Open Software One-Step Coupled Neutronics and CFD Thermalhydraulics Calculation

Vitor Silva¹, Andre Campagnole dos Santos², German Theler³, Claubia Pereira⁴

¹²Centro de Desenvolvimento da Tecnologia Nuclear, Comissão Nacional de Energia Nuclear, Av. Pres. Antônio Carlos, 6627-30270-901 Belo Horizonte, MG, Brazil
³Seamplex, Santa Cruz 205, 2300, Rafaela, Argentina
¹⁴Departamento de Engenharia Nuclear (DEN), Universidade Federal de Minas Gerais (UFMG), Av. Pres. Antonio Carlos, 6627 - 30270-901 Belo Horizonte, MG, Brazil

Abstract-- A one-step coupled neutronic and CFD thermal-hydraulic methodology is presented. The contribution proposed goes toward the use of the computational fluid dynamics (CFD) software OpenFOAM and the flexible reactor core analysis code milonga to perform coupled calculations for advanced nuclear reactor analysis. The developed methodology was applied to simulate a fuel pin from CDTN’s TRIGA-IPR-R1 reactor and assess its behavior in steady-state mode for different power levels. A set of two-group macroscopic cross-sections data was generated using WIMSD-5B code for different expected temperatures. The results show that this coupled system gives consistent results, encouraging system further development and its use for full core simulation.

Keywords—Coupling, milonga, Neutronics, OpenFOAM, CFD, Thermal-hydraulics.

I. INTRODUCTION

The goal is to present a coupled neutronic and Computational Fluid Dynamics (CFD) thermal-hydraulic methodology for nuclear reactors calculations. The thermal-hydraulic calculations are performed by the CFD toolbox called OpenFOAM [1]. For neutron calculations, a nuclear reactor core analysis code called milonga is used to solve the steady-state multigroup neutron diffusion equation [2]. Both codes solve the discretized equations for an unstructured mesh using finite volumes method. In this coupled framework, both codes use the same mesh for domain discretization, allowing both codes to solve their problems with the same degree of detail.

With the increase of computational power and parallel processing capability observed over the past decade, numerical simulations using highly discretized domains, as finite volume CFD, has grown and is quickly becoming the main numerical tool for analysis in engineering. With this new available capacity, the trend is to perform increasingly complex simulations coupling different codes so that multiphysics analysis can be performed, increasing the understanding of the behaviors of a physical system as a whole [3]. For the nuclear field, researchers now strive to achieve complex coupling of neutronics and thermal-hydraulics as their physics is intrinsically connected by feedback effects.

The objective of this paper is to present a one-step coupling of open source neutronic and CFD thermal-hydraulic codes. The decision to adopt open software is so that the development can be freely distributed so it can be used and improved by the nuclear academic and industrial communities.

II. METHODOLOGY

Figure 1 shows the basic schematic for the coupling methodology. Open CFD software OpenFOAM [1] is used to calculate thermalhydraulic variables temperature profile based on an initial guess of power distribution. These results are used to select the appropriate neutron parameters (diffusion coefficients and cross sections) for the neutronic calculation. Open neutronic code milonga [2] is used to solve the neutron fields and compute power distribution. This distribution is then fed back to OpenFOAM [1] for proper temperatures and densities calculation. This loop is repeated until a convergence criterion is met.
The methodology developed by DEN/UFMG [4,12] for cross-sections processing using WIMSD-5B code was applied in this work. In this methodology, a 69 groups cross-section library generated from ENDF-VI is used to generate a set of two-group cross-sections for three different materials, coolant, cladding, and fuel, at different temperatures, corresponding to the modelled fuel element temperatures variation.

In the following section, details of the methodology and simulations performed are presented.

A. Geometrical model and mesh

The coupled methodology was assessed simulating one of CDTN’s TRIGA IPR-R1 reactor fuel pins and evaluating the physical coherence of the results. This fuel was selected for this paper due to its strong temperature coefficient in terms of reactivity.

The geometry of the simulated cylindrical fuel pin comprised of a 1.78 cm radius fuel with a 1.865 cm external radius aluminum cladding surrounded by a square water section of 4.57 cm, as shown in Fig. 2. The total axial length of the model was 35 cm, equal to the active length of the CDTN’s TRIGA IPR-R1 reactor fuel pins. To simplify the model, no gap between the fuel and the cladding was considered. The volume of water was defined to maintain the same water to fuel ratio found in the reactor core.

The mesh was generated using Gmsh [5] that is an open source software for three-dimensional unstructured mesh generation compatible with both used software. A 2D mesh for the transversal section of the domain was defined with a global maximum mesh size of 4.0 mm for the whole domain and 0.3 mm local sizing at the cladding with a growth ratio of 1.2. These parameters resulted in a smoothly growing mesh in the 2D plane. The axial mesh was set as 35 extrude mesh layers of the 2D mesh. Some details of the mesh are also shown in Fig. 2.

The use of these parameters resulted in a mesh with 346,675 elements.

B. Thermalhydraulics

OpenFOAM is a C++ library used to create solvers for problems in continuum mechanics and utilities for data manipulation [1]. There is a large array of implemented solvers for CFD simulations that are verified by the OpenFOAM Foundation and is quickly being adopted by several companies and academic institutes as their main CFD solution. Amongst the available solvers, the chtMultiRegionSimpleFoam solver [1] was chosen for this work as it couples single phase flow simulations to solid conduction simulation.

The selected solver solves the RANS momentum, continuity and energy conservation equations for the fluid region and energy conservation equation for the solids. A modification of the energy equation for the fuel region was implemented in the code to include a variable source term in the solution. This is one of the main advantages of OpenFOAM [1] as it allows equations assembly directly using objects in the solver code.

The RANS two equations standard k-ε turbulence model [6] was selected to calculate the turbulent viscosity. The model assumes that the turbulence viscosity is related to the turbulence kinetic energy (k) and dissipation (ε).

Thermo-physical properties are defined for each region as a function of temperature or constant based on the work by Veloso [7], as presented in Tab. I.
C. Neutronics

The milonga nuclear code is a free and open source piece of software released under GNU license [8]. It heavily relies on other well-known GNU libraries, like GNU Scientific Library [9], bringing to it the robustness of this established software. It solves the steady-state multi-group neutron transport equation using different methods. In the present work, the diffusion approximation method is used. Milonga can discretize the spatial coordinates using either a finite-element or a finite-volumes scheme.

This ability to use finite-volumes discretization schemes over unstructured grids allows the use of the same mesh for both thermal-hydraulics and neutronics. With identical meshes, there is no need of fields mapping or balancing between codes, making coupled calculations straightforward. Despite the inaccurate results and limitations of the diffusion approximation under some circumstances [10], it is the method used in this work due to its relatively fast execution time.

The cross-sections dependence on temperatures does not affect the formulation of diffusion equation as linear since in the iterative calculation all coefficients are constant during time steps.

Milonga works by reading an input file which defines the characteristics of the problem to be solved. A simple input file for milonga must define a mesh (by selecting its filename and path), chose a numerical formulation and define the number of neutron groups to be calculated, two for this specific work.

Macroscopic absorption cross-sections, macroscopic scattering cross-sections, and diffusion coefficients must be obtained from the table generated by WIMSD-5 beforehand defined for each mesh. These coefficients are used in the solution of the partial differential equation representing the diffusion of neutrons in the system and must match the physical properties of the mesh.

Moreover, the coefficients must be defined for each group of energy defined for the calculations. After material definitions, the appropriate boundary conditions are set matching the physical entities defined in the mesh. Table II shows the boundary conditions used for the simulation.

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Type</th>
<th>Corresponding region</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet</td>
<td>Zero current</td>
<td>Coolant</td>
</tr>
<tr>
<td>Outlet</td>
<td>Zero current</td>
<td>Coolant</td>
</tr>
<tr>
<td>Extremes</td>
<td>Zero current</td>
<td>Cladding and fuel</td>
</tr>
</tbody>
</table>

The calculations are started by a command call which builds the eigenvalue problem and solves the system. Fig. 3 shows a simple input file for milonga code. The material definitions are made in lines 10-16. The values can be constants like in the example below but can also be a function of a value or position. This feature of milonga code makes coupling to external values straightforward.

D. Cross-sections

The beginning of life TRIGA IPR-R1 fuel composition was considered in this study.

In order to have a simulation with a real physical behaviour, it is fundamental to model the materials characteristics as close as possible to their physical aspects. This is achieved having a set of representative cross-sections of the materials neutronic behaviour.

These sets of cross-sections were generated for three different materials representing fuel, cladding, and coolant at the tabulated temperatures presented in Tab. III and their corresponding densities, while the materials composition are depicted in Tab. IV, following an established cross-section generation methodology developed by DEN/UFMG [4,12].
WIMS-D5 presents the macroscopic cross section homogenized in the cell and the value for each material. These macroscopic cross sections were used to feed milonga.

As explained before, calculations are performed separating neutrons from the whole energy spectrum in two energy groups. All coefficients used by milonga to solve the equation diffusion were previously calculated [4,12]. Coefficients values are obtained for the materials listed in Tab. IV for the temperatures listed in Tab. III. WIMSD-5B processing gives cross-sections and diffusion coefficients for each material, with an exception for scattering cross-sections, which are given for a homogenized region formed by all materials. For this reason, scattering cross-sections are the same for all materials.

These data are written in milonga format as constant values for each material and group.

### TABLE III
**Temperatures for materials based on Veloso [7].**

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel</td>
<td>300</td>
<td>300</td>
<td>500</td>
<td>600</td>
</tr>
<tr>
<td>Cladding</td>
<td>300</td>
<td>396</td>
<td>403</td>
<td>410</td>
</tr>
<tr>
<td>Coolant</td>
<td>300</td>
<td>308.5</td>
<td>317</td>
<td>341</td>
</tr>
</tbody>
</table>

### TABLE IV
**Materials composition for cross-sections generation with WIMSD-5B [4,12].**

<table>
<thead>
<tr>
<th>Material</th>
<th>Material code</th>
<th>Mass</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel H (in zirconium hydrate)</td>
<td>5001</td>
<td>3.7525e-02</td>
</tr>
<tr>
<td>Zr</td>
<td>91</td>
<td>3.7727e-02</td>
</tr>
<tr>
<td>U235</td>
<td>2235</td>
<td>2.5744e-04</td>
</tr>
<tr>
<td>U238</td>
<td>8238</td>
<td>1.0167e-03</td>
</tr>
<tr>
<td>Cladding Al</td>
<td>27</td>
<td>6.0261e-02</td>
</tr>
<tr>
<td>Coolant H</td>
<td>3001</td>
<td>6.6653e-02</td>
</tr>
<tr>
<td>O</td>
<td>6016</td>
<td>3.3327e-02</td>
</tr>
</tbody>
</table>

### TABLE V
**Averaged temperatures (K) for materials after first step thermal-hydraulic simulations.**

<table>
<thead>
<tr>
<th>Material</th>
<th>Simulation power by pin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material</td>
<td>1.98 [kW]</td>
</tr>
<tr>
<td>fuel</td>
<td>339.8 [K]</td>
</tr>
<tr>
<td>cladding</td>
<td>327.2 [K]</td>
</tr>
<tr>
<td>water/moderator</td>
<td>303.5 [K]</td>
</tr>
</tbody>
</table>

Temperatures from OpenFOAM simulations were used to generate the cross sections and fed back to milonga that calculated the neutron flux distribution. Fig. 4 shows the axial distribution of the neutron flux in the center of the fuel. It can be seen that the fluxes follow a physically expected sinusoidal shape distribution [11] for all simulated powers.

Based on flux distribution, milonga generates a power distribution with reference to a defined power value, the same value used by OpenFOAM.
The power distributions obtained from *milonga* and the temperatures along the axial center line of the fuel are shown in Fig. 5 and 6. As expected, the power profiles for all simulations have a sinusoidal like shape [11], since there are neutrons escaping from the top and bottom of the model. Temperature profiles have a non-symmetric shape due to the cold water entering the system. The water flow is heated when in contact with cladding, generating the non-symmetrical profile observed.

![Figure 4: Axial neutron flux distribution taken from the center line of the fuel.](image)

![Figure 5: Axial power profiles used by OpenFOAM from milonga.](image)

![Figure 6: Axial temperature profiles of the fuel calculated by OpenFOAM with power distribution from milonga.](image)

The solid region power distribution corresponding to the fuel material is presented in Fig. 7 illustrating its relative variation among simulations.

![Figure 7: Axial power profiles of fuel solid regions.](image)

**IV. CONCLUSIONS AND FUTURE WORK**

In this paper, a one-step coupling methodology is developed to allow thermal-hydraulic calculations based on neutronic generated power profiles.
The coupled calculations show expected results for power profile when compared to former calculations [11]. The effectiveness of this methodology can be extended by the use of scripts to make the temperatures average process fully automatic and also using the script already wrote to process milonga output generating OpenFOAM input. Moreover, since both codes used for calculations are distributed with source-code, an iterative coupling scheme can be envisaged. The framework offered by milonga has built-in functions to read, write and process external files in different ways, making coupled calculation straightforward.

REFERENCES