Coupled Neutronics and Thermal-Hydraulics Calculations on the Molten Salt Fast Reactor: Identification and Study of Cliff Edge Effects

T. Sornay[1,2], T. Boisseau[2], A. Laureau[1], A. Lemarchand[2], E. Merle[1], F. Vaiana[3]
[1] Univ. Grenoble Alpes, CNRS, Grenoble INP*, LPSC-IN2P3, 38000 Grenoble, France
* Institute of Engineering Univ. Grenoble Alpes
[2] Framatome, 2 rue du Professeur Jean Bernard, 69007 Lyon, France
[3] Newcleo, 9 rue des Cuirassiers, 69003 Lyon, France
thomas.sornay@lpsc.in2p3.fr

ABSTRACT

This paper presents a new coupled code called TFM-STAR to perform coupled neutronics and thermal-hydraulics simulations. It is the implementation of the Transient Fission Matrix (TFM) neutronic approach with the Computational Fluid Dynamics (CFD) code Star-CCM+. This CFD code developed by Siemens provides meshing and Computer Aided Design (CAD) tools that are useful to perform parametric studies. The coupling method is developed in the frame of research on the Molten Salt Fast Reactor (MSFR) initially developed by CNRS (National Centre for Scientific Research). The circulating fuel induces a strong coupling between neutronics and thermal-hydraulics, caused mainly by temperature feedback, but also by the transport of delayed neutron precursors. The code considers those effects to perform steady state and transient calculations like reactivity insertion, load following, loss of flowrate or loss of heat removal. Based on this code, the application aims at looking for cliff edge effects on alternative version of the MSFR, especially Small Modular Reactor design (SMR). It investigates design, operating and safety aspects.

KEYWORDS: coupling, neutron-kinetics, thermal-hydraulics, transient, simulation

1. INTRODUCTION

This paper presents a new coupled code called TFM-STAR to simulate the multi-physics phenomena inside the Molten Salt Fast Reactor (MSFR) [1] and especially to identify and study possible cliff edge effects in terms of operation, safety, or design aspects. Due to the circulating liquid fuel in this kind of reactors, there is a strong coupling between neutronics and thermal-hydraulics that requires dedicated calculation codes.
TFM-STAR is an adaptation of the TFM-OpenFOAM code [2][3] developed at CNRS (National Centre for Scientific Research) which connect the TFM neutronic model to the Star-CCM+ code. The two simulation codes (OpenFOAM and Star-CCM+) provide a high-fidelity Computational Fluid Dynamics (CFD) modelling. They are coupled with the TFM (Transient Fission Matrix) neutronics model based on a fission matrices approach for neutron kinetics simulation. The latter consists in generating, with a stochastic code, fission matrices plus a time matrix to combine accuracy and a reduced computational cost.
TFM-STAR has been validated using a code-to-code comparison with TFM-OpenFOAM [4][5]. The use of Star-CCM+ will bring some useful alternative features not included in OpenFOAM. For instance, it has computer-aided design (CAD) and meshing features, but it also allows more easily to add components or other physical phenomena. The objective of this work is to perform easily systemic studies of alternative versions of the MSFR, focusing on small modular designs. These studies should emphasize possible cliff edge effects, safety aspects or design optimisations. To do so, this work is based on coupled neutronics thermal-hydraulics associated with various constraints, such as salt composition during the enrichment adjustment process.

At steady state, the cliff edge effects should be identified on thermal-hydraulic parameters such as temperature or velocity flow but also on neutronic parameters like neutron flux, effective delayed neutrons, and others.

2. COMPARISON BETWEEN COUPLING CODES APPLIED ON THE MSFR

2.1. MSFR Presentation

The reference MSFR is a $3GW_{th}$ reactor with a circulating liquid fuel that acts also as the coolant. It is composed of three circuits: the fuel circuit represented in Fig. 1, the intermediate circuit, and the power conversion system. Studies led to a first optimised design "EVOL" [6] for the fuel circuit, its heat extraction part is composed of 16 recirculating loops that each includes a pump and a heat exchanger. It contains 18 m^3 of molten salt, half of it composes the active core region. The salt can be a fluoride salt or chloride salt with heavy nuclei dissolved inside (fissile and/or fertile material) and a third specie can be added to obtain a ternary mixture and decrease the melting temperature. For the fluoride version, the liquid fuel circulation period in the fuel circuit is around 4 s. To simplify the problem and reduce computational cost, only a 16^{th} of the fuel circuit, represented in Fig. 2., is simulated thanks to its periodicity. At this state of the studies, the pump is modelled by a source of momentum and the heat exchanger as a porous media with an associated heat transfer coefficient.

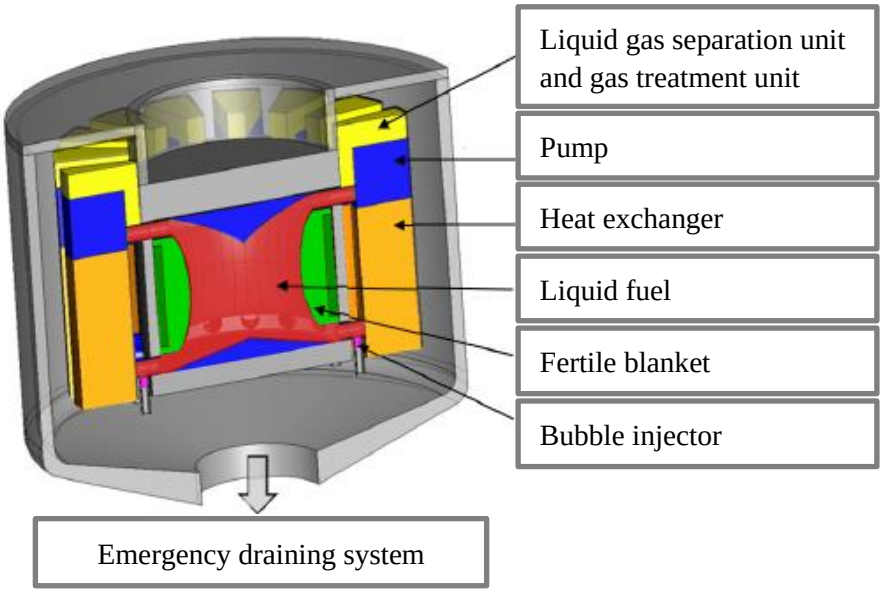

Figure 1 - Schematic view of MSFR fuel circuit [3]

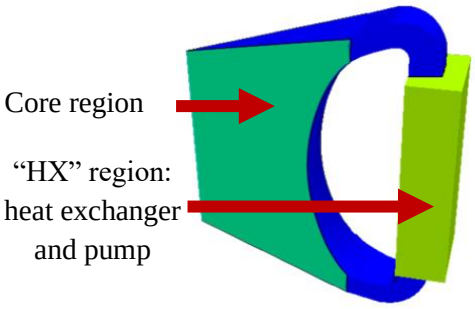

Figure 2 - Schematic view of a 16th MSFR slice for simulation [5]

2.2. Coupling Scheme

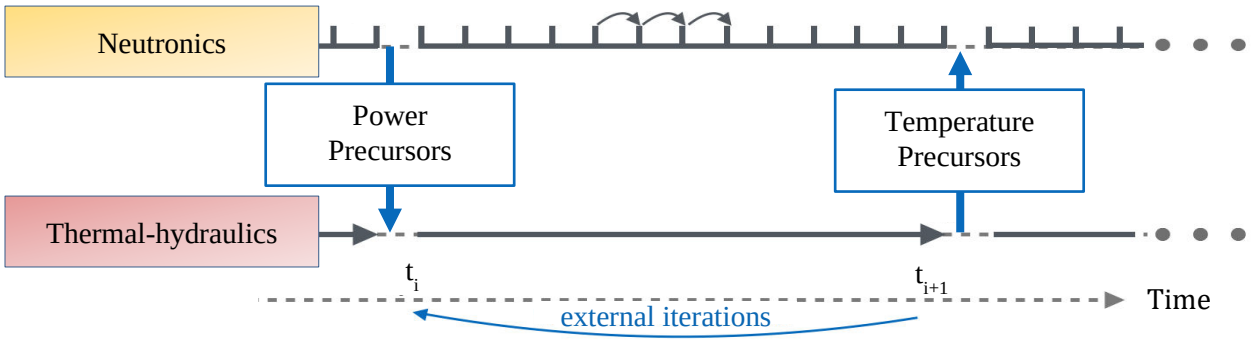

Figure 3 - Coupling scheme between neutronics and thermal-hydraulics codes [3][5]

As explained above, TFM-STAR is an adaptation of the TFM-OpenFOAM code to the STAR-CCM code, they both have the same calculation scheme shown in Fig. 3. The main difference is that TFM-STAR uses an external coupling between neutronics and thermal-hydraulics whereas TFM method is directly included into the OpenFOAM code, but both implementations are implicit. The iterations are made on the temperature and the power given by the thermal-hydraulics and neutronics, respectively. The distribution of delayed neutrons precursors is generated by the neutronics and the CFD code transports them. The neutronics thus generates the power field and the thermal-hydraulics generates the temperature field. Finally, external iterations are added to ensure the convergence of the different fields for a coupling time step because the thermal feedbacks are important, and power may be overestimated because the temperatures are not converged at the end on one single coupling iteration.

2.3. Comparison between TFM-STAR and TFM-OpenFOAM

As mentioned before, the first step of the TFM-STAR validation is to make a "code-to-code" comparison on various calculations made by TFM-OpenFOAM [5]. Steady state comparisons are first presented, followed by comparisons on a reactivity insertion. The comparisons are made on the reference version of the MSFR which uses a fluoride salt, in a Thorium/Uranium cycle. We consider fresh fuel in the present calculations, i.e. a fuel isotopic composition composed of ^{232}Th and ^{233}U fluorides in a LiF solvent.

2.3.1. Comparison at steady state

TFM-STAR also needs an implementation verification. As no prototype is working yet, a code-to-code comparison is the first way to check the new code. It can be noted that both the neutronic model TFM and

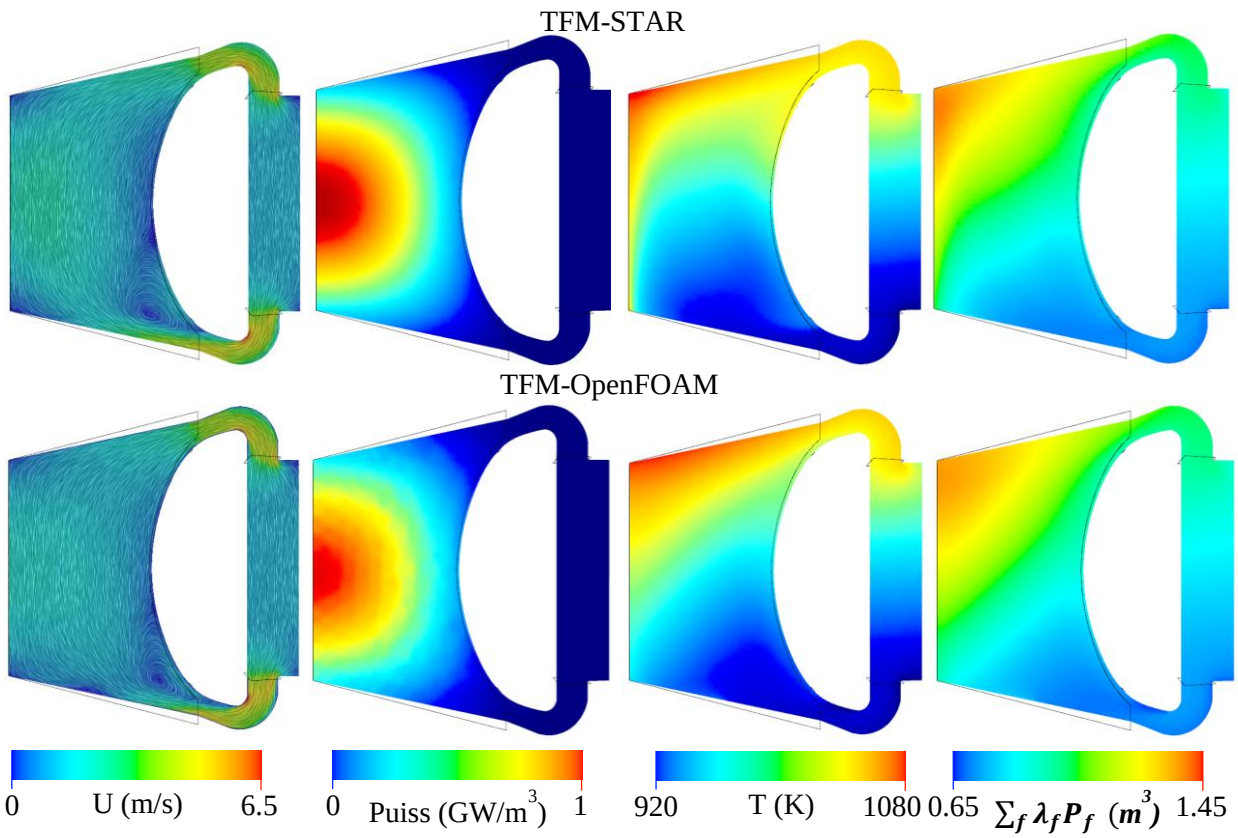

Figure 4 - Comparison between TFM-STAR (top) and TFM-OpenFOAM (bottom) of velocity field, power field, temperature field and precursors decays field at steady state

Star-CCM+ calculation schemes have been validated each other independently on reference codes and real experiments and benchmarks [3]. However, the coupled code-to-code comparison is not easy to perform because the models and/or correlations used may not be exactly the same between the two coupled codes, especially concerning turbulence model and wall function. Another point is the fact that the EVOL design of the MSFR considered here has been optimized using RANS calculations, where instabilities on the stall point and thus on velocities may appear at the heat exchanger outlet [8]. These two points lead to minor differences in results that are not possible to avoid but are not incoherent neither. Nevertheless, there is a good agreement between the results as displayed in Fig. 4.
The differences observed may come from the difference of velocity field. The stall is not at the same place and thus changes the flow in the core that directly impacts the temperature and precursors distribution. Another parameter of interest is the effective delayed neutron fraction equals at steady state to the prompt criticality margin:

$$\begin{cases} k = k_p + \beta_{eff} k \\ critical\ core : k = 1 \end{cases} \Rightarrow \beta_{eff} = 1 - k_p \quad (1)$$

There is a very small 7 pcm difference on the circulating β_{eff} between the two codes due to the difference on the velocity field and then on the distribution of delayed neutrons precursors.

2.3.2. Comparison on a reactivity insertion transient

It is also important to evaluate how the coupled code reacts during transient simulations. In this part, a neutronic transient is studied: a 1000 pcm reactivity insertion in one second. This reactivity insertion is not representative of a specific event because no initiator to insert such reactivity has been identified yet. However, it is a very efficient way to test our codes, how they react and their limits. The comparison on key parameters such as the power and the prompt criticality margin does not show significant differences in Fig. 5. The effect of the fluid recirculation period of around 4 seconds is visible on both codes. The steady state difference on the prompt criticality margin remains almost constant during the transient.

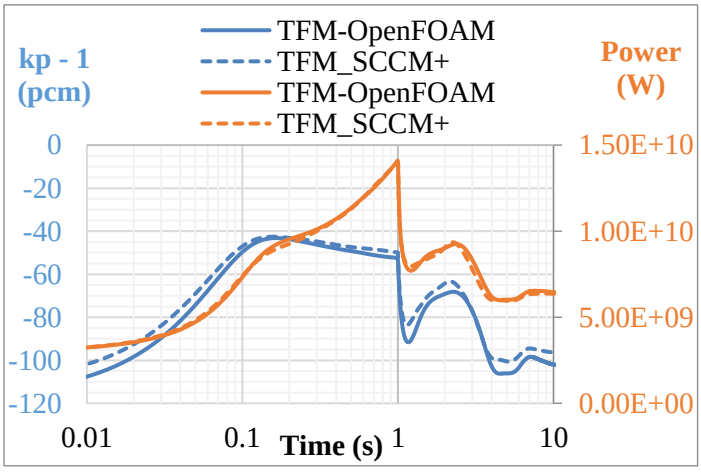

Figure 5 - Evolution of power and prompt criticality margin during 1000 pcm reactivity insertion in 1 s

3. SIMULATION OF ALTERNATIVE MSFR DESIGNS

The objective of this work is to identify and quantify some possible cliff edge effects that appear when the reactor design is modified. This work is not exhaustive as there are a lot more options for the conception, but this work aims to explore some of them. It has been chosen to focus on the reactor size and the loops number. Finally, to make comparison consistent, hypothesis and constraints have been taken and listed below.

Table I. Fuel isotopic composition table: Depleted uranium and plutonium from aged UOX fuel

Isotope	^{235}U	^{238}U	^{238}Pu	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu
Atomic proportion (%)	0.25	99.75	1.61	61.80	26.56	3.82	6.21

Studies are led on a chloride version of the MSFR and a Uranium/Plutonium fuel cycle. The salt is composed of depleted uranium at 0.25% of ^{235}U and plutonium from UOX fuel after aging [9] in a NaCl solvent. Isotopic compositions are presented in Table I.
Then, some parameters must be constrained:

- The salt composition is based on a ternary salt between NaCl, UCl_3 and $PuCl_3$[10]. It has been decided to be on a eutectic composition to minimize the fusion temperature and to minimize the risk of fissile matter precipitation. The consequence is that the fraction of each element of the ternary mixture is fixed by one of them. Then we simply adjust the proportion of plutonium (mainly fissile) over uranium to have a critical configuration
- The volume ratio between the core region and the out-core region is conserved. The core region is about half of the total volume
- The difference of temperature between the heat exchanger inlet and outlet is kept constant and around 100K
- The mean temperature is fixed at 880K
- The volumetric power remains constant
- The circulation time is constant

The variables on which the studies will focus are the effective delayed neutrons fraction β_{eff} (static and circulating values) and the temperatures (distribution and absolute values) because they may be representative of some behaviours of the reactor and may give some orientations for the reactor conception and safety features. The β_{eff} evaluated by the Monte Carlo simulation is "static" whereas in the coupling simulation, the "circulating" β_{eff} depends on the delayed neutrons precursors circulation.
A last point is the creation in Star-CCM+ of a parametric CAD to allow sensibility studies and so to make easier the design optimization. The EVOL MSFR design has been adapted with a modification on the junction between the loop and the heat exchanger, and with minor modification on core shape. It avoids some recirculation zones at the heat exchanger entrance. This modified design is our new reference case and presented in section 3.1. The studies presented then will focus on the reactor size and on the reactor loops number.

3.1. Reference chloride MSFR

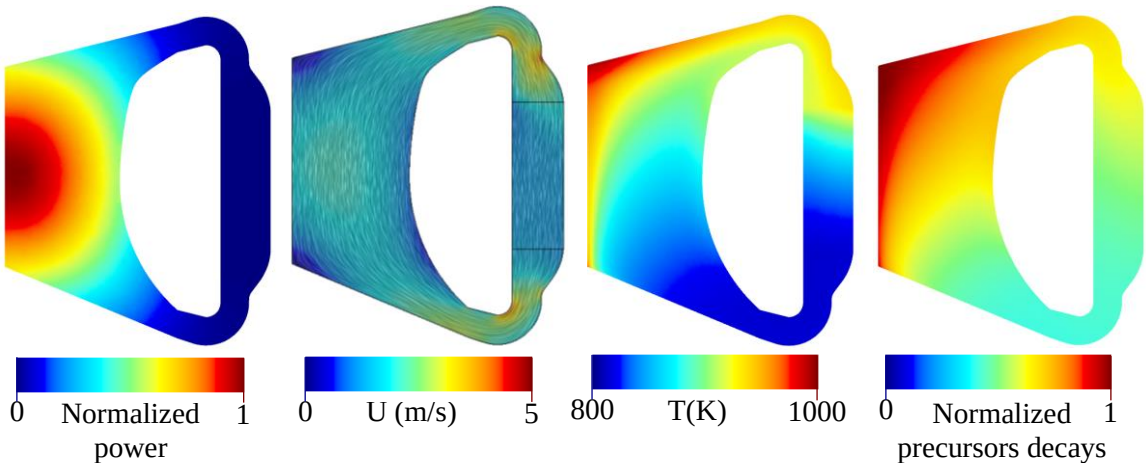

Figure 6 - Normalized power field ($Pvol_{max}$ = 213 MW/m^3), velocity field, temperature field and normalized precursors decay field at steady state

To be consistent with the reference MSFR version, the volumetric flow rate and the difference of temperature at heat exchanger inlet and outlet are retained. As the chloride salt is lighter and not as good coolant as the fluoride salt, the mass flow is decreased from 1170 kg/s to 833 kg/s and the power of the core

is reduced from 3GW to 900MW. Another main difference between the two salts is the operating mean temperature: 100K lower for chloride salt due to lower fusion point.
This design has been optimized to avoid recirculation zone at the core bottom and to reduce the velocities compared to the EVOL design. Otherwise, the different field presented in Fig. 6 are similar to the previous design. This calculation is the reference for the following studies lead on the volume reduction and on the number of loops.

3.2. Volume Reduction

With a constant reactor volumetric power to keep a point of comparison, it is interesting to change the size of the reactor to know how much it could be reduced, which parameters are affected and to quantify this. To do so, a simple homothetic transformation is made on the original geometry. The upper limit is the 18 m^3 (900 MW) design because the study focuses on small design. Then the design will be also limited by the heat exchanger minimal size, the pipes sizes, and the velocities. An overview of the dimensions is given in Fig. 7 for an 18 m^3 down to a 0.6 m^3 reactor.

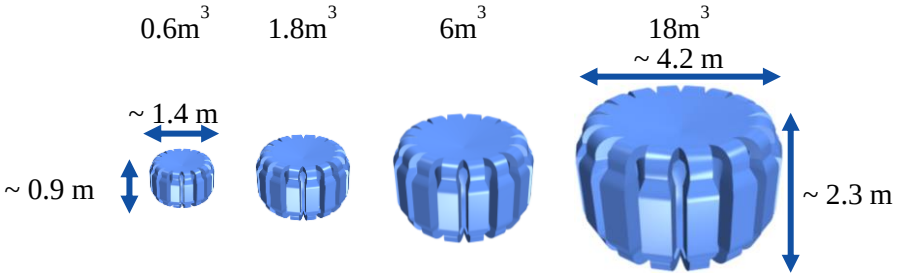

Figure 7 - Alternative versions with a total volume of 0.6 m3, 1.8 m3, 6m3 and 18m3

Another limitation in terms of volume reduction is the plutonium isotopic composition because a smaller size means a higher need of fissile material. For this reason, the 0.18m^3, initially considered, is too small and will not be studied. The "enrichment" of plutonium $\frac{Pu}{Pu+U}$ is presented Fig. 8.

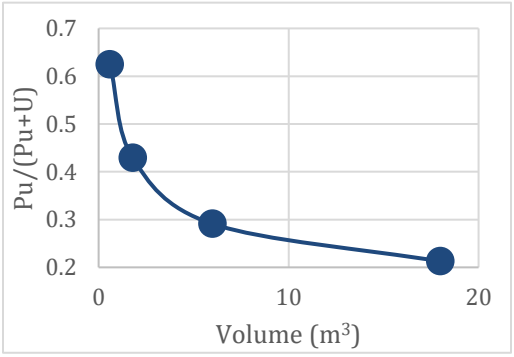

Figure 9 - Enrichment in function of the reactor size

The Fig. 9 shows that the different distributions of velocity are only affected in amplitude due to the fact the ratio of the surface over the volume increase with downsizing. The circulation time is however conserved.

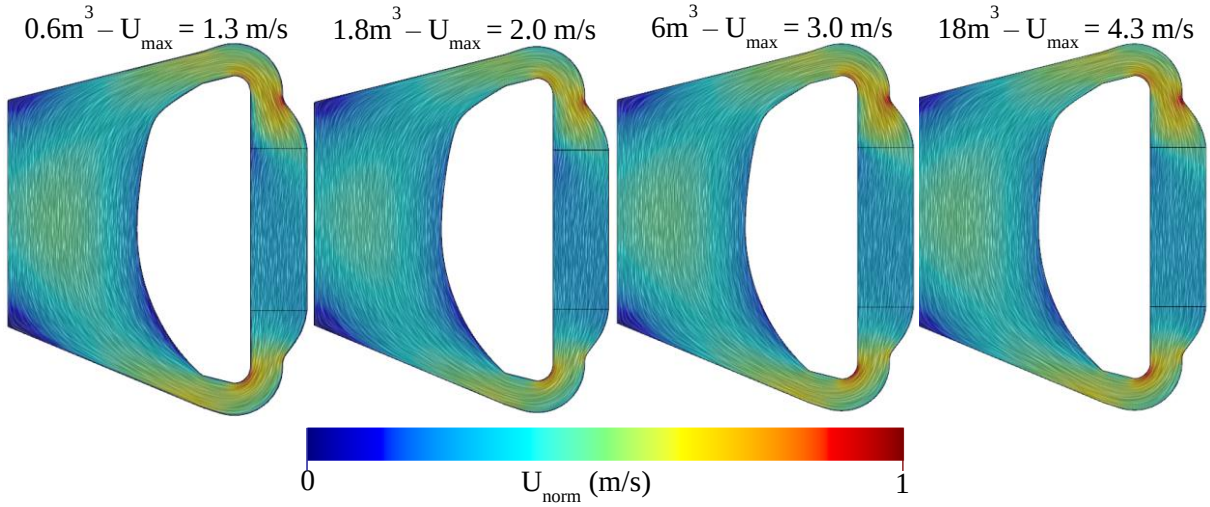

Figure 8 - Evolution of the normalized velocity for different reactor sizes and their normalization factor (maximum velocity amplitude)

3.2.1. Neutronics aspects

A first consequence of size reduction is the modification of geometry from a neutronic point of view. A smaller size means a higher probability for neutrons to leak outside the core and the flux will be more homogeneous in the core. This effect is visible in Fig. 10. Otherwise, the higher enrichment also means a modification of the "static" β_{eff}. Nevertheless, the fuel is circulating, and so a "circulating" β_{eff} has to be considered. Their evolution is shown in Fig. 11. Even if the static β_{eff} is lower for smaller versions, the circulating β_{eff} increases. Their ratio, see Fig. 12, is better for smaller versions that means delayed neutrons are better used for the fission reaction.

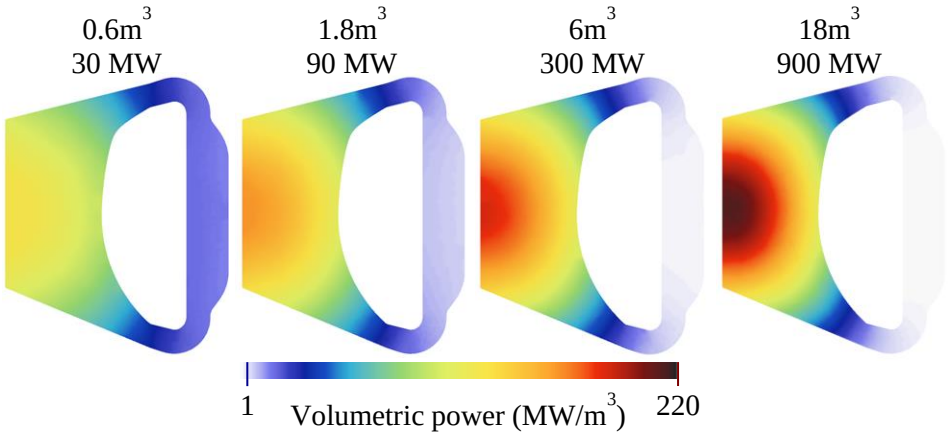

Figure 10 - Volumetric power for different core sizes (0.6m3 to 18m3) and various levels of power

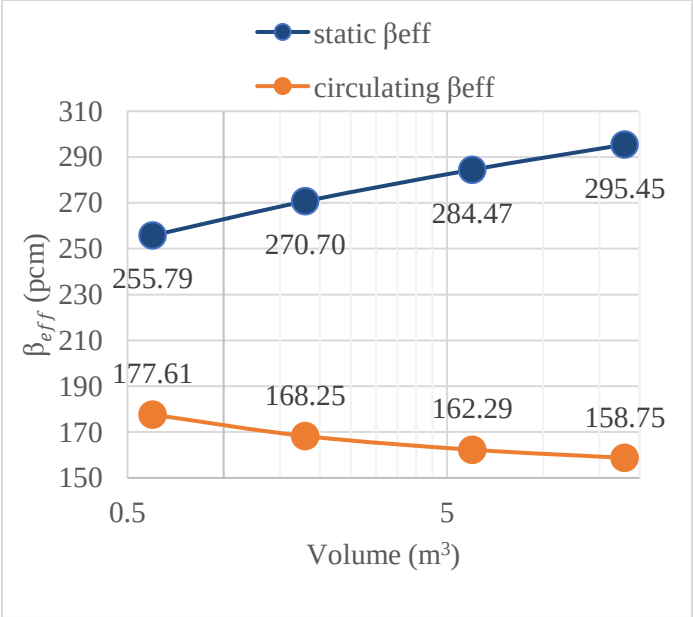

Figure 11 – Evolution of static and circulating β_{eff} as a function of the reactor size

That can be explained in terms of importance of neutrons. The weight of neutrons for the fission reaction is linked to the adjoint flux, approximately equals at first order to the flux [8]. Fig. 10 shows that the flux is more important and more homogenous in the core region, meaning that the delayed neutrons produced there matter more and lead to a higher value of the circulating β_{eff}. The delayed neutrons are produced in the top part of the core as in Fig. 6.

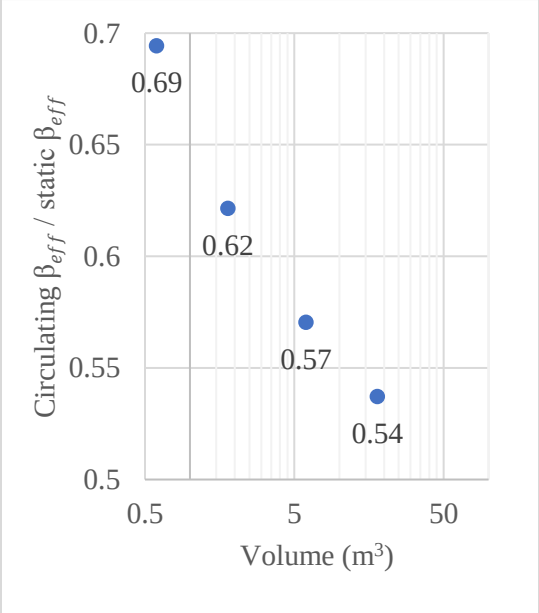

Figure 12 - Evolution ratio between the circulating and the static β_{eff} as a function of the reactor size

3.2.2. Thermal aspects

The flow is concerned by a modification of the size because the ratio surface over volume is changed. It leads to a modification of velocities that may have an influence on the temperatures. The temperatures are rather more homogeneous for smaller versions, which leads to lower high temperature. Fig. 13 shows the effect of the flow on the temperatures at core top and core bottom. Smaller sizes decrease the hot point at the core top but increase the one at the bottom.

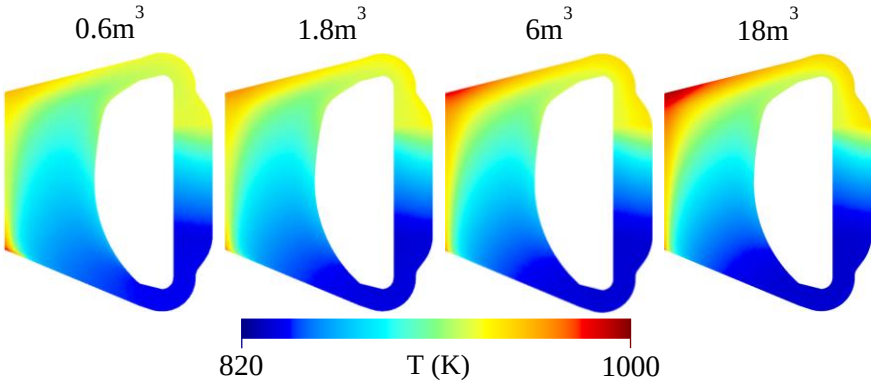

Figure 13 - Temperature field for different reactor sizes

3.3. Loop number optimization

As mentioned before, the MSFR fuel circuit is composed of 16 loops. The idea here is to decrease the number of loops while extracting enough power with reasonable mass flow and temperature gradient. Each loop contains a pump and a heat exchanger so it is a lot of components, especially if we focus on small modular designs. Star-CCM+ allows to easily adjust the number of loops for alternative designs (Fig. 14) thanks to the parametric CAD.

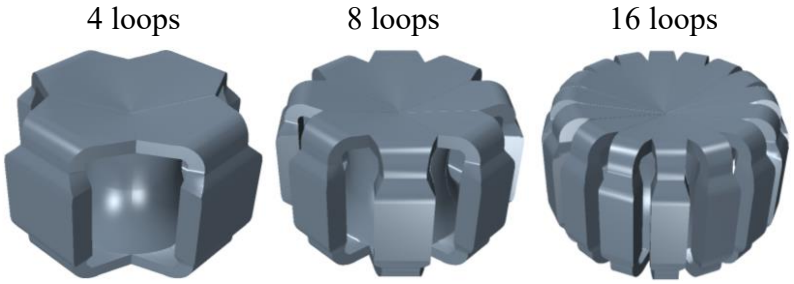

Figure 14 - Alternative versions with 4, 8 and 16 loops

In this study, the distribution of velocity is really affected by the number of loops because it may create recirculation zones in the core region as shown in Fig. 15.

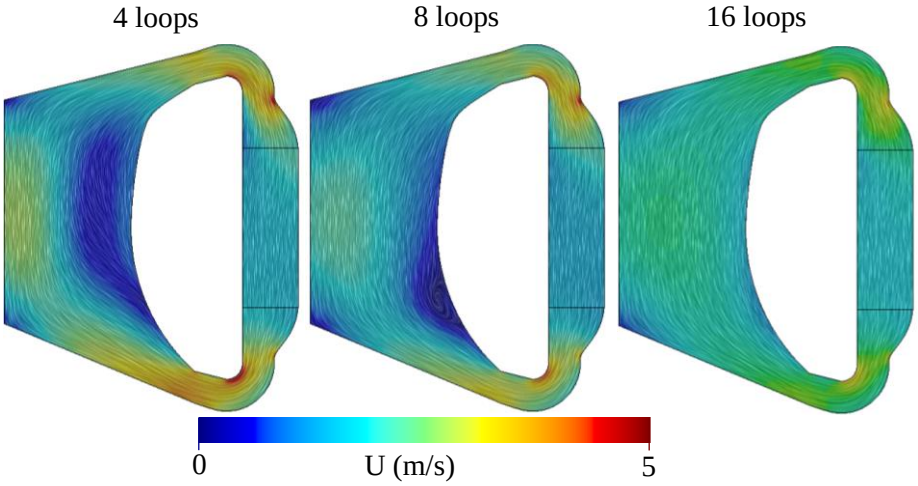

Figure 15 - Distribution of velocity for different loops numbers

3.3.1. Neutronics aspect

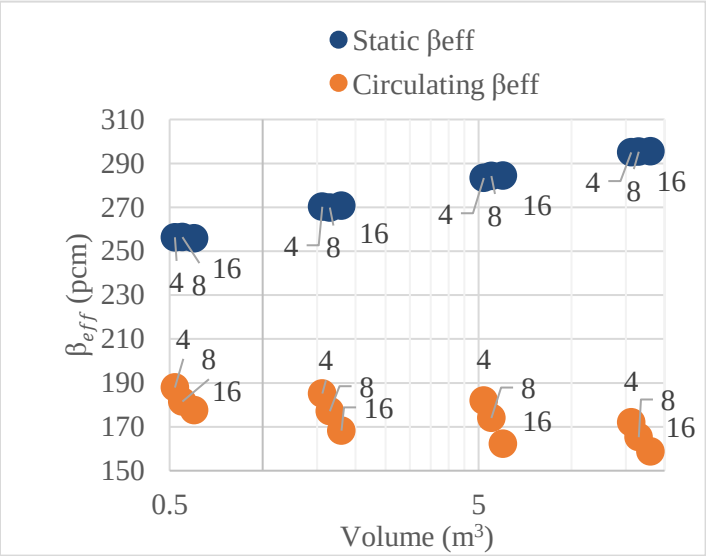

Figure 16 - Evolution of static and circulating β_{eff} for different loops numbers and for different reactor sizes

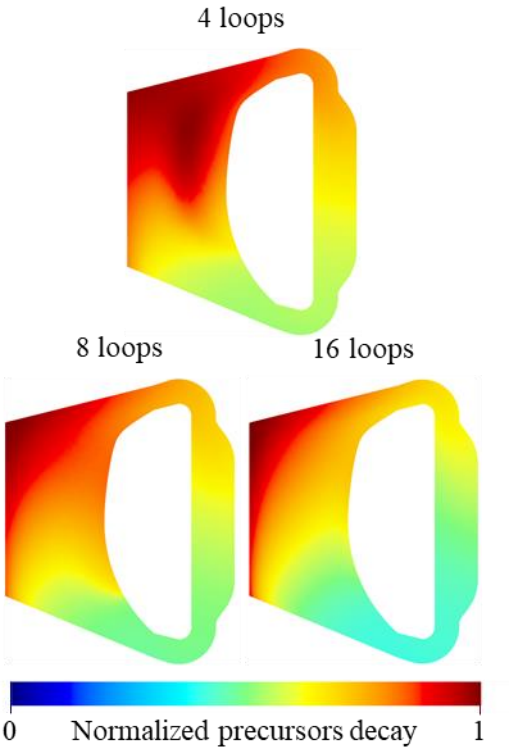

Figure 17 - Distribution of normalized precursors decays for different loops numbers for an 18 m³ reactor size

Fig. 16 shows β_{eff} for different loops number. On one hand, the static β_{eff} is not really affected by the number of loops because it is rather linked with the fuel composition and the core geometry that do not change significantly. On the other hand, the circulating β_{eff} is directly impacted because the flow inside the core changes. The greater importance of delayed neutrons is also visible in Fig. 17, with more decays in proportion in the core region. The modification of the distribution of velocity directly affects the distribution of precursors decays in the core and thus the β_{eff} whatever the reactor size.

3.3.2. Thermal aspects

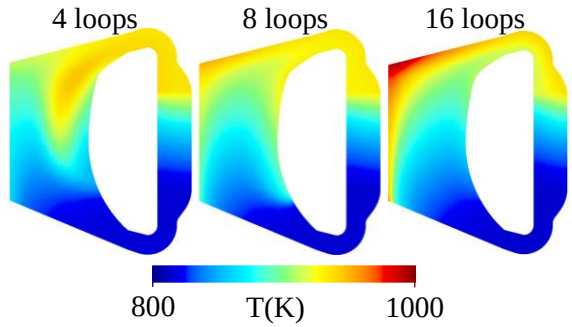

Figure 18 - Distribution of temperature for different loops numbers (18 m³ reactor)

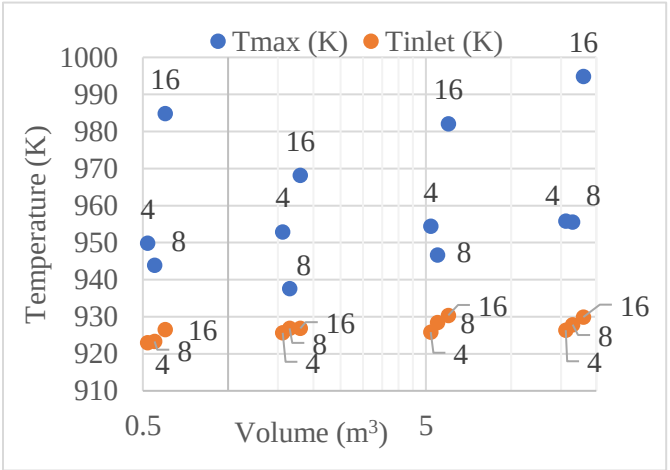

Figure 19 - Evolution of T_{max} and T_{inlet} for different loops numbers and for different reactor sizes

The differences of flow lead also to significant differences on the temperature. The maximum temperatures in Fig. 18 and Fig 19. decrease

with the lower loops number, but a too small amount may not be optimal neither, because of bigger recirculation zones leading to other hotter points.
One issue that could occur with a low loops number version is an instable asymetric flow as in Fig. 20. This is due to the too large core entrance that creates instability in the flow. That may lead to unwanted effects like hot points. To avoid this effect, some blades can be added to break the large eddies and to make the velocity field more homogeneous. Otherwise, new designs can be explored to improve the flow in the core [8].

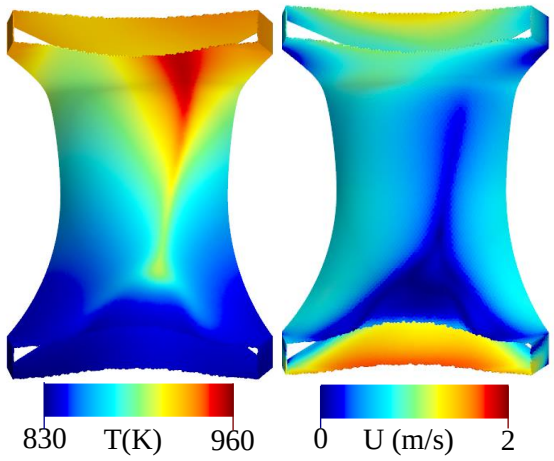

Figure 20 - Temperature and velocity distributions near the core wall for the 4 loops 1.8m^3 reactor

4. CONCLUSIONS

The implementation of the TFM approach coupled to the Star-CCM+ code provides promising results and has been compared to the TFM-OpenFOAM original code. This new coupled code brings useful features not included in OpenFOAM such as Computer Aided Design (CAD) and meshing tools. The first studies presented in this paper show that there is an opportunity to develop small modular versions of a molten salt reactor. Both neutronics and thermal-hydraulics seem to evolve positively to the downsizing. The temperatures are generally lower and the fraction of delayed neutrons β_{eff} is better. There is also a margin to increase the velocities in pipes and thus to decrease the gradient of temperature.
Nevertheless, these are still early-stage results on one particular design and this design could limit our optimisations due to the instability of flow on low loops number design. For this reason, it could be interested to develop another preconceptual design that prevent from these undesirable effects. To complement these first tendencies for normal operation, transient studies would be relevant to enrich this analysis, in order to include safety considerations.

REFERENCES

[1] M. Allibert et al., “Handbook of generation IV nuclear reactors”, Elsevier, pp. 157–188 (2016)
[2] A. Laureau et al., “Transient Fission Matrix: kinetic calculation and kinetic parameters βeff and Λeff calculation”, Annals of Nuclear Energy, volume 85, 1035–1044 (2015)
[3] A. Laureau, "Développement de modèles neutroniques pour le couplage thermohydraulique du MSFR et le calcul de paramètres cinétiques effectifs", PhD Thesis, Grenoble Alpes University, France (2015)
[4] G. Bourdon, “Développement d’outils pour la simulation de la physique des réacteurs à sels fondus”, Master Thesis, Framatome Lyon (2020)
[5] T. Sornay, "Développement d’outils pour la simulation de la physique des réacteurs à sels fondus", Master Thesis, Framatome Lyon (2021)
[6] E. Merle-Lucotte et al., “Optimization of the pre-conceptual design of the MSFR”. Rapport technique, EVOL European FP7 project, Work-Package WP2, Deliverable D2.2 (2014)
[7] A. Laureau et al., “Transient coupled calculations of the Molten Salt Fast Reactor using the Transient Fission Matrix approach”, Nuclear Engineering and Design, volume 316, 112–124 (2017)
[8] A. Laureau et al., “Unmoderated molten salt reactors design optimisation for power stability”, Annals of Nuclear Energy, volume 177, 109265 (2022)
[9] J. Guidez et al., “Molten Salt Reactor to close the fuel cycle: example of MSFR multi-recycling applications”. ICAPP 2019, Juan-les-pins, France (2019)
[10] O. Beneš & R. J. M. Konings, “Thermodynamic evaluation of the NaCl–MgCl2–UCl3–PuCl3 system”. Journal of nuclear materials, volume 375(2), 202-208 (2008)