Nuclear Engineering and Technology xxx (xxxx) xxx

Contents lists available at ScienceDirect

Nuclear Engineering and Technology

journal homepage: www.elsevier.com/locate/net

Original Article

Assessing the impact of DIONISIO-SubChanFlow code coupling in nuclear fuel performance simulations

Mauricio Exequiel Cazado [a,b,*], Victor Hugo Sánchez-Espinoza [a], Alejandro Soba [c,d]

[a] Institute for Neutron Physics and Reactor Technology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, Eggenstein-Leopoldshafen, 76344, Baden-Württemberg, Germany
[b] Instituto Sabato, UNSAM-CNEA, Avenida General Paz 1499, San Martín, 1650, Buenos Aires, Argentina
[c] Sección Códigos y Modelos, Gerencia Ciclo del Combustible Nuclear, CNEA, Avenida General Paz 1499, San Martín, 1650, Buenos Aires, Argentina
[d] Consejo Nacional de Investigaciones Científicas y Técnicas - CONICET, Godoy Cruz 2290, 1425, Ciudad Autónoma de Buenos Aires, Argentina

ARTICLE INFO

Keywords:
DIONISIO
SubChanFlow
Nuclear fuel performance
Cladding oxide layer

ABSTRACT

Realistic simulation of nuclear fuel performance requires not only validated models capable of describing the thermomechanical phenomena that take place within the fuel under irradiation conditions, but a detailed description of the thermal hydraulics of the channel surrounding the fuel rods, which provides the boundary conditions of the system. In this work, the main results and outlooks of coupling the thermal hydraulics code SubChanFlow with the fuel performance code DIONISIO are presented. To achieve this, an internal coupling was implemented, wherein DIONISIO is used as a master code controlling SubChanFlow as a thermal hydraulics subroutine replacing the simplified version already embedded in DIONISIO. Several tests were conducted to ensure the performance and quality of the coupling under normal operation conditions as a first approach. In addition, it was observed that the coupling demonstrated a significant improvement in the description of the cladding temperature and related variables, such as oxide thickness and hydrogen uptake, when compared with experimental data.

1. Introduction

The Codes and Models Section of the Nuclear Fuel Cycle Management (GCCN) of the National Atomic Energy Commission of Argentina (CNEA) has developed a code called DIONISIO. This code simulates the behavior of a nuclear fuel rod under irradiation inside a reactor, in both under normal operating conditions and in Loss-of-Coolant Accident (LOCA) scenarios. DIONISIO is a multidimensional code, incorporating uni–, bi–and tri–dimensional models coupled to one another. These models allow the simulation of the thermomechanical evolution of a fuel rod during irradiation [1–4]. Since DIONISIO aims to simulate the main phenomena occurring inside an irradiated fuel rod, in particular, those related to the pellet and cladding materials, the code estimates the thermal hydraulics of the channel surrounding the rod by means of a simplified one–dimensional model. However, the physical processes that take place in this channel domain have a crucial effect on the performance of the fuel, since the functions of the coolant are to extract the heat generated by the fuel and to determine the thermal boundary conditions for the code [5,6]. In a LOCA event, the analysis of the behavior of the fluid becomes even more important, since the main relevant phenomena affecting the safety of the reactor depend on its evolution. So far, the simple thermal hydraulics model used in DIONISIO has enabled it to become an effective tool for predicting fuel performance under different conditions when comparing its results against comprehensive databases, as well as with the COBRA IV and RELAP codes [3]. However, in some specific cases under very high power irradiation condition or with relatively high coolant temperature, some departured from the experimental data have been noticed. Therefore, to extend the range of conditions that DIONISIO can evaluate when performing a comprehensive analysis of a fuel rod, a more detailed description of the surrounding fluid is necessary.

Consequently, the possibility of using a thermal hydraulics code for nuclear reactors and coupling it with DIONISIO has been raised. In this context, the Karlsruhe Institute of Technology (KIT) developed the SubChanFlow code, which allows a detailed description of the behavior of the cooling fluid and the fluid–structure interaction under irradiation conditions. The thermal hydraulics code can provide accurate and dynamic boundary conditions for the fuel performance code in order to improve the simulations. It is important to consider that DIONISIO is

* Corresponding author at: Institute for Neutron Physics and Reactor Technology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, Eggenstein-Leopoldshafen, 76344, Baden-Württemberg, Germany.
E-mail addresses: mauricio.cazado@kit.edu (M.E. Cazado), victor.sanchez@kit.edu (V.H. Sánchez-Espinoza), soba@cnea.gov.ar (A. Soba).

https://doi.org/10.1016/j.net.2024.06.048
Received 26 March 2024; Received in revised form 10 June 2024; Accepted 27 June 2024
Available online 3 July 2024

Please cite this article as: Mauricio Exequiel Cazado et al., *Nuclear Engineering and Technology*, https://doi.org/10.1016/j.net.2024.06.048

primarily conceived as a fuel performance code and the ultimate goal of a coupling is to extend the domain of DIONISIO to be used for bundles (groups of fuel rods) or even a core in future research.

For the reasons stated previously and in order to obtain more realistic fuel rod simulations, this paper presents the coupling of the codes, taking advantage of the capabilities of the thermomechanical models included in DIONISIO and the detailed description of the thermal hydraulics phenomena in SubChanFlow.

In this work, the general description of the coupling methodology carried out is presented. In a first step, the main objectives of this work is to test the coupling of these tools and to assess the effect on the thermomechanical modeling of a single fuel rod by incorporating more complex models for the treatment of the fluid under normal operation conditions. This will lay the groundwork for future extensions in order to use the complete subchannel capabilities of SubChanFlow.

This paper is organized as follows: in the next section, a brief description of both codes is introduced. In section three, the description of the coupling methodology used is presented. Section four contains the academic tests used to study the performance of the newly developed tool. In section five, the comparison of the coupled codes with experimental data is displayed. Finally, in the last section, some final observations and remarks are provided.

2. Codes description

2.1. DIONISIO

The DIONISIO code simulates the behavior of an irradiated fuel rod during the operation of a Nuclear Power Plant (NPP). This code is able to perform both three-dimensional analyses as well as two-dimensional analyses with axial symmetry. The calculation methodology consists of dividing a fuel rod into a certain number of axial sectors, to which a linear power value is assigned in order to represent a power distribution along the entire rod. For each sector, a domain consisting of a representative pellet with the corresponding cladding and gap is considered. DIONISIO describes the pellet-gap-cladding domain and the mechanisms that occur there by means of the Finite Element Method (FEM). The phenomena modeled include temperature distribution, thermal expansion, elastic and plastic strains, creep, irradiation growth, pellet-cladding mechanical interaction (PCMI), fission gas release, gas mixing, swelling and densification, among others. The strain–stress and heat conduction problems are non-linear due to plasticity and temperature dependence of the thermal conductivity [2,7]. This requires an iterative procedure in order to calculate the variables at each node of the discretization. In addition, the fission gas inventory is calculated with a diffusion model, considering spherical fuel grains and a one-dimensional finite element scheme. Moreover. the code includes a group of subroutines dedicated to the calculation of fuel behavior under high burnup conditions [8].

The evolution of the set of physical phenomena and their mutual interaction is simulated using a linear power history as input data. In order to solve the heat diffusion equation in the corresponding domain, in addition to the linear power input, the temperature values at the outer surface of the cladding obtained from the thermal hydraulics model is required and in the case of the two-dimensional domain, a zero temperature gradient at the fuel pellet centerline must be specified.

The simple thermal hydraulics model used in DIONISIO considers a vertical channel with an annular geometry around a fuel rod, through which the cooling fluid is transported in single phase. The coolant temperature at a given position z can be obtained from an energy balance [9] as:

$$T_C(z) = T_0 + \frac{1}{Q_m C_p}\int_{-\frac{L}{2}}^{z} P_l(z)dz \tag{1}$$

in which T_0 in K is the inlet coolant temperature, Q_m in kg/s is the mass flow rate, C_p in $\mathrm{Jkg^{-1}K^{-1}}$ is the specific heat capacity of the fluid, L in m is the active rod length and P_l in $\mathrm{Wm^{-1}}$ is the linear power distribution along the length of the rod. The outer surface cladding temperature is calculated as follows [9]:

$$T_v(z) = T_C(z) + \frac{P_l(z)}{\pi D h_{eff}} \tag{2}$$

in which D in m is the outer cladding diameter and h_{eff} in $\mathrm{Wm^{-2}K^{-1}}$ is the convective heat transfer coefficient between the metallic cladding surface and the coolant.

Under normal operating conditions, the fluid exhibits turbulent behavior. Despite the great progress in understanding this phenomenon, limitations due to its complexity make it necessary to use empirical correlations. For a turbulent fluid in a channel around a rod, the following expression can be used:

$$h_{eff} = \frac{Nu \cdot k_w}{D_h} \tag{3}$$

in which, Nu is the Nusselt number, k_w in $\mathrm{Wm^{-1}K^{-1}}$ is the thermal conductivity of the fluid and D_h is the hydraulic diameter. The Dittus–Boelter correlation for the turbulent regime is the most widely used one for Nu [10]:

$$Nu = 0.023 Re^{0.8} Pr^{0.4} \tag{4}$$

in which, Re is the Reynolds number and Pr is the Prandtl number.

When water is in contact with the cladding material, under the operation conditions, it is possible to observe the growth of a layer of zirconium oxide (ZrO_2). The oxide has a poor thermal conductivity and consequently reduces the heat transfer and increases the temperature of the system. Then the temperature difference between the oxide interfaces with the fluid and metal bulk material is:

$$\Delta T_{ox} = \frac{P_l(z) e_{ox}}{\pi D k_{ok}} \tag{5}$$

where e_{ox} and k_{ok} are the oxide thickness and thermal conductivity, respectively, which are obtained using the correlations suggested by Hagrman and Reyman [11].

The different parameters used in Ec. (1)–(5) can be found in [11].

Although this simplified model performed well in the tests and validations carried out with DIONISIO and when compared with experimental data [1–4,7,8,12], there is a need to increase the range of validity of the code, especially to consider the subcooled boiling that is well known to occur within the PWR cores in both steady-state and transient behavior. In order to accomplish this, a coupling with the thermal hydraulics code SubChanFlow is proposed.

2.2. SubChanFlow

SubChanFlow is a thermohydraulic subchannel code developed by KIT, based on the legacy subchannel programs COBRA-IV-I and COBRA-EN. The code is capable of assessing fuel rods, rectangular and hexagonal fuel assemblies and core geometries, providing a detailed description of the processes taking place in the coolant domain and the coolant-structure interaction during the irradiation period. SubChanFlow does not describe the flow by simulating the microscale phenomena, but taking profit of many important empirical correlations related to heat transfer, pressure losses and void generation, among others. The coolant properties and the state functions used within the code are implemented for water using the IAPWS-97 formulation (The International Association for the Properties of Water and Steam). It also contains a library with property functions for liquid metals, such as sodium and lead.

Details of the basic balance and constitutive equations can be consulted in multiple Refs. [13–16]. The following are some of the most relevant features present in SubChanFlow version 3.5:

- For the simulation of the fluid, a three-equation two-phase flow model is applied for the steady-state and transient mass, momentum and energy balance. The system of equations is solved for each subchannel, considering the transfer between the coolant with its corresponding rods, including friction against solid surfaces.
- The phenomenon of fluid friction against a solid surface produces a loss of pressure as it travels along its path. The code has different models to deal with this phenomenon. The most commonly used correlation is the simple Blasius model. Armand's friction correlation is the standard one when evaluating a two-phase fluid [10,16].
- The heat flux emitted from fuel rod surfaces is the main source of energy in the energy equation. The code uses either the simple Dittus–Boelter model or the more sophisticated Gnielinski model for single-phase heat transfer cases. In two-phase cases, the correlation used depends on the transfer mechanism in the boiling curve. Under a subcooled nucleate boiling mechanism, correlations like Levy, Bowring, and Saha–Zuber allow for determining the regions along the rod where the conditions for action are met. Among these correlations, the Levy correlation has been particularly successful.
- The code contains a simplified thermomechanical model that allows to calculate the key parameter of the fuel rod such as fuel and cladding temperature distribution, gap conductivity, fuel swelling, and the thermal expansion of the fuel and cladding.

SubChanFlow has undergone validation through diverse experiments using different core designs and geometries [13,15,17–20]. However, the current version of the thermomechanical model for the fuel rod does not account for the evolution of porosity due to densification and swelling, as it maintains a constant value throughout the simulation, which has an impact in the thermal conductivity of the pellet. Moreover, the model used for the thermal conductivity depends only on the fuel temperature and initial porosity value, neglecting the burnup effect. Additionally, the model does not include cladding growth correlations due to irradiation and creep.

3. Coupling methodology

The coupling of the codes consists of an internal coupling, where DIONISIO is used as the main code and controls SubChanFlow as a thermohydraulic subroutine. Since DIONISIO evaluates only one representative fuel rod of an assembly, the geometry used in SubChanFlow during coupling consists of a single rod centered channel.

In this first coupling approach, the main purpose is to analyze irradiated fuel rods under normal operation conditions, which involves time steps on the order of days. The general concept is using the thermal hydraulics results obtained with SubChanFlow at each time step as boundary conditions for solving the thermomechanical problem in DIONISIO. The solution from DIONISIO then serves as a boundary condition for SubChanFlow in the subsequent time step, thus repeating the process. Specifically, SubChanFlow is run at each time step using the power history provided in the input of the code and the rod geometry calculated previously by DIONISIO and it calculates the coolant temperature and heat transfer coefficient distribution along the channel. This information is transferred and used by DIONISIO to calculate the outer cladding temperature, including the effect of oxide growth, which is then used as a boundary condition to solve the thermomechanical problem in the *pellet-gap-cladding* domain in all sectors of the rod. Fig. 1 shows a general scheme of the domain used by both codes and the main variables that are exchanged. In particular, Fig. 1 (b) shows the two-dimensional domain with axial symmetry of the *pellet-gap-cladding* system (half a pellet in height) solved by DIONISIO for each sector in which the active length of the fuel rod is divided. Moreover, the number of axial zones or levels into which the channel is divided can be independent of the number of sectors of the fuel rod.

In order to replace the thermohydraulic subroutine used in DIONISIO with SubChanFlow several modifications were necessary as listed below:

- An internal interface was added so that SubChanFlow can receive the input parameters that are managed by DIONISIO, such as: rod geometry specification, power and fast neutron flux history, initial conditions of the fluid, thermal hydraulics models options and the required numerical parameters.
- SubChanFlow possesses a subroutine to calculate the heat flux and the fuel-cladding temperature distribution. In this coupling, these calculations are skipped and instead all required variables used later in the coolant simulation are updated with the values computed with DIONISIO.
- An internal subroutine was created to handle the variable exchange for both codes in each time step. This subroutine applies a linear interpolation when the axial discretization of the fuel rod and the coolant channel are independent, in order to exchange the information. In addition, for each sector in DIONISIO, axially averaged values for the fuel and cladding temperature is calculated to transfer to the domain used in SubChanFlow.

4. Coupling tests

In order to evaluate the DIONISIO/SubChanFlow coupling (hereafter referred to as DIO-SCF), several tests have been performed considering a rod surrounded by a cooling channel. The most representative results and their comparison with the stand-alone codes (DIONISIO — DIO, SubChanFlow — SCF) are presented below.

During the tests performed, the geometrical parameters for the fuel rod and coolant channel used, and the general operating conditions were taken from a rod designated TSQ002 in the US-PWR 16x16 LTA Extended Burnup Demonstration Program experiment [21]. To run the code, a hypothetical power history consisting of three consecutive steady states with nominal values of 100, 200 and 300 W/cm at the center of the fuel rod height was considered. In addition, a cosine profile with a maximum value at the center of the height (P_M) and an extrapolated length factor (l_e/L) equal to 1.3, $P_l(z) = P_M \cos\left(\pi z/l_e\right)$ were assumed. The inlet temperature of the coolant was 563.15 K. The experiment provides data for the linear power along the rod in 25 zones, which are equispaced. Therefore, the same discretization is used for both the channel and the fuel rod. Based on the geometry and operating conditions of the TSQ002 rod, preliminary tests were performed using different models for the SCF heat transfer regimes, among which no significant difference was found. Therefore, unless otherwise indicated, the Blasius and Armand correlations were used in the simulations for the single-phase and two-phase friction models, respectively, the Levy correlation was used to evaluate the subcooled nucleate boiling phenomenon, and the Dittus–Boelter correlation was used for the single-phase heat transfer.

A first academic evaluation was performed, consisting of comparing the results of the pellet temperature evolution using the coupled code and stand-alone SCF. Fig. 2 shows the linear power history used together with the comparison between SCF and the DIO-SCF coupling for the evolution of the centerline temperature of the fuel in the most demanding sector (central sector of the rod). At the beginning of the history, a difference between the codes can be observed because in DIO, a certain number of initial steps, chosen by the user, are defined in which the boundary conditions are shielded in order to avoid an abrupt jump in the values of the variables involved, which could cause instabilities in the calculation. This shielding consists of multiplying the boundary condition variables, such as pressure and temperature, by a factor that increases linearly with each time step until it reaches the full nominal value at the step where the shielding ends. For low

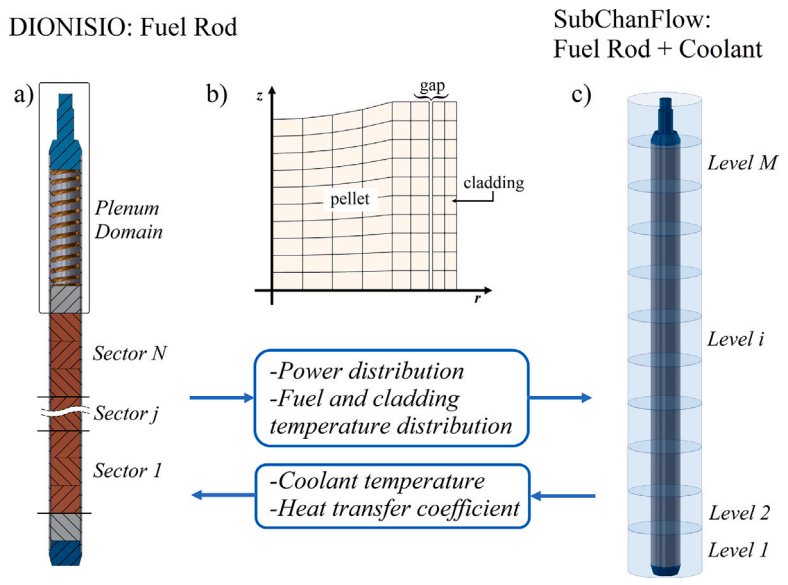

Fig. 1. Domain scheme used in DIONISIO and SubChanFlow and variables exchange between the codes.

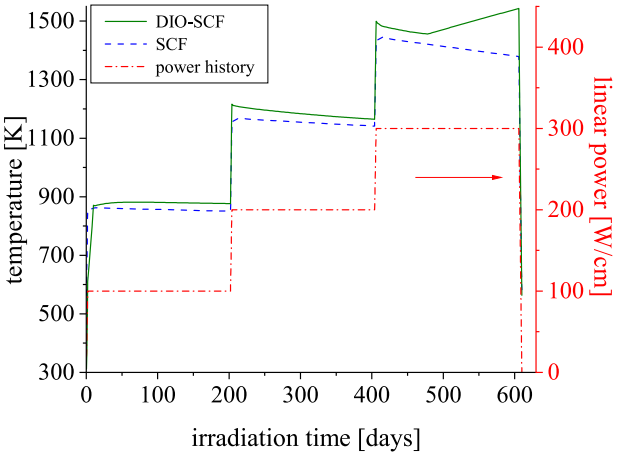

Fig. 2. Power history used in the academic tests and centerline temperature evolution obtained with SubChanFlow and the coupling.

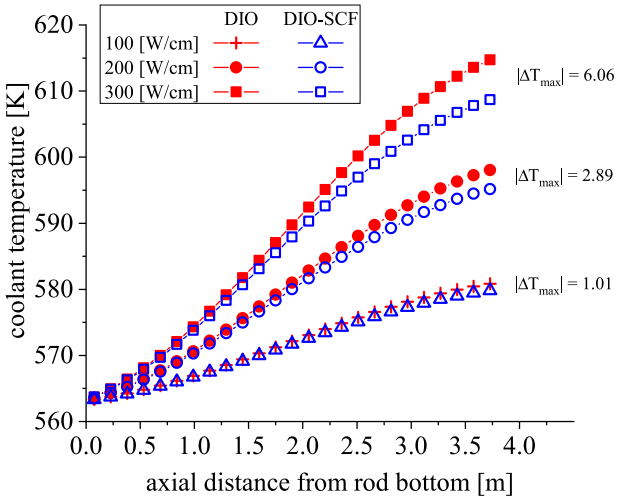

Fig. 3. Comparison of coolant temperature profile between DIO and DIO-SCF for different power levels.

powers (100–200 W/cm) it is observed that the temperature behavior is very similar in both cases, with differences of less than 50 K. These differences are mainly due to differences in the thermal conductivity coefficient of the pellet and to the fact that SCF has a relocation model, which at the beginning of its execution imposes a deformation on the pellet, reducing the size of the gap, so that the temperature is slightly lower. The largest differences in temperature and behavior are observed at the highest power tested. Once the maximum rated power is reached, SCF shows a decrease in temperature over time as a consequence of the decrease in gap. However, DIO-SCF exhibits a similar trend until a point where the temperature starts to rise. As the gap decreases, the temperature of the pellet decreases due to the increase in gap conductivity. It should be noted that in SCF, the gap size evolution is modeled considering the thermal expansion, swelling, and radial relocation of the fuel pellets, as well as the thermal expansion of the cladding. In contrast, DIO models the thermal expansion of both the pellet and cladding, the densification and swelling of the fuel pellets, and the creep and irradiation growth phenomena in the cladding. Moreover, the thermal conductivity model used for the pellet material in DIO-SCF depends primarily on the burnup, the temperature, and the porosity [22]. In DIO-SCF, the porosity first decreases due to densification and then begins to increase due to swelling. This porosity evolution competes with the gap width evolution for the conductivity effect of the system. The change in behavior for DIO-SCF occurs when the gap completely closes, ceasing its role in the conductivity evolution, while porosity continues to increase due to the swelling phenomena, thereby reducing the thermal conductivity of the pellet and increasing its temperature. On the contrary, although SCF calculates swelling, its effects are only including in the progression of the gap closure, but it does not account for the porosity evolution within the fuel pellet and the thermal conductivity model neglects the burnup effect.

The behavior of the coolant temperature along the fuel rod has been evaluated to observe the effect of the coupling with the thermal hydraulics code in comparison with the simplified model included in DIO. Fig. 3 shows the results of the coolant temperature profile as a function of the position with respect to the rod bottom for different power levels calculated with DIO and DIO-SCF. As expected, the higher the linear power, the higher the overall coolant temperature. As for the comparison between the codes, it is observed that in all cases the temperature reached in the coupling is lower than in DIO. These differences can be explained by the fact that the correlations used

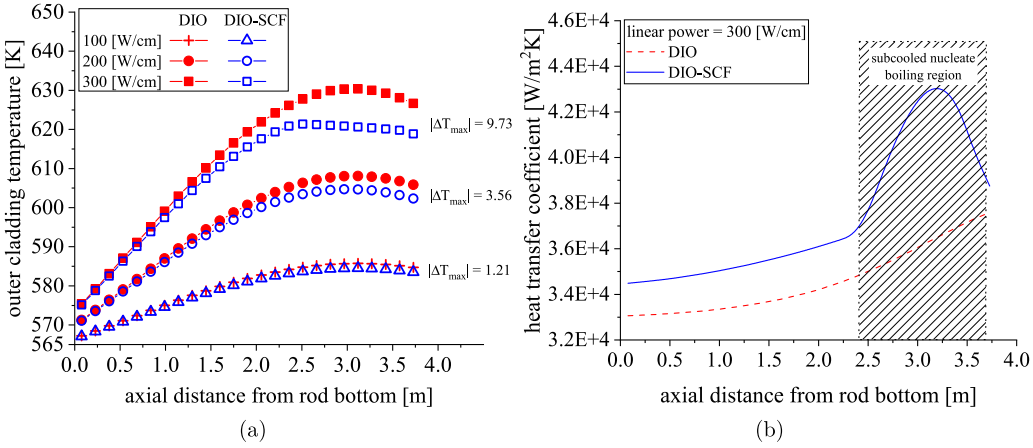

Fig. 4. (a) Comparison of the outer cladding temperature profile between DIO and DIO-SCF for different power levels. (b) Heat transfer coefficient profile along the rod for the maximum power.

in DIO is slightly different from the ones obtained with the IAPWS-97 formulation in SCF. It is highlighted that for the lowest power evaluated, the maximum observed difference is 1.01 K, while for the highest it is 6.06 K, corresponding to approximately 5% and 15% of the temperature increase along the channel obtained in DIO, respectively. In addition, the larger difference for 300 W/cm is due to the fact that the SCF model is able to evaluate the double phase heat transfer, as it is shown in Fig. 4(b).

Fig. 4(a) shows a comparison between the calculation with DIO and DIO-SCF of the outer cladding temperature as a function of the fuel rod height for the different powers used in this evaluation. It is observed that for 100 and 200 W/cm, the temperature variations between DIO and DIO-SCF are less than 3.6 K, while for 300 W/cm, there are differences of up to approximately 10 K. Since both codes use the single-phase heat transfer mode for the lower powers, the observed differences are mainly due to the fact that SCF uses correlations for water properties that depend on the temperature and pressure of the system, while DIO uses an approximation that depends only on temperature for an average pressure in a PWR reactor, which may differ from the analyzed experiment. In addition, for the 300 W/cm power, the DIO-SCF thermal hydraulics model determines that, under the conditions tested, the heat transfer occurs by the phenomenon of subcooled nucleate boiling in the upper third of the rod, which would explain the observed behavior and the higher thermal difference found. This can be verified in Fig. 4(b), where the profile of the heat transfer coefficient along the rod calculated with both codes is shown. As can be seen, in the upper third of the fuel rod, SCF evaluates the heat transfer in the subcooled nucleate boiling mode, for which the h_{eff} coefficient increases considerably with respect to the one evaluated during the liquid phase transference. This behavior cannot be evaluated with DIO as it does not provide the appropriate model for it, hence the importance of coupling the codes to take advantage of the detailed thermal-hydraulic description of SCF.

Although the cladding temperature differences obtained with the codes may be relatively small, this can have important implications for oxide layer growth, which degrades the thermal properties of the material, and hydrogen absorption, which degrades the mechanical properties. This can be seen in Fig. 5, which shows the final profiles of the oxide layer and hydrogen absorption along the fuel rod for the numerical test described above. It is observed that a decrease of up to 10 K in the temperature of the cladding corresponds to a decrease of up to 28.6% in the hydrogen absorption and up to 26.6% in the oxide layer thickness when comparing between DIO and DIO-SCF. In addition, it is observed that the maximum value reached in these variables for the coupling is slightly shifted towards the left with respect to DIO.

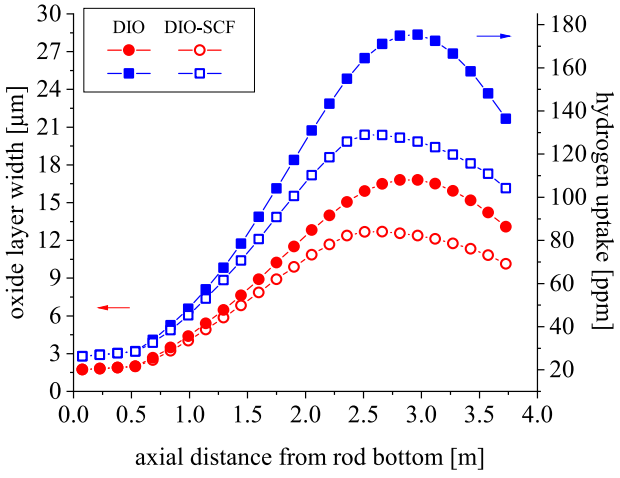

Fig. 5. Final oxide layer and hydrogen uptake profile simulations along the fuel rod for the academic test for the same power history presented in Fig. 2.

5. Comparison with experimental data

5.1. US-PWR 16x16 LTA extended burnup demonstration program experiment

Following the initial evaluation of the coupling and the main observations of its behavior, a first approach to validating it was made using data from the US-PWR 16x16 LTA Extended Burnup Demonstration Program [21] experiment. For this purpose, four fuel rods designated TSQ002, TSQ004, TSQ022 and TSQ024, irradiated up to 53.2, 50.5, 58.1 and 54.7 MWd/kgU, respectively, were selected. The first two rods contained solid pellets and the latter ones, annular pellets. In all cases studied, the fuel consisted on UO_2 with an enrichment of 3.48% and the cladding material was Zircaloy-4. All geometric dimensions and operation conditions are given by Lyon and Turnbull [21].

The mentioned experiment provided values for the outer cladding temperature along the fuel rod and at different values of the average power over the rod. However, these data do not correspond to experimental measurements, but to a calculation from the coolant inlet temperature (563.15 K) and an outlet temperature averaged over the entire operating time (595.15 K), assuming that the coolant temperature increases linearly. This means that in order to evaluate the effect of coupling in this experiment, it is necessary to compare with variables that are strongly influenced by the thermohydraulic ones, such as oxide thickness growth and hydrogen uptake by the cladding.

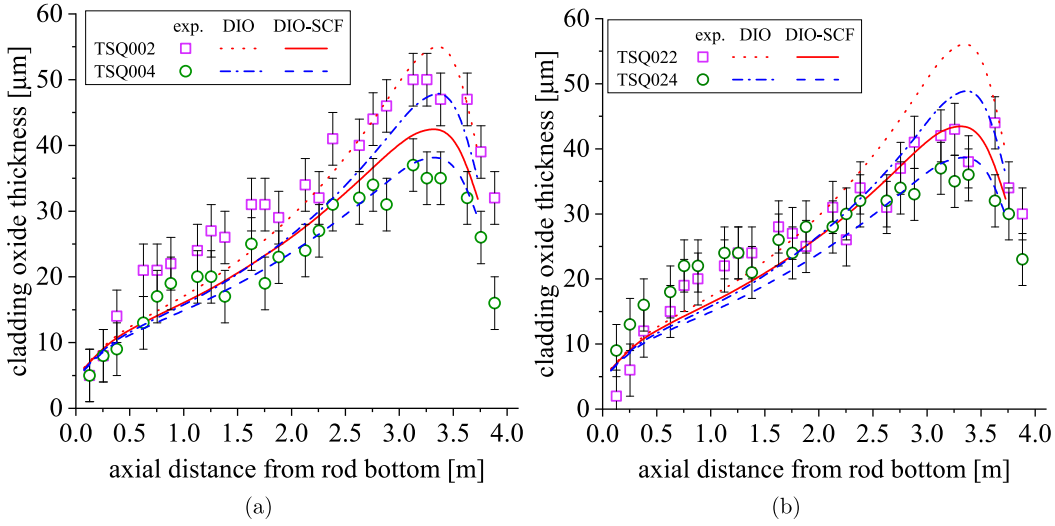

Fig. 6. Comparison of oxide thickness along the cladding between simulations and experimental data from different rods of the US-PWR program. [21]. The error bars correspond to ±4 μm.

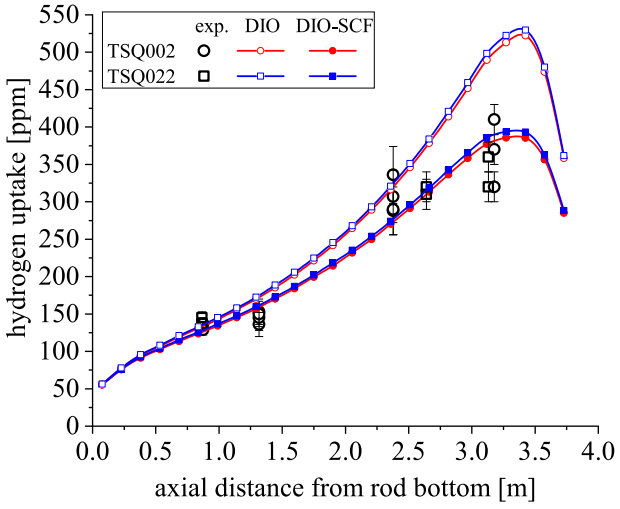

Fig. 7. Cladding hydrogen uptake comparison between DIONISIO and the coupling DIONSIO-SubChanFlow with experimental data of the US-PWR 16x16 LTA Program [21].

Fig. 6 shows the comparison of the outer oxide thickness of the cladding between the values calculated by the codes and those measured in the experiment. Here the improvement introduced by the coupling is more evident, since the oxide thickness is highly dependent on the temperature of the cladding. When the stand-alone DIO is used, the differences with the experimental values can reach up to 30%, while DIO-SCF achieves a good agreement with the experimental data for all the rods, except for TSQ002 where DIO shows a better fit. No specific reason was found for the behavior of the TSQ002 rod. Generally, it can be observed that around the lower third of the rod, the experimental values are higher than those calculated numerically. CRUD deposition in this area (corrosion products dragged by the coolant) can decrease thermal conductivity, which would increase the cladding temperature and oxide layer thickness. This hypothesis was investigated by Krasnorutskyy and Slyeptson [23], who included a model for CRUD deposition, achieving a slight improvement in their code. Despite this, no related information was available in the experiment reports to support this assumption.

The calculated hydrogen uptake profiles and the experimental data for the rods on which they were measured: TSQ002 and TSQ022 are shown in Fig. 7. This parameter is closely related to the mechanism of oxide formation, so the cladding temperature plays an important role in hydrogen capture [11]. DIO-SCF shows better agreement in the range of measured values, especially in the higher absorption zone, where DIO calculates a maximum value 34% higher than that obtained with coupling. Regarding the pellets used, simulations showed no significant differences for the hydrogen uptake between the rods with solid and hollow pellets, TSQ002 and TSQ022, respectively.

5.2. IFPE/OSIRIS R3 experiment

Additionally, the IFPE/OSIRIS R3 experiment was used to test the coupling developed in this work. In particular, PWR rods designated G07 and H09 were selected and irradiated up to ~34 and ~46 MWd/kgU, respectively. The fuel rod materials were UO_2 for the pellet and Zircaloy-4 for the cladding. All geometrical parameters and operating conditions are given by Menard [24,25].

In this case, the fuel rods are divided into 18 irregular axial sectors based on information obtained from the experiment reports. Some sectors were only a few centimeters long and corresponded to axial positions where spacers were located. On the other hand, SubChanFlow only accepts a regular discretization, and 18 sectors were also considered.

The oxide thickness profiles for the rods studied are shown in Fig. 8. There is good general agreement between the calculations and the experimental measurements. Consistent with observations from previous cases, the results obtained with DIO-SCF are lower than those obtained with DIO, achieving a good agreement with the experimentally measured maximum values. The largest deviations occur in the lower zone of rod H09, where the measured data are slightly higher than the calculated data, while a slight underestimation occurs in the calculation in the lower zone for G07. The strong “depressions” in the oxide layer measurements correspond to regions near the spacers of the fuel rods. This could be due to a great reduction in power in these areas caused by the spacers. However, the reports do not provide an explanation for this behavior in the oxide profile. Although, in DIO-SCF an oxide growth model with dependence on the irradiation profile is used, the particular mentioned behavior could not be reproduced. Despite these differences, a good coupling behavior is achieved and the general profile trend is captured, providing improved results comparing with the stand-alone version of DIO.

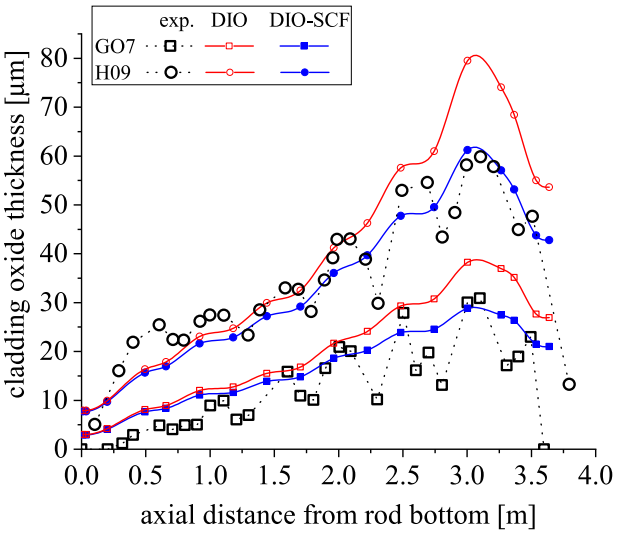

Fig. 8. Cladding oxide growth comparison between DIONISIO and the coupling DIONSIO-SubChanFlow with measured values in the IFPE/OSIRIS R3 experiment [24, 25].

6. Concluding remarks

The internal coupling between DIONISIO and SubChanFlow has been successfully implemented, bringing together the strengths of both codes. The preliminary tests carried out with the coupling showed a good performance of the system and the codes work together in a satisfactory way. In particular, small variations in fluid and cladding temperature can lead to considerable differences in thermally activated mechanisms, such as oxide growth and hydrogen uptake processes.

The coolant and cladding temperature description by the coupling and their related variables such as the oxide thickness and hydrogen uptake showed a significant improvement under normal operation conditions when comparing with experimental results from the US-PWR 16x16 Extended Burnup Demonstration Program and OSIRIS R-3 experiments. Despite these good results, additional validation with experimental data is needed to test the performance of the coupling in special operation conditions.

Although the simplified DIONISIO thermal hydraulics subroutine has been successfully used in numerous cases, it is observed that the use of the new coupled code system improves the overall response of the code, being able to represent not only better quantitative results, but also to provide a better description of the phenomenology involved in the evaluation of two-phase fluid conditions.

So far, the work has focused on analyses under normal operating conditions using a single fuel rod and its corresponding channel. Therefore, an important next step is to extend the coupling conditions to LOCA-type accident scenarios and subsequently extend DIONISIO's domain to analyze a set of fuel rods. This will further capitalize the capabilities of a subchannel code like SubChanFlow, thereby providing adequate boundary conditions for each analyzed.

CRediT authorship contribution statement

Mauricio Exequiel Cazado: Writing – review & editing, Writing – original draft, Validation, Software, Methodology, Investigation, Data curation, Conceptualization. **Victor Hugo Sánchez-Espinoza:** Writing – review & editing, Validation, Supervision, Software, Resources, Investigation, Funding acquisition. **Alejandro Soba:** Writing – review & editing, Writing – original draft, Validation, Supervision, Software, Resources, Investigation, Data curation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

This work was supported by the Strategic Partnership UNSAM-KIT (SPUK) and partially by the Agencia Nacional de Promoción de la Investigación, el Desarrollo Tecnológico y la Innovación, Argentina (PICT-2018-01568).

References

[1] A. Soba, M. Lemes, M.E. González, A. Denis, L. Romero, Simulation of the behavior of nuclear fuel under high burnup conditions, Ann. Nucl. Energy 70 (2014) 147–156, http://dx.doi.org/10.1016/j.anucene.2014.03.004.

[2] A. Soba, A. Denis, DIONISIO 2.0: New version of the code for simulating a whole nuclear fuel rod under extended irradiation, Nucl. Eng. Des. 292 (2015) 213–221, http://dx.doi.org/10.1016/j.nucengdes.2015.06.008.

[3] M. Lemes, A. Soba, H. Daverio, A. Denis, Inclusion of models to describe severe accident conditions in the fuel simulation code DIONISIO, Nucl. Eng. Des. 315 (2017) 1–10, http://dx.doi.org/10.1016/j.nucengdes.2017.02.015.

[4] E. Goldberg, M.E. Loza, A. Soba, DIONISIO 3.0: Comprehensive 3D nuclear fuel simulation through PCMI cohesive and PLENUM models, J. Nucl. Mater. 523 (2019) 121–134, http://dx.doi.org/10.1016/j.jnucmat.2019.06.005.

[5] R.H. Pletcher, J.C. Tannehill, D.A. Anderson, Computational fluid mechanics and heat transfer, Taylor & Francis, 2013.

[6] L.S. Tong, Y.S. Tang, Boiling Heat Transfer and Two-Phase Flow, Taylor & Francis, 1997.

[7] A. Soba, A. Denis, Simulation with DIONISIO 1.0 of thermal and mechanical pellet-cladding interaction in nuclear fuel rods, J. Nucl. Mater. 374 (2008) 32–43, http://dx.doi.org/10.1016/j.jnucmat.2007.06.020.

[8] M. Lemes, A. Soba, A. Denis, An empirical formulation to describe the evolution of the high burnup structure, J. Nucl. Mater. 456 (2015) 174–181, http://dx.doi.org/10.1016/j.jnucmat.2014.09.048.

[9] A. Soba, Simulación del comportamiento mecánico de una barra combustible en operación (Ph.D. thesis), Universidad Nacional de Buenos Aires, 2007.

[10] L.S. Tong, J. Weisman, Thermal Analysis of Pressurized Water Reactors, American nuclear society, 1996.

[11] D.L. Hagrman, G.A. Reyman, MATPRO-Version 11: a handbook of materials properties for use in the analysis of light water reactor fuel rod behavior, NUREG/CR-0497,TREE-1280, 1979, http://dx.doi.org/10.2172/6442256, URL https://www.osti.gov/biblio/6442256.

[12] A. Soba, A. Denis, L. Romero, E. Villarino, F. Sardella, A high burnup model developed for the DIONISIO code, J. Nucl. Mater. 433 (2013) 160–166, http://dx.doi.org/10.1016/j.jnucmat.2012.08.016.

[13] A. Gómez Torres, V. Sánchez Espinoza, U. Imke, R. Macián Juan, Pin level neutronic - thermalhydraulic two-way-coupling using DYN3D-SP3 and SubChanFlow, in: International Conference on Mathematics and Computational Methods Applied To Nuclear Science and Engineering, M&C 2011, Rio de Janeiro, RJ, Brazil, 2011, p. 20.

[14] J.C. Almichi, V.H. Sanchez, U. Imke, Extension and validation of the SubChanFlow code for the thermo-hydraulic analysis of MTR cores with plate-type fuel assemblies, Nucl. Eng. Des. 379 (2021) 111221, http://dx.doi.org/10.1016/j.anucene.2014.02.028.

[15] M. García, Y. Bilodid, J. Basualdo Perello, R. Tuominen, A. Gommlich, J. Leppänen, V. Valtavirta, U. Imke, D. Ferraro, P. Van Uffelen, M. Seidl, V.H. Sanchez, Validation of serpent-SUBCHANFLOW-TRANSURANUS pin-by-pin burnup calculations using experimental data from pre-konvoi PWR reactor, Nucl. Eng. Des. 379 (2021) 111173, http://dx.doi.org/10.1016/j.nucengdes.2021.111173.

[16] U. Imke, V.H. Sanchez, Validation of the Subchannel Code SUBCHANFLOW Using the NUPEC PWR Tests PSBT, Sci. Technol. Nuclear Install. 2012 (2012) 12, http://dx.doi.org/10.1155/2012/465059.

[17] W. Jaeger, J. Perez Manes, U. Imke, J. Jimenez Escalante, V.H. Sanchez, Validation and comparison of two-phase flow modeling capabilities of CFD, sub channel and system codes by means of post-test calculations of BFBT transient tests, Nucl. Eng. Des. 263 (2013) 313–326, http://dx.doi.org/10.1016/j.nucengdes.2013.06.002.

[18] M. Calleja, U. Jimenez, V.H. Sanchez, R. Stieglitz, J.J. Herrero, R. Macían, Implementation of hybrid simulation schemes in COBAYA3/SUBCHANFLOW coupled codes for the efficient direct prediction of local safety parameters, Ann. Nucl. Energy 70 (2014) 216–229, http://dx.doi.org/10.1016/j.net.2021.04.023.

[19] M. Daeubler, A. Ivanov, B.L. Sjenitzer, V. Sanchez, R. Stieglitz, R. Macian—Juan, High-fidelity coupled Monte Carlo neutron transport and thermal-hydraulic simulations using Serpent2 - SubChanFlow, Ann. Nucl. Energy 83 (2015) 352–375, http://dx.doi.org/10.1016/j.anucene.2015.03.040.

[20] M. García, R. Vocka, R. Tuominen, A. Gommlich, J. Leppänen, V. Valtavirta, U. Imke, D. Ferraro, P. Van Uffelen, L. Milisdörfer, V.H. Sanchez, Validation of Serpent-SubChanflow-TRANSURANUS pin-by-pin burnup calculations using experimental data from the Temelín II VVER-1000 reactor, Nuclear Eng. Technol. 53 (2021) 3133–3150, http://dx.doi.org/10.1016/j.net.2021.04.023.

[21] W.F. Lyon, J. Turnbull, IFPE/US-PWR-16 X 16 Lead Test Assembly Extended Burnup Demonstration Program, Nuclear Energy Agency of the OECD (NEA), 2005.

[22] K.J. Geelhood, W.G. Luscher, P.A. Raynaud, I.E. Porter, FRAPCON–4.0: A Computer Code for the Calculation of Steady–State, Thermal–Mechanical Behavior of Oxide Fuel Rods for High Burnup, Pacific Northwest National Laboratory, Richland, Washington, USA, 2015.

[23] V. Krasnorutskyy, O. Slyeptson, Fuel Rod Performance Evaluation of CE 16x16 LTA Operated at Steady State using TRANSURANUS and PAD Codes, Technical Report, National Science Center "Kharkov Institute of Physics and Technology", 2009.

[24] M. Menard, Rapport d'Assurance Qualite Crayon FF06E2BV/G07/1067, Nuclear Energy Agency of the OECD (NEA), 1998.

[25] M. Menard, Rapport d'Assurance Qualite Crayon FF0EFELX/H09/5007, Nuclear Energy Agency of the OECD (NEA), 1998.