Numerical techniques in neutronic-thermohydraulics coupling models of CAREM-25 nuclear reactor

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I. Introduction

The spatial distribution of the power generated in the core of a nuclear reactor depends on various factors, such as the position of control rods, fuel elements and other materials, and physical parameters such as fuel temperature, coolant temperature or void fraction. The neutronic equations that are used to capture this dependence model all these factors simply through a spatial arrangement of effective cross sections. The spatial power distribution, in turn, generates modifications on the cross sections, either because it is acting as an energy source, modifying temperatures and densities of fuels, coolants and other materials, or due to the required future movement of materials, such as the control rod movements necessary to search for flat power profiles, or fuel replacement by loss of criticality. In addition, in the temporal evolution, the fuel burnup generates alterations in the concentration of existing elements and appearance of new elements, which also modify the effective cross sections.

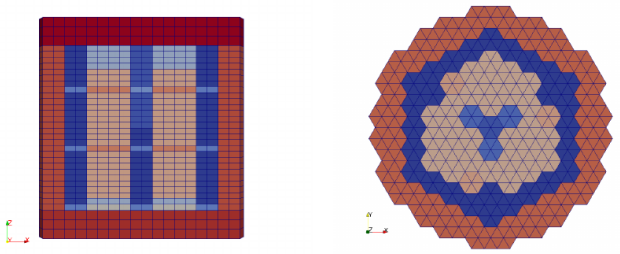
The dynamics of a nuclear core reactor strongly couple multiple phenomena, and any model that is used to study it must approach the coupling by some strategy. In general, the calculation codes used in the nuclear area are validated to solve only one of these phenomena, so a coupling between them is usually required to solve the complete dynamics. Commonly, the temporal evolution is discretized in different burnup steps, and in each of them the coupling is solved by explicit *Picard* iterations. In this work we use a previously developed program, Newton [1], that allows solving non-linear problems in the *master-slave* paradigm by coupling different codes using explicit and implicit techniques. The analysis system is a simplified model of the core dynamics of the CAREM-25 reactor.

CAREM-25 is an integrated natural convection reactor with 100 MW thermal generation. It uses light water as coolant and enriched uranium as fuel, and has innovative designs in security systems [2]. The analysis of this reactor is a complex problem with a large number of coupling unknowns. The simple model we present here analyzes one burnup cycle, considering only the neutron and thermohydraulic phenomena.

II. Subsystem Models

A. Neutronic model

The domain of neutron calculation consists of a core of 1.4 meters of height and 1.312 meters of equivalent diameter. This core is composed of 61 fuel elements. Each fuel element has a hexagonal cross-section with 127 positions, between which there are bars of fuel and absorbent material. A diagram of the reactor core can be seen in Figure 1.



(a) (b)

Figure 1. (a) CAREM-25 core reactor model cross-sectional view. (b) CAREM-25 core reactor model axial-sectional view.

The core calculation is performed using a stationary diffusion model [3]. In the proposed model the effective cross sections depend on the coolant density N_{cool}, the coolant temperature T_{cool}, the fuel temperature T_{fuel}, and the historical burnup value B of the material [4], for each spatial point and each energy group , so that:

$$\Sigma = \Sigma\left(N_{cool}, T_{cool}, T_{fuel}\right) \quad (1)$$

Neutronic difussion equation requires extra conditions in the boundary of the compute domain. In the case of study analyzed, null inlet flow boundary conditions are imposed. These are modeled by an artifact of total absorption of the protruding neutrons, extending the mesh of the calculation. Once the neutron flux is obtained, the power distribution P can be calculated from the rate of fission reactions [4]. The P power distribution found is used as the energy source in the coupled termohydraulics calculations.

The calculation mesh used is composed of pentahedral cells. The different colors in Figure 1 represent different fictional materials homogenized per zone in previous cell calculations. The differences correspond to the degree of enrichment of each fuel and to the possibility that some have to accommodate control materials. The Control and Adjustment System (SAC, for its acronym in spanish) control rods are inserted up to half the active length of the core during the entire burnup cycle. The material arrangement is not detailed because it is not considered relevant for the study objective.

Neutronic equations are solved with PUMA [5] using five energy groups. PUMA is a core code developed by CNEA that calculates the neutron flux from a finite difference scheme of the diffusion neutronic equation. The core model developed for its calculation with PUMA was provided by the Department of Physics of Advanced Reactors of CNEA (DIFRA, for its acronym in spanish).

B. *Termohydraulics model*

The thermohydraulic calculation domain consists of a simplification of the core geometry. A single cooling channel is modeled in contact with a heat structure containing the entire mass of the fuel elements. The length of this structure is equivalent to the length of the sum of all the pins present in the fuel elements. Radially, it respects the distribution of fuel, gap and cladding.

The hydrodynamic and heat transfer phenomena are modeled with uni-dimensional and transient equations. The heat transfer through the fuel structures is modeled with diffusion differential equation, considering a source that has the power distribution information generated in the reactor core. The model is completed with suitable edge conditions. The coolant flows around the structures and the energy transferred between them is given by convection.

The hydrodynamic model of coolant behavior considers a mixture of fluid in liquid and gaseous phases. The basic differential equations of this model are six [6]. The first two are the continuity equations in each phase. The following two equations are the moment equations of each phase. The last two hydrodynamic equations are the energy conservation equations for each phase. A series of coefficients are not defined in these equations. All these coefficients are modeled from extra closure equations. These equations strongly depend on the flow regimes, and basically model the mass transfer calculation at the interface of phases, heat transfer at the interface and with structures, interface friction and structures, and viscous dissipation. All these hydrodynamic equations are solved with RELAP5 [6].

III. Coupling strategy

The neutronic-thermohydraulic coupling is studied during a 400-day burnup cycle. The temporal evolution is discretized in intervals of a 5 and 10 days. In the first calculation step, it is assumed that the B burnup value is null for all definite physical zones, and from the second step the burnup value is updated locally assuming that the last calculated fission rate in that zone remains constant. In each burnup step, the coupling strategy implemented is to consider the thermohydraulic variables as data in the neutron calculation, and the power distribution as data in the thermohydraulic calculation. The core is discretized axially in a 28 zones in which are worked with mean values of the coupling variables.

The thermohydraulic calculation yields variables averaged in the different axial zones of the channel. In the neutronic calculation, axial zones are defined based on the same discretization, in each of which the effective cross sections are calculated from the thermohydraulic variables of the corresponding zone, and from the burnup historical value stored in different predefined physical regions. Σ functions dependent in T_{fuel}, T_{cool}, N_{ref} and the burnup value B were constructed from tables of effective sections provided by DIFRA. The power distribution calculated from the neutronic model is also integrated in each axial zone. With this model, 4 coupling variables are defined at each axial position i: T_{fuel}, T_{cool}, N_{ref} and P_i. With the resolution model previously discussed, a total of 112 coupling unknowns are defined.

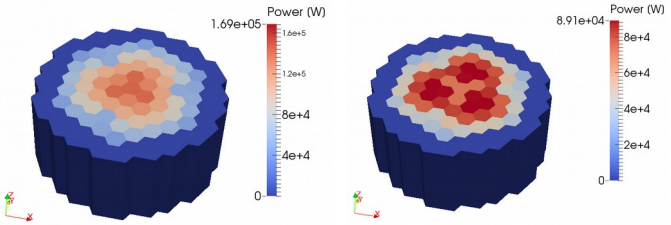
During the burnup evolution, no movement of control rods was performed to maintain criticality. Up to the middle of the core were kept inserted throughout the cycle so that the excess or lack of reactivity is not so abrupt at the ends. The movement of control rods would have incorporated an extra model in the coupling and here was not considered for simplicity.

This scheme is solved with iteratives schemes. The convergence at each burnup step is considered to be achieved when the residuals, the differences between the proposed guess values and the calculated values, are less than a certain predetermined tolerance. The Newton code was used as a *master* code to implement communication functions and solve these residual equations. The communication with *slave* codes is given by file handling, and for this purpose specific reading and writing functions were developed for PUMA and RELAP5 files.

IV. Results

The resolution of the coupled system was carried out using different methods. Differences in performance are discussed later. Each burn step was considered converged when the infinite norm of the residue became lower than a predetermined absolute *tol* tolerance. This *tol* tolerance was set at 0.1. This proposition involves iterating with the solution until the residual in each variable falls below 0.1, which is the precision of the results printed by RELAP5. Requiring greater precision in the printing of results is not justifiable due to the models and approximations used.

Figure 2 shows the evolution of the power distribution in an axial section to the middle of the core, and Figure 3 shows the evolution of the corresponding burn distribution. The power distribution is attenuated in the center and concentrated in the intermediate rings of the core as the burn cycle progresses.



(a) (b)

Figure 2. Evolution of power distribution in cross-sectional view of the middle of the core of CAREM-25 reactor: (a) Power distribution in day 10. (b) Power distribution in day 400.

(a) (b)

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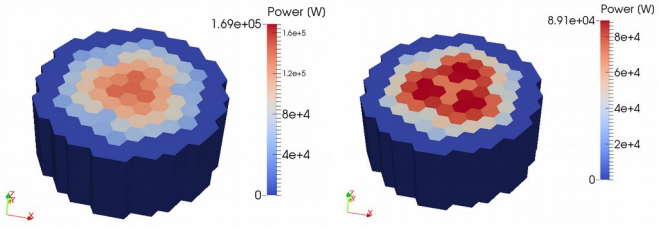


Figure 3. Evolution of burnup distribution in cross-sectional view of the middle of the core of CAREM-25 reactor: (a) Burnup distribution in day 10. (b) Burnup distribution in day 400.

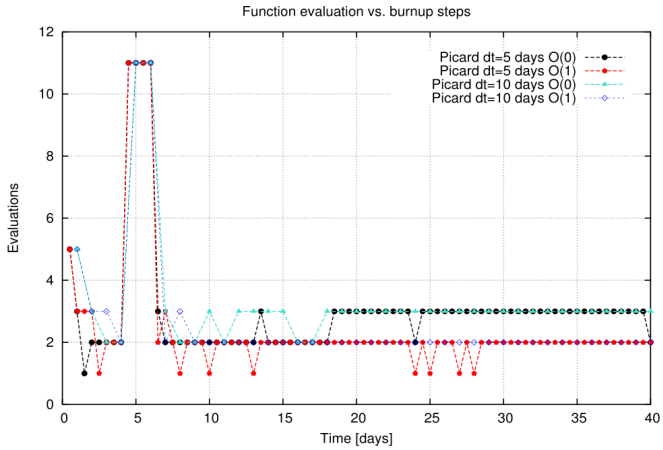
Extrapolations of order 0 and order 1 of the previous solutions were used for the seed x_n at the first iteration of each burnup step. Also, there were used different temporal discretization. Explicit methods complete the burnup cycle in a robust and stable manner. Two explicit methods were used, the *Picard's* method, that solves the equations by iterating in 2 fractional steps, and the *fixed point* method, that solves them by iterating monolithically. *Picard's* method has problems in some burnup steps, in which iterates between values that are repeated in cycles. As the residue in these steps was only one order of magnitude greater than the set tolerance, it was decided to consider them to be converged after 10 iterations and to continue evolution. The *fixed-point* method, on the other hand, converges at each burnup step. While the number of function evaluations at each burnup step is comparable between the two methods, the *fixed point* method solves each iteration by parallelizing the code runs and thus completes the cycle in the least amount of time.

Table 1 summarizes the amount of function evaluations and the temporal resources consumed by each explicit method studied. In explicit methods function evaluations are directly related with the iterations of the method. In Figures 4 and 5 we report the amount of function evaluations required by different schemes at each burnup step, using *Picard's* method and *fixed point* method respectively.

TABLE I. TOTAL EVALUATIONS AND TOTAL TIME REQUIRED BY EACH NONLINEAL METHOD SOLVING THE BURNUP CYCLE WITH RELAP5 AND PUMA.

Nonlinear method	*Delta t [days]*	*Xn extrapolation*	*Total evaluations*	*Total time [s]*
Picard	5	O(0)	243	11019
Picard	5	O(1)	195	9085
Picard	10	O(0)	131	5898
Picard	10	O(1)	104	4774
Fixed point	5	O(0)	139	5415
Fixed point	5	O(1)	186	6990
Fixed point	10	O(0)	101	3755
Fixed point	10	O(1)	107	3919

Figure 4. Function evaluations using *Picard* scheme to solve the residual equations in neutronic-termohydrauilics coupling model, using different extrapolation orders for the seed at the first iteration of each burnup step..



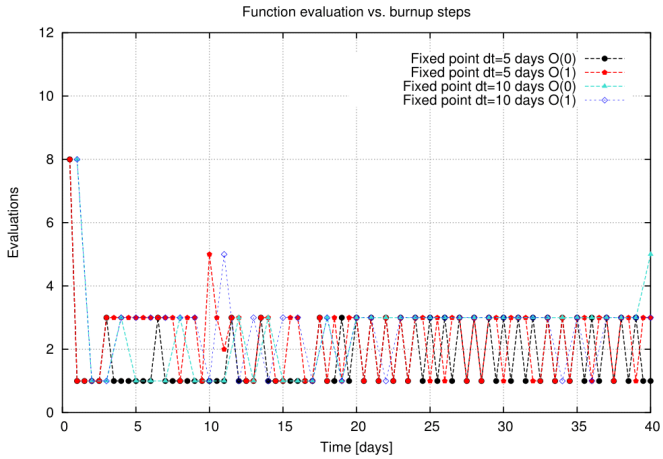


Figure 5. Function evaluations using *fixed point* method to solve the residual equations in neutronic-termohydraulics coupling model, using different extrapolation order for the seed at the first iteratoin of each burnup step..

Implicit techniques like *Newton-Raphson* method and other *quasi-Newton* methods were also tested. The implicit *quasi-Newton* method *Broyden* was studied in detail because it was the one that gave the best results throughout coupling models previously tested in fluidic systems [8]. Multiple trials were carried out including initialization by finite difference of *jacobian* matrix, reinitialization of the *jacobian* matrix, extrapolation orders for the unknown vector x_n^0 and the matrix B_n^0 and different seeds to start the calculation. The temporal discretization parameter was also varied. Most of the models required an excessive amount of function evaluations, mainly due to the approximate calculation of the Jacobian matrix. In the simulations with the *Broyden* method and initialization of the *jacobian* matrix, solutions for each burnup step converge with an average of 1 iteration during the first 20 steps approximately. This result is very good, since the explicit methods converge with an average between 2 and 3 iterations in each burn step. However, these simulations could not be completed, because the evolution was destabilized later. This instability generates a bad update of the *Broyden* matrix and

finally the method ends up proposing guess values without physical sense.

V. Conclusions

In this work, the coupling methodology of different programs was implemented to solve the neutronic-thermohydraulic problem using the *master-slave* paradigm. A neutronic-thermohydraulic coupling model was developed to study fuel burnup cycles and the efficiency of resolution of different numerical schemes was evaluated. The CAREM-25 core reactor was analyzed and it was found that the *Picard* technique commonly used is not the most efficient since it requires serialized evaluations that can well be paralleled using the *fixed point* method. The *Broyden* method proved efficient only during the first half of the burnup cycle, but then encountered instabilities.

Acknowledgment

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