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Molten Salt Reactor thermal-fluid dynamics evaluation using a CFD code for a theoretical power density distribution

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ABSTRACT

The molten salt reactors are a kind of nuclear reactor that had received additional attention worldwide due to their inherent safety features and the possibility of use the Thorium, a more abundant resource than Uranium, as a fuel. Despite of this promise concept and works being developed or under course, some aspects related to their thermal hydraulics should be better understand. In this work, the initial thermal-hydraulics results obtained using the ANSYS-CFX® code are presented. The simulations were conducted in 3D for 1/16 of a cylinder volume that represents the molten reactor core. The results show a good agreement for this simplified geometry and for a theoretical power density distribution between the benchmark work and those obtained within this for the temperature. An evaluation for the other properties and for different turbulence models, among others, are planned for future.

Keywords: **Molten salt, CFD, Thermal-hydraulics, Properties.**

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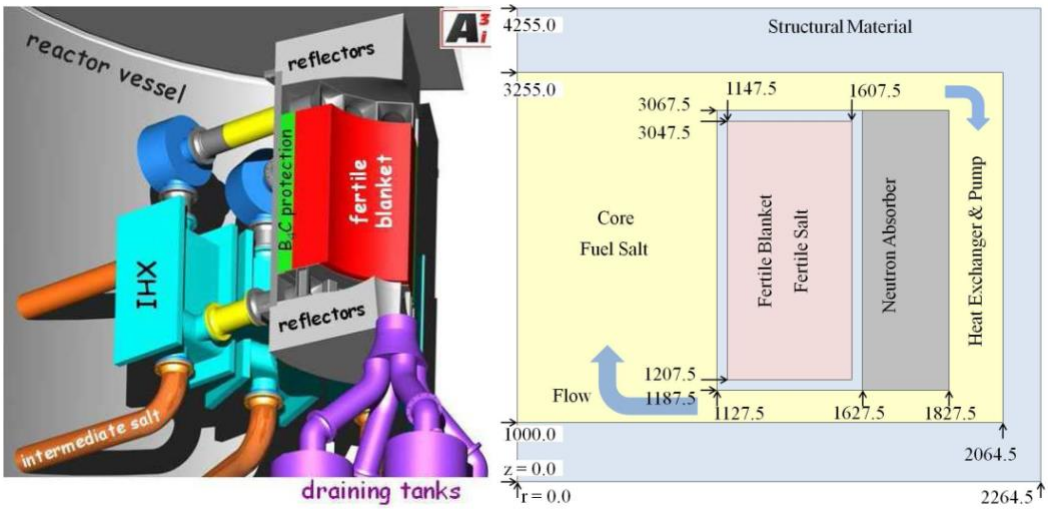
1. INTRODUCTION

The Molten Salt Reactors (MSR) are reactors in which the fuel is mixed with the coolant, thus flowing through the reactor core and system components. This coolant-fuel mix is a salt, having interesting physical properties that allows the reactor to operate with low pressure and high temperatures without compromise its safety since the reactor remains operating only while the salt is flowing, which requires the salt to be above a minimum temperature to become liquid (melting point). In addition, since the salt have an elevated vapour pressure, it does not boil even with the operational pressure being low [1].

The MSR have being proposed initially by the Oak Ridge National Laboratory (ORNL) to aircraft propulsion during the Cold War but, despite of the good results and the prototype that have been constructed, the program was closed. Recently, the EVOL project have being proposed, this being based on the initial concept of the ORNL. The EVOL reactor is a fast reactor in which the core has a cylindrical shape surrounded by a Thorium blanket, where the fuel, ^{233}U, is produced [1]. A schematic view of the reactor and some of its equipment is given in Figure 1.

Figure 1: *3D view of reactor internals and main equipments (left) and main dimensions (right)*



Source: [1]

Despite of its simple concept, the thermal hydraulics of the MSR, such as the EVOL, is still object of research because a change in the molten salt flow properties (the coolant) could affect other physical salt properties and, as consequence, the reactor kinetics, its power and operation. A better understand of the properties of the salt flow could be accessed by using a CFD (Computational Fluid Dynamics) code, in which the flow domain is discretized in small volumes and the governing equations are solved (mass, momentum and energy conservation equations). In this manner, the CFD codes are an important tool to investigate how and the extension in which a change in the coolant flow properties affects other reactor properties or is affected by changes in the reactor neutronics [1].

In this work, the ANSYS-CFX® code was used to perform an initial evaluation of EVOL's molten salt coolant properties using a theoretical power density distribution. The simulations were performed considering two turbulence models, the κ-ε and SST (Shear Stress Transport), this last being a hybrid model between the κ-ε and κ-ω models suitable to treat flows close and far from walls with smooth walls. The results were them compared with the work [1], used as benchmark, in which some thermal-hydraulic CFD simulations were performed. At the aware of the authors, there is no experimental data available for validation purpose of simulations results [[1], [2]].

The initial results obtained in the present work consist in flow properties distributions, which were compared with the benchmark work. The pressure and temperature distributions agree well with the benchmark work [1] for both turbulence models while the turbulence viscosity and other flow properties have a better agreement for the SST model, indicating that a wall function have been used in the benchmark work to simulate the flow next to the walls. The κ-ε model typically requires an adjustment by a wall function to simulate the boundary layer next to the walls. On the other hand, the SST model as implemented in the CFD code used in the present work includes a wall function that is automatically [3].

Additional investigation is under course to evaluate the dependency of the results within the turbulence models, mesh refinement and the coolant flow properties for other power density distributions.

2. MATERIALS AND METHODS

The present work has been performed numerical simulations using a commercial CFD code – ANSYS-CFX® academic license – which have models implemented suitable for the simulations performed in the present work in which a turbulent flow, heat generation and change in properties are of interest. In literature it is often found works in which the EVOL reactor is simulated only in 2D using CFD codes developed for this specific reactor and its geometry. On the other hand, the CFX® is a CFD code able to simulate a wide variety of flows, heat transfer and coupled fluid flow and heat transfer that occur in several equipment and industrial application [[1], [3]].

The choose of the code was based on its robustness and versatility. Despite of these and other advantages that the code brings, the simulations should be performed only in 3D. In this manner, due to this characteristic, the simulations were performed in a 3D flow domain, for 1/16 of the EVOL cylindrical core due to the core symmetry in the "z" coordinate (considering cylindrical coordinate system). This approach aid to reduce the mesh volumes required to discretize the flow domain and the computational effort [[1]-[3]].

Two simplified branches were added to simulate the inlet and outlet tubes through the molten salt flows into and outer of the reactor core. These tubes are only of secondary importance for this stage of the research since there is no fission and power being produced inside them and the main objective is to understand if there is any influence of the flow properties change to the power distribution and neutronics. The neutron precursors and other features are subject of future works in which a more detailed simulation is planned.

In this work, two turbulence models were used to perform the simulations: the κ-ε and SST. The former is the same used in the benchmark work [1] while the last was choose due to its ability to simulate flows next to and far from the smooth walls. As mentioned, the SST model is a hybrid model between the κ-ε and κ-ω models developed to overcome some difficulties found to simulate certain flows with one or another model [3]. In this manner, a comparison of the results using the ANSYS-CFX® with the benchmark work could be done as well as a first evaluation of the influence of the turbulence models on the results.

The turbulence level was setup as medium (5%), the intermediate level pre settled available in ANSYS-CFX® code. Briefly, the turbulence level is a measure of the variation in local flow velocity of the flow compared with its average velocity. Thus, as higher the turbulence level, as greater would be the variation of local flow velocity [3]. By choosing the intermediate value, it would be possible to evaluate how much turbulence is involved in the molten salt flow, serving as a guide to adopt values above or below as need.

The RMS (Root Mean Square) residuals were used as the convergence criteria. The simulations converge for residuals below $1x10^{-5}$ threshold for any of the governing equations (mass, momentum and energy). The residuals represent the difference between the values of properties and other quantities calculated within an iteration and those that were obtained in the previous. This threshold value was adopted to all governing equations since it does not impose a severe computational effort at all as well as it is low enough to improve the quality of results obtained [3]. As part of the convergence evaluation, also the imbalances of governing equations were monitored aiming to ensure the quality of the results, as recommended by the user's guide of the CFD code [3]. The imbalances are in percentage form and represents the extent to which the conservation of mass, momentum and energy is achieved. In this manner, as close of 0% as better is the results.

Since the library of the code does not include a fluid with the properties of the molten salt, it was necessary to implement it. The properties of the molten salt were inserted in the CFD code considering the equations and values available in literature and in the benchmark work [[1], [2]]. Some of the most relevant are: thermal conductivity, physical density, buoyance coefficient, morphology (physical state), reference enthalpy and entropy, reference pressure and temperature, etc.

After selecting the turbulence model, it was performed 4 different runs. In the first run, it was assumed that properties of the molten salt such as thermal conductivity and physical density are constant. In the second run, the thermal conductivity was let to vary according to the relation as given by equation (1). In the third run, only the physical density of the salt was let to vary, according to the relation as given by equation (2). Finally, in the fourth, both properties – thermal conductivity and physical density of the salt – were let to vary according to equations (1) and (2).

The equations (1) and (2) are recommended by [1] for the operational conditions expected for the MSR with the geometry simulated.

$$k = 0{,}928 + 8{,}397 \times 10^{-5} T \tag{1}$$

$$\rho = \left(4{,}094 - 8{,}82 \times 10^{-4}(T - 1008)\right) \times 10^{3} \tag{2}$$

In which T [K] is the salt temperature in an arbitrary point of the molten salt flowing and to which the thermal conductivity and physical density are calculated. Equations (1) and (2) are valid in the interval of 891-1020K (618-747°C) and 893-1126K (620-850°C), respectively [2].

The initial power density distribution assumes the theoretical case of a bare and finite cylinder. This power density distribution is given by equation (3) according to the neutron diffusion theory [4].

$$q'''(r,z) = \frac{3{,}63 P J_0(2{,}405 \frac{r}{R}) \cos(\pi \frac{z}{H})}{V} \tag{3}$$

In which r and z are an arbitrary radius and height in core, respectively, R is the core radius, H is core height, V is the core volume and J_0 is the Bessel function of order zero [4]. The r and z in equation (3) considers that the coordinated system origin is centered in the core (r=0 and z=0 in the middle of the core's height at the core's center). It means that the blanket of Thorium surrounding the core does not have any influence in the power density distribution and core neutronics, an assumption adopted by. Notwithstanding, it was considered that the blanket region does not produce significant thermal power [1]. Thus, to comply within these assumptions, every wall of the 1/16 cylinder representing a slice of the core was assumed to be adiabatic (blanket wall, top and bottom walls, external walls. Due to the symmetry of the volume domain, the two faces of the slice that represents the calculus domain simulated was assumed to be periodic. In this manner, the CFD code assumes that there is an exchange of heat and flow through these two walls while the salt flows from the core inlet to the outlet [[1], [3]]. Figure 2 illustrates these main regions, the symmetry axis and the mesh used in this first approach.

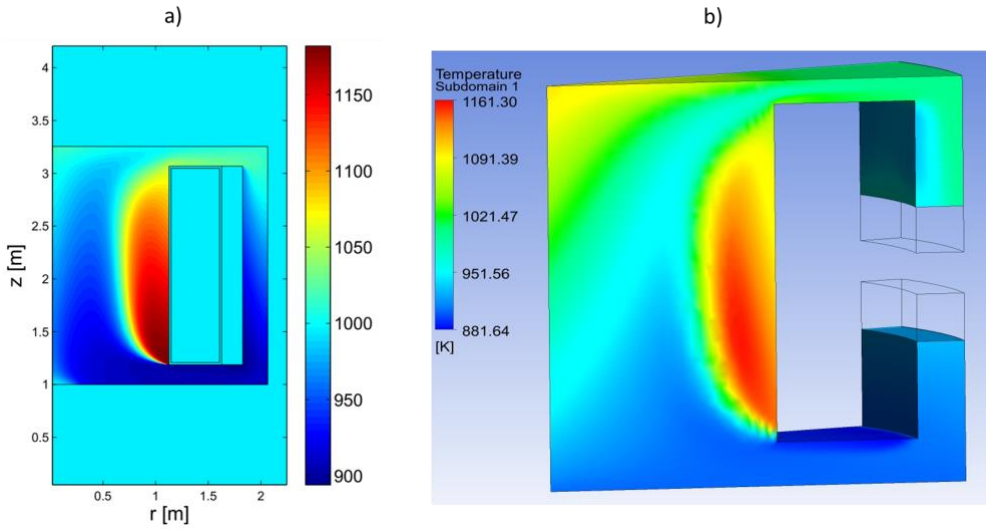
Figure 2: *Schematic view of fluid domain simulated - MSR.*

Regarding the mesh, it was applied a non-structured mesh of mainly composed by tetrahedral elements. In the regions where the gradients are higher (walls, inlet and outlet), it was applied 20 layers of prisms each one within different thickness to better capture the gradients in these regions, improve the quality of results and numerical stability. A total of about 89,000 elements of volume were used in this first mesh. In this first evaluation a mesh dependency study was not performed since the objective is primarily evaluating the influence of turbulence models on the results. For future, it is planned such study together with additional evaluations addressing the molten salt properties and its relation within the flow and reactor neutronics. This mesh reveals to have a good cost-benefit balance among the results quality and computational effort, requiring a common personal computer and only few minutes (about 12 minutes) to perform completely each simulation run.

3. RESULTS AND DISCUSSION

The results obtained in this first part of the research demonstrated, for the theoretical power density distribution (see equation (3)), a good agreement of the temperature profile within the benchmark work [1] for both turbulence models. The other flow properties are still under evaluation since, according to equations (1) and (2), they have no influence over properties such as physical density and thermal conductivity of the salt. The distributions obtained in the present work for the SST model and in the benchmark are given in Figures 3 a) and b).

Figure 3: *Temperature distributions a) in the benchmark work, b) in the present work for the SST model. Temperatures are in [K].*



Source: a) adapted from [1].

As could be observed, the values obtained in present work are similar to that in the benchmark, being only slightly above that in benchmark work [1]. A plume of hot salt is formed close to the blanket wall due to the lower flow in this region. It should be emphasized that in this region the power density is lower than in the center of the core. Another reason for this plume location refers to the assumptions made for the blanket walls. Since they are assumed as adiabatic, no heat could be transferred through them and thus, it accumulates in regions with lower flow.

Some additional and important remarks regarding these initial results are:

- The turbulence level seems to be adequate considering the temperature distribution only. In future works when other properties would be under evaluation, it would be changed aiming to check its influence over the results;
- The mesh seems to be refined enough, since it does not compromise the results quality, have a reduced computational effort and good numerical stability;
- Despite both turbulence models had shown very similar results, an evaluation regarding their influence over the distributions of other properties is planned for future. It is expected that the SST model presents a better agreement since it incorporates a wall function that is automatically adjusted by the CFX® code accordingly required. Even considering that the code allows to introduce such function for the κ-ε model, since there is no previous experience with this adjustment for such coolant and there is no indication regarding the function eventually used in the benchmark work, the reference results would be difficulty to be achieved, requiring a high computational time.

4. CONCLUSION

The ANSYS-CFX® code was able to simulate the molten salt flow. The temperature distribution agrees well within the benchmark work, with values only slightly above that available in the benchmark work, for both turbulence models tested. For future works, it is planned to evaluate other properties, turbulence models and perform a mesh dependency study aiming to evaluate more completely the thermal-hydraulics of the molten salt flow.

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