is necessary.

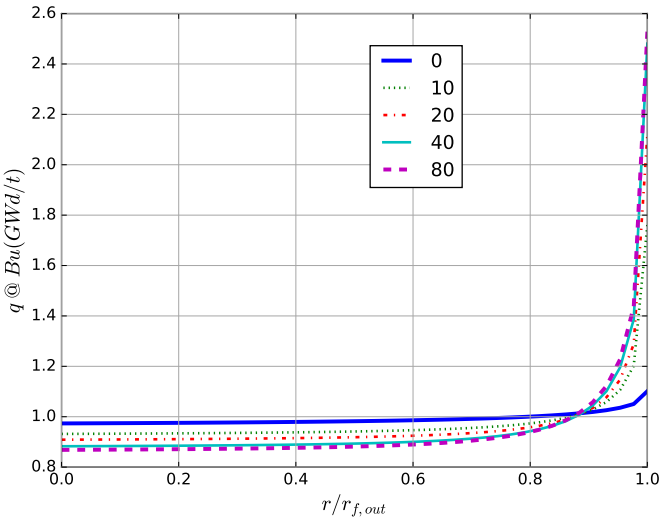

Figure 1: Behavior of the radial power profile in uranium fuel along exposure.

In this work, we use the same mesh in both models of APOLLO3® and ALCYONE of an axial slice of a fuel rod to avoid the use of complex reconstruction techniques for the radial power profile. However the unknowns of ALCYONE are located on the bounds of the annular rings, whereas APOLLO3® works with average quantities in the ring volumes. Also, ALCYONE considers all variables linearly dependent on the radius, thus the temperature in the i-th ring is:

$$T_i(r) = a_i T_{i,in} + (1 - a_i) T_{i,out}, \text{ with } a_i = \frac{r_{i,out} - r}{r_{i,out} - r_{i,in}}; \tag{3}$$

volume-averaged temperature values become:

$$\begin{aligned} \bar{T_i} &= \frac{1}{S_i} \int_{r_{i,in}}^{r_{i,out}} 2\pi r T(r) dr = b_i T_{i,in} + (1 - b_i) T_{i,out}, \ \forall i \text{ with} \\ b_i &= \frac{1}{3} \left(\frac{r_{i,out} + 2r_{i,in}}{r_{i,out} + r_{i,in}} \right), \ S_i = \pi (r_{i,out}^2 - r_{i,in}^2), \end{aligned} \tag{4}$$

in and out respectively as the inner and the outer boundaries of the given ring. An additional constraint is necessary for the determination of the boundary values of the radial power profile, being the central symmetry condition $\nabla q(r_{1,in}) = 0$. Due to the first order approximation used, we use $q_{1,in} = q_{1,out}$. The other values $q_{i>1,out}$ follow from Eq. 4 by substitution of the known power at the inner bound of each ring. This simple choice may yield non-monotone functions with coarse meshes. This event however is prevented here by the fine meshing used to model accurately the RIM. Specifically, the meshes are obtained by geometric progressions with the smaller ring width of 100 μm at the pellet surface.

5. THE COUPLING SCHEME

Alcyone models a fuel rod as an ensemble of multiple slices coupled through the gap physics. The numerical scheme used in ALCYONE to solve the multi-physics fuel rod problem is presented in detail by Marelle [17]. This scheme is resumed briefly hereafter.

Three nested levels of iterations are noticed within each time step. About all physical models applied on each fuel slice, only heat transfer, mechanics and gaseous diffusion and release enter the lowest level of iterations. The fixed point on all models is sought by successive substitutions, according to the Gauss-Seidel scheme. The Steffensen's method is used to accelerate the convergence on gas swelling due to intragranular bubbles. Under-relaxation on the temperature distribution prevents unwanted oscillations. A loop on all slices determines the new state of the rod to then run possible additional coupling with the closed-channel thermo-hydraulics in case of fast transients.

Neutronics does not enter the inner loop since the effects of the temperature on the nuclear cross sections is neglected. This approximation can be fully acceptable when reliable temperature profiles (parabolic-like) are considered in the derivation of the simplified neutronics models. Indeed, the Doppler reactivity coefficient rising from the heavy isotopes in the fuel is of a few pcm per temperature degree, thus justifying this approximation. In this work, the multi-physics inner iterations are extended up to neutronics, to eventually account also for possible thermal feedback on cross sections in the fuel, see Fig. 2. A tolerance of 0.1% on the volume-specific values is adopted to establish the convergence of the radial power profile on the heated surface of the pellet.

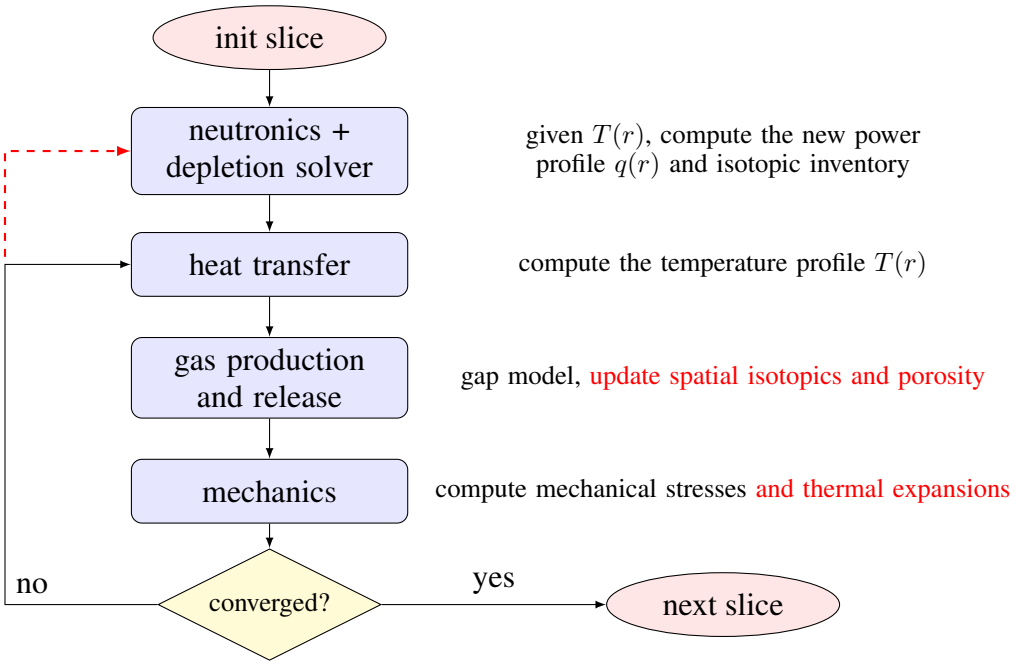

Figure 2: Extension of the multiphysics loop to neutronics (dotted red line). The text in red at right suggests new possible improvements.

5.1. Coupling at the pin-cell level

The previous realizations of the APOLLO3-ALCYONE coupling [7] have been applied in the context of whole reactor calculations where the multigroup cross sections where processed according to the standard homogenization procedure and put in form of multi-entry interpolation tables. The state points are characterized with burnup, average fuel and coolant temperatures and boron concentration. The neutronic part of the coupled multiphysics problem here was solved using simplified models within ALCYONE. In the present work the coupling is realized at the level of the fuel pin, where the temperature dependency is explicitly used in self-shielding and neutron flux calculation. The power distribution is thus calculated by APOLLO3® using the updated temperature distribution in each coupling iteration.

The current implementation of the coupling with APOLLO3® is limited to the steady state problems during fuel exposure, and it does not cover fast transients yet. Although the internal time manager of ALCYONE may insert additional time steps for error control and prevention, the synchronism in time with the APOLLO3® depletion is ensured all along the fuel irradiation.

This study is limited to a single axial slice of a single fuel pin. The generalization of the procedure to the axially dependent problem of fuel assembly is straightforward, where the ALCYONE calculations could be performed simultaneously for each fuel rod and each axial layer.

6. RESULTS

The coupling of ALCYONE and APOLLO3® is demonstrated in this section on a PWR-UO_2 fuel slice problem. The slice belongs to a homogeneous rod with active length of 340 cm and flat axial power distribution. The exposure at the mass-specific power density of 38.25 W/g is reproduced up to 60 GWd/t, first using the recommended model PRODHEL and then by the APOLLO3-ALCYONE coupling. The wall cladding temperature is set at 600 K.

APOLLO3® models one eighth of pin cell, whose pitch is 1.26 cm. The outer diameter of the pellet is 3.9 mm, which is discretized in 12 annular rings with the volume of the smaller ring at the outer surface of 5%, that means a width of about 100 μm. The inner and outer radii of the Zircaloy-4 clad are respectively 4.0 and 4.6 mm. Self-shielding by the fine structure Livolant-Jeanpierre formalism [15] is applied to the cross sections of the following isotopes $^{234-238}$U, $^{239-242}$Pu, ^{241}Am and ^{243}Am. The radial meshes in the fuel region are the same in the two codes, with volume-averaged reaction rates for APOLLO3® and unknowns located on the radial surfaces for ALCYONE. The reconstruction of surface or volume quantities is operated as in section 4.

The maximum relative differences of the temperature distribution and of the radial power density are plotted in Fig. 3 (left). Differences follow as the values computed using APOLLO3® as neutronic model minus that produced with PRODHEL. Although differences of more than 6% are noticed on the power profile at high burnup, the temperature differences at the hotter center of the pellet are less than 1%. The gap conductance is plotted on the right of Fig. 3, showing differences mainly due to different amounts of gas released in the gap. In fact, reaction rates computed by APOLLO3® are also used to set quantities like the ratio of Xe/Kr needed in the gas release models. The average neutron flux and the fast flux ($E > 1$ MeV) calculated in the clad by APOLLO3® are also part of the dataset transferred to ALCYONE. The gap conductance does not show significant

differences until the gap closure occurring at about 30 GWd/t, but at different times with the two neutronic models. After, the contact pressure shows differences which are reducing as long as the irradiation continues.

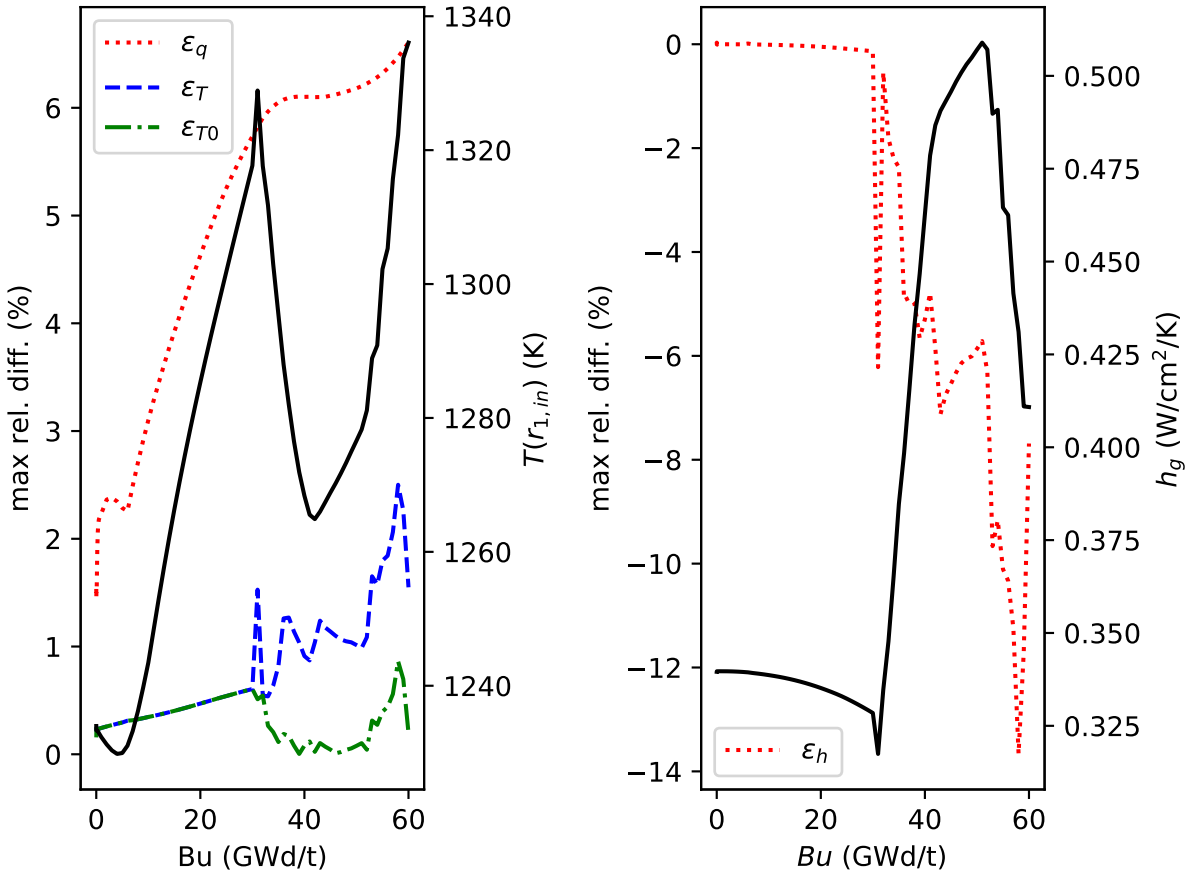

Figure 3: Maximum relative differences along exposure of the temperature distribution ϵ_T and of the radial power density ϵ_q (left), and of the gap conductance ϵ_h (right); ϵ_{T0} indicates the differences at the center of the pellet (i.e. at $r_{1,in}$). Absolute values are on right axes.

Fig. 4 illustrates the radial distributions of the relative differences of the fuel temperature and of the radial power profile. The power profile is always overestimated of a few percents by PRODHEL in the center of the pellet. Whereas in outer zone, the power deposited by APOLLO3® in the RIM region becomes higher without showing the asymptotic increase typical of the Palmer's function, and of PRODHEL. Lower temperature values are computed by APOLLO3® at the center of the pellet when the gap is opened. After its closure, different gap conductance values at the same burnup cause higher temperature at the pellet surface when using APOLLO3®, without however inducing significant increase of the temperature at the center.

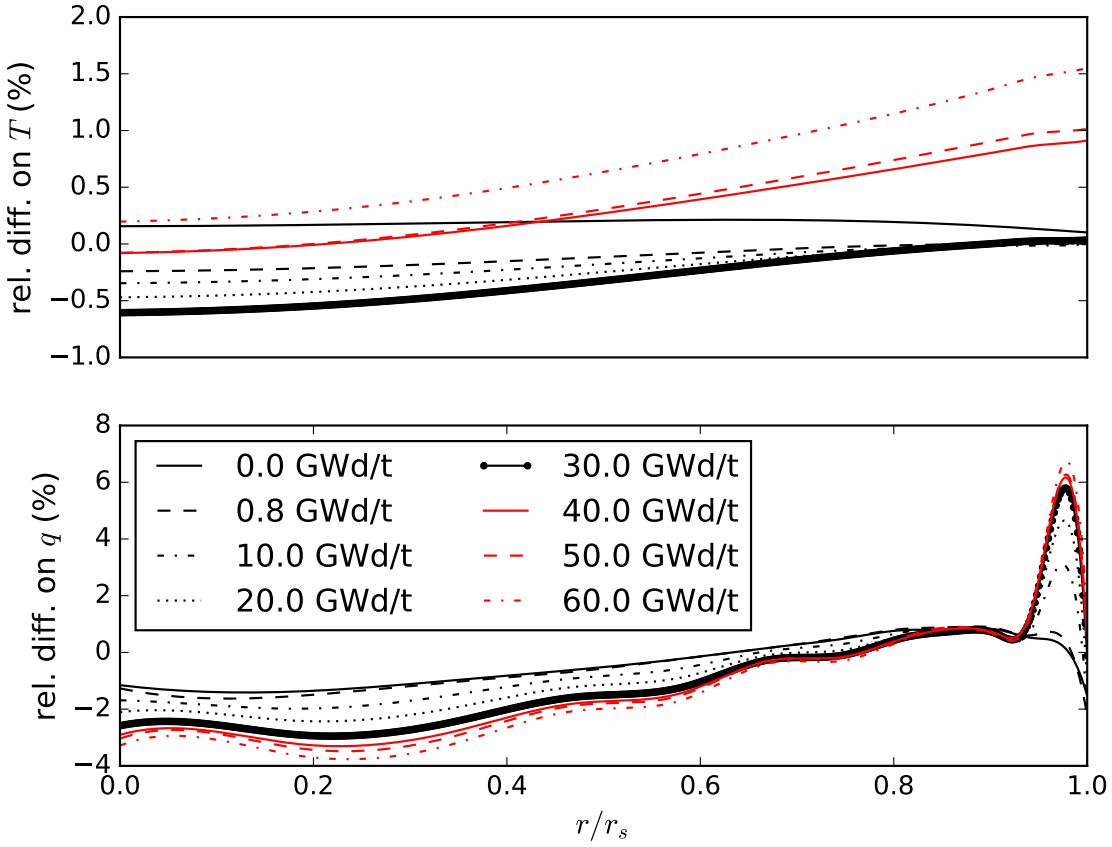

Figure 4: Radial distribution along exposure of the relative differences of the temperature distribution T (top) and of the radial power density q (bottom).

7. CONCLUSIONS

In this paper we show the first works on the coupling between the neutron code APOLLO3® and the fuel performance code ALCYONE v1.4. Development versions of the codes have been used to ease the coupling effort. The objective is to replace all simplified neutronic models integrated in ALCYONE by APOLLO3®. The exchange between power and temperature distributions in the iterative procedure is done at the level of the fuel pin.

The example calculation presented here is limited to a single axial layer of a fuel pin cell, but the application to the axially dependent problem of the fuel assembly is straightforward. It serves indeed the purpose of verification for the current implementation, provided that the stand-alone ALCYONE calculation with its recommended model PRODHEL provides already excellent results on this test case. The comparisons of the radial temperature and of the power density distributions along the exposure are encouraging. Results compare well, with slightly lower temperature values at the center of the fuel pellet produced by APOLLO3®.

At the current stage of the work, APOLLO3® calculations are much longer and resource demanding than the calls to the ALCYONE modules. However, we observed only two or three radial power profile updates by APOLLO3® before achieving the convergence according to the selected criterion. The whole stand-alone simulation by ALCYONE takes overall a few minutes, whereas the problem coupled with APOLLO3® runs in about five hours on a 64bit Intel Xeon CPU 2.4GHz with openMP parallelism on 20 processors. Regarding this simple use case, the stand-alone ALCYONE execution shows outstanding performances compared to the much more computationally intensive problem coupled with APOLLO3®.

It seems then mandatory to use coarser and non-overlapping meshes with the neutron transport solver to attain feasibility for practical cases. This means either developing more accurate reconstruction techniques or allowing the solver to treat non-uniform cross sections within the spatial cells. The computation time overhead in the current implementation is mainly due to the detailed self-shielding calculations that are done every time the temperature changes during the iterations. This involves the interpolation of self-shielding data and the calculation of effective cross sections for as many spatial regions as radial fuel meshes. Different options are considered for future developments based on coarser spatial meshes for both the self-shielding and flux calculations.

The proposed coupling is here presented in steady state problems offering the advantage of modelling any fuel type with a single implementation. The interest in this coupling is even higher for fast transient cases, where temperature distributions are very different from the classic parabolic-like shape. Extension to full fuel rod and transient problems are expected as future developments.

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