ABSTRACT

This paper presents a preliminary approach to thermo-hydraulics of the molten salt, which plays the role of both heat generator and coolant in the Molten Salt Reactor (MSR). This kind of nuclear reactor represents one of the "Generation IV International Forum" concepts that can be used for actinides burning, production of electricity, production of hydrogen, and breeding of nuclear fuel.

Physics of circulating nuclear fuels, as the molten salt, is featured by a strong coupling between neutronics and thermo-hydrodynamics. In the present study, analyses are performed assuming that the neutronic term is decoupled from fluid dynamics and appears like an energy source term, and taking into account the thermodynamic and transport properties of the molten salt as well as its local flow conditions and heat transfer. Even if this assumption simplifies the equations to be solved, the thermo-hydrodynamic behaviour of the molten salt remains complex.

The graphite-moderated channel type molten salt breeder reactor based on a previous research at Oak Ridge National Laboratory (ORNL) is considered: a preliminary study of the heat transfer and pressure losses in a typical MSR core channel is proposed referring to a simple axial-symmetric cylindrical geometry with the aim to investigate the specific behaviour of such system as well as to test and compare two different commercial computer codes – namely, COMSOL® (Multiphysics finite elements software) and FLUENT® (Computational Fluid Dynamics finite volumes software) – on the basis of an analytic framework, in view of their adoption for more realistic, design-oriented and multi-physics simulations.

1 INTRODUCTION

Molten Salt Reactor (MSR) represents one of the promising high temperature nuclear reactor types for future generation of electricity and of heat for hydrogen production. It also could be used as transmuter to burn plutonium and other transuranium elements occurring in the spent nuclear fuel of nowadays nuclear power plants [1]. MSR is usually labelled as a non-classical reactor type because of the specific character of its fuel, which is constituted by a molten fluoride salt mixture circulating in the primary circuit. The fission material (uranium and/or transuranium elements) is dissolved in carrier molten salt, which is also a heat-transferring agent.

Thanks to the potentialities of this liquid fuel based on molten fluorides [2], several MSR concepts were investigated by ORNL in the past, and in the last years MSRs have been the subject of a renewed interest mostly within the European activities in the framework of
Generation IV nuclear reactors [3]. These concepts differ mainly by neutron balance (critical or subcritical), neutron spectra (thermal, epithermal or fast), the presence/absence of the graphite matrix as moderator and the fuel salt chemical composition.

In the present work, the Molten Salt Breeder Reactor concept, proposed by ORNL in the frame of the MSR Program [4,5], is considered: this reactor was designed to produce 1000 MW\textsubscript{e} and is featured by a thermal neutron spectrum and thorium fuel cycle; the core is formed of hexagonal graphite-moderated blocks, each one with a central molten salt fuel/coolant channel. The salt composition in the primary circuit is the following: $^{7}$LiF(71.7 mol%), BeF\textsubscript{2}(16 mol%), ThF\textsubscript{4}(12 mol%) and $^{233}$UF\textsubscript{4}(0.3 mol%). Such a system is featured by a strong coupling between neutronics and thermo-hydrodynamics as well as between the fuel and the graphite matrix [6].

In the present study the neutronic term has been decoupled from fluid dynamics, and appears like a heat source within the molten salt fuel/coolant, with the aim to investigate only the thermo-hydrodynamic behaviour specific to such system, with reference to an axial-symmetric geometry representative of a typical reactor core channel. A preliminary analytic approach to evaluate the temperature radial profile in both fuel and graphite is discussed, and offers a useful validation framework for testing commercial tools, in view of their adoption for more realistic and complex 3-D geometry analyses. At this purpose, a necessary validation step has been individuated in the assessment and comparison of the numerical solutions achieved by two different codes, namely COMSOL (Multiphysics) and FLUENT (CFD), on the basis of the well-established analytic solution of flow in long smooth pipes both in laminar and turbulent regimes. This validation procedure referring to the pipe flow has been carried out in analogy with recent works performed for other innovative reactors, like the Super-Critical Water Reactor (SCWR) [7] and the Accelerator Driven Systems (ADS) [8]; it is also an “excellent building-block case for testing turbulence models” [9], but this last investigation has not been the object of the present study.

2 VALIDATION

In this section COMSOL and FLUENT computational fluid dynamics (CFD) results have been compared with the analytic solution of radial temperature profile in presence of a volume heat source within the fluid for a circular-pipe system in cylindrical coordinates $(r,\theta,z)$ in the cases of both laminar and turbulent flows [10]. The analytic solution was found by Poppendiek [10] under the following hypotheses:
- Axial-symmetric conditions are taken into account.
- Thermal and hydro-dynamic patterns are established (long pipes).
- Fluid axial conduction is neglected.
- Steady state exists.
- Uniform volume heat source exists within the fluid.
- Physical properties are not function of temperature.
- Heat is transferred uniformly to or from the fluid at the pipe wall.
- In the case of turbulent flow, an analogy exists between heat and momentum transfer.

Under the above assumptions, the differential equation and the boundary conditions describing the heat transfer in the pipe system for laminar or turbulent flow can be written according to the following 1-D formulation:

$$\frac{d}{dr} \left[ (\alpha + \varepsilon) r \frac{d\Theta(r)}{dr} \right] = \frac{u(r)}{v_m \rho c_p} \left[ q^* - \frac{2}{r_0} q^*_{\Phi} \right] r - \frac{q^* r}{\rho c_p},$$

(1)
where $T$ is the fluid temperature, function of the radial coordinate $r$; $\alpha$, $\lambda$, $\rho$, and $c_p$ are the thermal diffusivity, the thermal conductivity, the density and the specific heat capacity of the fluid, respectively; $\varepsilon$ is the fluid eddy diffusivity and it is a function of both the radial coordinate and the axial component of the fluid velocity $u(r)$; $u_m$ is the mean fluid velocity; $r_0$ is the pipe radius; $q'''$ and $q''_{W}$ are the volume heat source and the uniform wall-heat flux, respectively. The second boundary condition, expressed by Eq. (3), is some reference temperature $T_D$ such as wall, centre-line, or mixed-mean fluid temperature.

As concerns CFD simulations, they have been performed in steady state conditions, with reference to a 2-D axial-symmetric ($r,z$) computational domain. It is assumed that the fluid is incompressible, homogeneous and independent on the concentration of chemical species, and its physical properties are not function of temperature; moreover, the action of gravity has been neglected. For the analyses in turbulent regime, the standard $k$-$\varepsilon$ model has been adopted, which is the most widely two-equation model used as reference among the several turbulence models available in literature [9].

As far as the approach for modelling the near-wall region is concerned, COMSOL adopts the logarithmic wall-functions, assuming that the computational domain begins at a certain distance, which depends on the mesh size, from the real wall, while the enhanced wall treatment approach has been chosen for FLUENT calculations.

Great effort was spent in setting up the mesh elements/cells size, particularly at walls and interfaces, by means of a mesh sensitivity analysis that is not reported here for brevity. It must be noted that, even for the simple circular-pipe geometry adopted in this work for the validation, the accuracy of numerical results depends on the fluid properties, on the meshing strategy and on the turbulence model, as clearly demonstrated by analogous studies performed for other fluids in the same geometry [7,8].

Concerning the numerical strategy, the segregated algorithm has been used in both codes for getting the solutions. The second order scheme and the SIMPLE algorithm for the pressure-velocity coupling have been adopted for FLUENT analyses, while the anisotropic diffusion (with the standard tuning parameter) has been chosen for COMSOL. A complete description of the fluid flow modelling and of the different available options is given in the FLUENT and COMSOL user’s guides [11,12].

### 2.1 Laminar flow

The solution of the boundary-value problem defined by Equations (1), (2) and (3) was achieved by Poppendiek [10] in the case of laminar flow, considering that the eddy diffusivity is null in laminar regime and the fluid velocity attains a parabolic profile along the pipe radius once the hydrodynamic pattern is established. The solution is given by Eq. (4):

$$
\frac{T(r) - T_C}{q^*_{W}/2\lambda} = \frac{2F - 1}{2} \left(\frac{r}{r_0}\right)^2 - \frac{F}{4} \left(\frac{r}{r_0}\right)^4
$$

where $T_C$ is the centre-line temperature and $F = 1 - (2q^*_{W}/q^*_{W_{0}})$, namely $\{1 - \text{fraction of heat generated within moving fluid that is transferred at wall}\}$ [13].
The dimensionless radial temperature profile given by Eq. (4) is plotted in Figure 1 for several values of the function F and compared with the CFD simulations results attained by means of COMSOL and FLUENT: both numerical solutions are practically superimposed to the analytic one.

2.2 Turbulent flow

For the case of turbulent flow, the boundary-value problem defined by Equations (1), (2) and (3) can be separated into the following two simpler boundary-value problems, whose solutions can be superimposed to yield the solution of the "original problem":

(i) a problem representing a flow-system with a volume-heat source, but with no wall-heat flux;
(ii) a problem representing a flow-system without a volume-heat source, but with a uniform wall-heat flux.

The solution for the first problem (i) was found by Poppendiek [10] with the following procedure: at first, the radial heat flux profile is calculated assuming that the velocity profile may be satisfactorily represented by two layers (a laminar layer and a turbulent core with the so-called "venerable" one-seventh power law for the velocity [14,15]); therefore, by replacing the radial heat flux by simple monomials and polynomials, it is integrated layer by layer (laminar sublayer, buffer layer, outer turbulent layer and inner turbulent layer) to find the radial temperature profile. The dimensionless radial temperature profile results a function of both Reynolds (Re) and Prandtl (Pr) numbers [10,16].

The solution for the second problem (ii) was originally found by Martinelli [16] assuming three layers (laminar sublayer, buffer layer, turbulent layer) for the calculation of both the velocity and the temperature profiles. It is worth mentioning that in the buffer and turbulent layer Martinelli prefers a logarithmic law for the velocity based on experimental data (i.e., the so-called generalized velocity profile). In the present work the authors follow an alternative analytic solution based on the same approach of Poppendiek, briefly described above for the problem (i), adopting the 1/7\textsuperscript{th} power law for the velocity and the same four layers of Poppendiek for the radial temperature. The comparison between the Martinelli and
the present work approaches is shown in Figure 2 in terms of the temperature difference with respect to the centre-line pipe temperature as a function of the dimensionless distance \( n \) from the pipe wall \( (n = 1 - r/r_0) \): these two approaches substantially agree with little differences at lower Reynolds numbers and in the centre of the pipe.

The temperature profile of the "original problem" can be easily achieved by superimposing the temperature profiles of the problems (i) and (ii). In Figure 3 the results attained by means of CFD analyses for the "original problem" are compared with the analytical ones achievable following the Martinelli and the present work approaches for the problem (ii).

![Figure 2: Comparison between the different evaluations of the radial temperature profiles in a pipe with turbulent flow for several Reynolds numbers and \( Pr = 1 \) – problem (ii).](image)

![Figure 3: Comparison between the different evaluations of a) the dimensionless velocity profile, and b) of the radial temperature profile in a pipe with turbulent flow for several Reynolds numbers and \( Pr = 1 \) – "original problem" = (i) + (ii).](image)

The numerical results in terms of velocity (Figure 3-a) and temperature (Figure 3-b) profiles follow very well those provided by both the analytic approaches, which result very close each other.

As concerns the temperature, it must be pointed out that a more accurate agreement can be found by means of FLUENT in the near-wall region thanks to the *enhanced wall treatment* approach of the boundary layer.
As concerns the velocity, numerical results provided by both codes are in a good agreement, whereas the analytical profiles show some little differences due to the modelling assumptions (logarithmic and 1/7th laws).

3 HEAT TRANSFER AND PRESSURE LOSSES IN THE MSR CHANNEL

It is specific to the MSR that, even if the energy from nuclear fissions is predominantly released directly in the fuel, the graphite channels are heated-up by the gamma and neutron radiation and the presence of this heat source causes that in most cases the direction of radial temperature gradient is from the fuel to the graphite: the liquid fuel practically cools down the graphite in steady-state operation [17].

The investigation of the heat exchange properties between molten salt and graphite has been performed with reference to an axial-symmetric geometry representing a typical MSR core channel, idealised as a circular pipe with circulating molten salt that is surrounded by a hollow cylinder of graphite.

By coupling the analytic approach of the present work described in the previous section for modelling the fully developed flow of molten salt inside the pipe with the heat conduction problem for the graphite, it is possible to find the radial temperature profile in the channel (graphite + molten salt). The previous solutions (i) and (ii) can be used for the molten salt, while for the graphite the following radial profile is obtained solving the 1-D heat conduction equation between the inner (R_i) and the outer (R_o) radii of graphite:

\[
T(r) = \frac{q''_g}{2\lambda_g} \left( R_i^2 - r^2 \right) + R_o^2 \ln \left( \frac{r}{R_i} \right) + T_w
\]

where \( q''_g \) and \( \lambda_g \) are the volume heat source and the thermal conductivity of the graphite, and \( T_w \) is the interface molten salt-graphite temperature. The heat flux at the interface, \( q''_{w} \), is given by Eq. (6):

\[
q''_w = -q''_g \left( R_o^2 - R_i^2 \right) / 2R_i
\]

To calculate the wall temperature \( T_w \), it is necessary to solve first the heat transfer problem in the molten salt applying as boundary condition the wall heat flux given by Eq. (6) and imposing the value of the volume-heat source in the molten salt (\( q''_s \)) as well as in the graphite (\( q''_g \)). In the next analyses a ratio \( q''_w / q''_s \) of about of 3% is adopted [18].

Once the radial temperature profile is known, it is possible to calculate analytically the Nusselt number as \( Nu = (D_h/\lambda) \cdot q''_{w} / (T_w - T_b) \), and consequently the heat transfer coefficient between the molten salt and the graphite as \( h = Nu \cdot \lambda / D_h \), where \( T_b \) and \( D_h \) are the bulk (or mixed-mean) temperature of the molten salt and the channel hydraulic diameter, respectively.

It must be pointed out that in the case of heat source within the fluid, the Nusselt number is not only function of Reynolds and Prandtl numbers, but also of the ratio between the heat source and the wall heat flux [10].

Two different cases have been considered for the CFD analyses: I) no volume-heat source within the molten salt; II) molten salt with volume-heat source. The first case is important both for the above comment about the Nusselt number and because molten salt heat transfer properties are of interest for its employment in the intermediate-heat exchanger [18]. The second case is more representative of a MSR core channel, and the respective results will be shown for brevity only in the turbulent flow, since it represents the case of operating regime.
For what concerns molten salt and graphite properties, MSR design specifications and the volume-heat sources, this work refers to [18], the most important data being reported in Table 1.

<table>
<thead>
<tr>
<th>Symbols/quantities</th>
<th>Molten salt</th>
<th>Graphite</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_p$, specific heat capacity [J·kg$^{-1}$·K$^{-1}$]</td>
<td>1357</td>
<td>1760</td>
</tr>
<tr>
<td>$D_h$, channel hydraulic diameter [m]</td>
<td>0.16</td>
<td>-</td>
</tr>
<tr>
<td>$H$, channel length [m]</td>
<td>4.8</td>
<td>4.8</td>
</tr>
<tr>
<td>$Pr$, Prandtl number [-]</td>
<td>11</td>
<td>-</td>
</tr>
<tr>
<td>$q''$, volume-heat source [W·m$^{-3}$]</td>
<td>$1.3 \cdot 10^8$</td>
<td>$3.4 \cdot 10^6$</td>
</tr>
<tr>
<td>$R_i$, interface radius [m]</td>
<td>0.08</td>
<td>0.08</td>
</tr>
<tr>
<td>$R_o$, outer radius [m]</td>
<td>-</td>
<td>0.12</td>
</tr>
<tr>
<td>$T_{in}$, channel inlet temperature [K]</td>
<td>900</td>
<td>-</td>
</tr>
<tr>
<td>$\eta$, dynamic viscosity [kg·m$^{-1}$·s$^{-1}$]</td>
<td>0.01</td>
<td>-</td>
</tr>
<tr>
<td>$\lambda$, thermal conductivity [W·m$^{-1}$·K$^{-1}$]</td>
<td>1.23</td>
<td>31.2</td>
</tr>
<tr>
<td>$\rho$, density [kg·m$^{-3}$]</td>
<td>3330</td>
<td>1843</td>
</tr>
</tbody>
</table>

### 3.1 Laminar flow

A Reynolds number $Re = 80$ has been chosen for the present analysis, referring to the case with no volume-heat source within the molten salt. In Figure 4 the local Nusselt number achieved by CFD simulations (considering a length of 15 m in order to reach fully developed flow conditions) has been compared with the following correlation given by Bird et al. [19], which is valid for thermally developing flow with constant wall heat flux:

$$
\begin{align*}
\text{Nu}_z &= \begin{cases} 
1.302 \left(z^*\right)^{1/3} - 1.0 & \text{for } z^* \leq 5 \cdot 10^{-5} \\
1.302 \left(z^*\right)^{1/3} - 0.5 & \text{for } 5 \cdot 10^{-5} \leq z^* \leq 1.5 \cdot 10^{-3} \\
4.364 + 8.68 \left(10^1 \cdot z^*\right)^{0.56} \cdot \exp\left(-41 \cdot z^*\right) & \text{for } z^* \geq 1.5 \cdot 10^{-3}
\end{cases}
\end{align*}
$$

(7)

where $z^* = z/(Re \cdot Pr \cdot D_h)$. COMSOL and FLUENT codes supply the same results, which are in a very good agreement with the correlation given by Bird et al. as well as with the analytical evaluation of the local Nusselt number (see also Table 2). The friction pressure losses have been numerically evaluated (considering a parabolic profile of the inlet velocity) and compared in Table 2 with the classical Darcy formula for the friction coefficient $f$ in the Hagen-Poiseuille flow (i.e., $f = 64/Re$): a very good agreement exists.

![Figure 4: Comparison between the different evaluations of the local Nusselt number in the MSR channel with laminar flow.](image)

Proceedings of the International Conference Nuclear Energy for New Europe, Portorož, Slovenia, Sept. 8-11, 2008
Table 2: Comparison between analytic and numerical calculations of the local Nu and friction pressure losses in the MSR channel with laminar (fully developed) flow.

<table>
<thead>
<tr>
<th></th>
<th>Analytic</th>
<th>COMSOL</th>
<th>FLUENT</th>
<th>COMSOL</th>
<th>FLUENT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Local Nu (z = 13 m)</td>
<td>4.364</td>
<td>4.393</td>
<td>0.7</td>
<td>4.389</td>
<td>0.6</td>
</tr>
<tr>
<td>Pressure losses (z = H)</td>
<td>9.00·10^{-2}</td>
<td>8.99·10^{-2}</td>
<td>0.1</td>
<td>8.97·10^{-2}</td>
<td>0.3</td>
</tr>
</tbody>
</table>

3.2 Turbulent flow

A Reynolds number Re = 8·10^4 has been chosen for the turbulent flow. In the present paragraph the effect of the standard k-ω turbulence model has been also investigated and results are compared with the analytic solution and with those obtained with the standard k-ε model by means of COMSOL and FLUENT codes for both the considered cases I and II. Radial temperature profiles are shown in Figure 5, while the Nusselt number and the friction pressure losses calculations are given in Tables 3 and 4, respectively.

![Figure 5: Comparison between the different evaluations of the temperature profile in the MSR channel with turbulent flow (z = 4.4 m): I) without, and II) with volume heat source.](image)

Table 3: Nu comparison with the analytic solution in the MSR channel (turbulent flow).

<table>
<thead>
<tr>
<th>Local Nu (z = 4.4 m)</th>
<th>Case I)</th>
<th>Case II)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Analytic solution</td>
<td>523</td>
<td>-</td>
</tr>
<tr>
<td>Dittus-Boelter correlation</td>
<td>502</td>
<td>4.0</td>
</tr>
<tr>
<td>COMSOL k-ε</td>
<td>512</td>
<td>2.1</td>
</tr>
<tr>
<td>COMSOL k-ω</td>
<td>517</td>
<td>1.2</td>
</tr>
<tr>
<td>FLUENT k-ε</td>
<td>584</td>
<td>1.2</td>
</tr>
<tr>
<td>FLUENT k-ω</td>
<td>526</td>
<td>0.7</td>
</tr>
</tbody>
</table>

Table 4: Pressure losses comparison with the McAdams correlation in the MSR channel for the turbulent flow (z = H).

<table>
<thead>
<tr>
<th>Friction pressure losses</th>
<th>[Pa]</th>
<th>Analytic</th>
<th>COMSOL k-ε</th>
<th>COMSOL k-ω</th>
<th>FLUENT k-ε</th>
<th>FLUENT k-ω</th>
</tr>
</thead>
<tbody>
<tr>
<td>McAdams correlation</td>
<td>2163</td>
<td>-</td>
<td>2163</td>
<td>2021</td>
<td>2332</td>
<td>2193</td>
</tr>
<tr>
<td>COMSOL k-ε</td>
<td>2021</td>
<td>6.6</td>
<td>2036</td>
<td>2036</td>
<td>2332</td>
<td>2193</td>
</tr>
<tr>
<td>COMSOL k-ω</td>
<td>2036</td>
<td>5.9</td>
<td>2036</td>
<td>2036</td>
<td>2332</td>
<td>2193</td>
</tr>
<tr>
<td>FLUENT k-ε</td>
<td>2332</td>
<td>7.8</td>
<td>2332</td>
<td>2332</td>
<td>2332</td>
<td>2332</td>
</tr>
<tr>
<td>FLUENT k-ω</td>
<td>2193</td>
<td>1.4</td>
<td>2193</td>
<td>2193</td>
<td>2193</td>
<td>2193</td>
</tr>
</tbody>
</table>
As a result, there is a good agreement of the numerical evaluations of both the Nusselt number and the temperature profiles with those obtained analytically. The well-known Dittus-Boelter correlation can be used for molten salt [13,18] giving a reasonable result in the case of no heat source with a discrepancy of 4% in comparison with the analytic solution, but it should be used carefully in presence of heat source within the fluid because it does not take into account the dependence of heat transfer on the ratio between wall heat flux and volume heat source; as a consequence, the heat transfer coefficient could be excessively overestimated (see Table 3), leading to an underestimation of the graphite temperature. A good agreement can also be found between the numerical evaluations of the pressure losses and the well-known McAdams correlation (see Table 4).

As a general comment on the analyses presented in this section regarding a typical MSR channel, both in laminar and turbulent flows, we can observe that the numerical results provided by COMSOL and FLUENT codes are very close each other in terms of temperature profiles, Nusselt number and pressure losses, and are in a good accordance with the analytical solutions within an error of maximum 13%: this is considered acceptable from an engineering point of view. Some differences have been found, which are related to the choice of different turbulence models, but it is not the aim of the present work to enter into such details. In short, this preliminary study has shown some relevant aspects of the thermo-hydrodynamic behaviour of the molten salt nuclear fuel/coolant, in particular the influence of the volume-heat source on the heat transfer properties. This influence has to be carefully accounted for in the case of more realistic and design-oriented 3-D geometry analyses together with the effects related to the choice of the meshing strategy as well as to the turbulence modelling.

CONCLUSIONS

With reference to a renewed interest on the molten salts technology in the framework of the "Generation IV International Forum", a preliminary study of the thermo-hydraulics of a typical MSR channel has been performed. By assuming that the neutronic problem is decoupled from fluid dynamics and referring to a simple axial-symmetric geometry, several aspects of this system, featured by the heat source within the fuel/coolant, have been analyzed. A validation framework has been thoroughly discussed in order to test two different computer codes (i.e., COMSOL and FLUENT), whose results - in terms of temperature profiles, Nusselt number and pressure losses - are very close and substantially in a good agreement with the analytical solutions and data given by empirical correlations. In particular, an analytical approach based on the 1/7th power law turbulent velocity profile has been adopted and compared with the work of Martinelli. However, more detailed analyses are required in the case of more complex and design-oriented geometries, taking into account the effects related to the geometry itself and to the choice of both the mesh structure and the turbulence model. For this purpose the strong coupling between neutronics and thermo-hydraulics, which is a specific and intrinsic feature of MSRs, needs also to be in-depth investigated.

REFERENCES


