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Development of CFD models and pre-test calculations for thermal-hydraulics and freezing experiments on Lead coolant

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ABSTRACT

Heavy Liquid Metals (HLM) are objects of interest in the nuclear research sector because of their optimal thermal and neutronic properties; the development and the validation of models allowing to predict their behaviour are fundamental for the future development of the Generation IV energy systems.

An experimental facility named SESAME-stand, is planned to be operated at Research Centre Rez (RC-Rez) under the framework of SESAME project. The aim of the facility is to study the solidification of Lead under GEN-IV Heavy Liquid Metal pool type nuclear reactors relevant conditions and to provide a database for the benchmarking and validation of

numerical models. Corresponding CFD models are developed using commercial software and are used for the pre-test assessment and to support the experimental work. The aim of this paper is to describe the CFD models, explain how they are tested and used in order to define a valuable experimental matrix that will be needed in order to run the facility itself. First of all, the facility is introduced together with the range of foreseen investigations. The numerical models are then presented. Emphasis is given to the geometrical and physical assumptions. Different approaches of modelling are compared and discussed. Results from the pre-test simulations are illustrated. Encountered challenges and their relevance with regard to the experimental matrix and setup are commented.

1 INTRODUCTION

Development, validation, and licensing of computational models for simulations of liquid metal thermal-hydraulic and freezing phenomenon is essential for development of liquid metal cooled Gen IV reactors and for their safety assessment ([1], [2], [3]). For this purpose, an activity focused on development and validation of computational models simulating a liquid lead natural convection and freezing is on-going within H2020 SESAME project. The first step of this work package is to develop a suitable computational model, which will be then validated on the experimental data obtained from an experimental stand, which will be operated within the project at RC-Rez in the next phases. The main goal of this article is to describe two CFD (Computational Fluid Dynamics) models, which were developed in parallel using different software and approaches for this application. Results of pre-test calculations obtained with the two models will be presented and compared.

2 SESAME EXPERIMENTAL STAND

The SESAME-stand facility [4] consists of a steel-casted Experimental Vessel (EV) in which all the thermal-hydraulic and freezing processes take place, electric heating rods inside the vessel itself provide the heating power while an obstacle enhances the natural circulation; an Air Channel (AC) designed to cool down the system works as a heat sink from the outside of the steel vessel, the cooling air-exposed region of the vessel is finned in order to increase the heat exchange area.

In the first experimental phase the temperature field, and therefore the solidification front, is monitored using 21 thermocouple (TC) probes with totally 110 measuring points. In the second experimental phase the planned transient ends with the fast draining of the liquid Lead, the vessel's cover is removed together with the connected internals and the obtained solidified structure is scanned using a 3D scanner and compared with the CFD results. In this second phase, the frozen Lead cannot reach the upper TC probes, the obstacle, and the heaters to allow the vessel's opening.

3 COMPUTATIONAL MODELS

The two numerical models were built in parallel with two different commercial CFD codes. RC-Rez used ANSYS 17 [5] and CRS4 used STAR-CCM+ [6]. RC-Rez's CFD model was created using ANSYS Design Modeler, ANSYS Meshing and ANSYS Fluent 17.

3.1 RC-Rez's modelling strategy

Due to different behaviour of the two fluids (Lead and Air), three different modelling approaches have been considered. The first approach consists of one CFD model including

only the EV. This solution implies heaters and a convection boundary condition on the finned surface to simulate the cooling air flow. The heat transfer coefficient can be calculated using proper correlations while the air's bulk temperature can be assumed equal to the inlet temperature. This approach does not allow accurate transient calculations because the behaviour of the air is heavily simplified.

A second approach is a CFD-CFD coupling. In the first model, the AC is simulated and provides a boundary condition for the EV, which is simulated in the second CFD model. This approach can grant higher sensitivity to the physical phenomena occurring in the system than in the previous case due to the exchange of information iteration after iteration between the two domains, and an additional great advantage: the different fluids are kept separated in the two models which can be set with different turbulence models and physical properties according to the specific fluid. The turbulent Prandtl number, for instance, is around 0.85 for air and 4 for Lead. On the other hand, this system is the slowest because of the time needed to exchange the data between the two calculations.

The third approach features one CFD model in which the two different fluids are simulated together, which introduces difficulties in the solver settings. This implies a good compromise in the calculation's time consumption and accuracy.

After the introduction of the k-ε RNG turbulence model in the calculations and after a careful tuning of the solver settings, the third approach was chosen. K-ε RNG includes a formulation able to calculate the turbulent Prandtl number as a function of the local variables: this feature allowed the proposed model to overcome one of the critical points presented.

3.2 Geometry and mesh with Fluent

EV and AC are the considered components and have been simplified with respect to the real geometry due to mesh generation needs and computational time economy. A first step toward those targets is the central symmetry applied: only ¼ of the domain was modelled.

The vessel's bottom in the real facility accommodates the draining pipe for the liquid Lead and was designed to help HLM's flow (2° of inclination). The filling and draining procedures are not of interest, consequently the bottom was supposed flat and the draining hole not included. On the contrary, the fitting connecting the bottom to the finned region of the vessel was carefully designed according to the original geometry: the solidification starts in this corner and is fundamental in the physics of the phenomenon. The level of the liquid metal is supposed constant for any operating condition. Thermocouples probes are not included in the geometry due to mesh requirements. The cooling heat flux is assumed to be only on the finned surface. Argon is simulated as a solid without any convective behaviour.

Detailed results and indications about the inner temperatures of the heaters were highly prioritized both for protection of the hardware and benchmarking reasons. To reach that target the heaters were modelled including the whole inner structure and the relative materials.

The volumes were designed and split to allow the mesher to create a structured mesh (Hexahedral) in the widest domain possible. Preliminary calculations revealed that a conformal mesh is required in the EV to get a stable transient simulation. This is not needed between the AC and the EV: a Coupled Wall was created on the finned surface. Details of the mesh are given in Figure 1. A grid independency study was performed in two steps using the operating conditions: air mass flow rate equal to 0.156 kg/s and heating power 3 kW. In the first step three different refinements of the air channel were tested while the EV's mesh wasn't modified; the considered variables are maximum and minimum temperatures and maximum velocity in the Lead volume: the results are summarized in the plots illustrated in Figure 2.

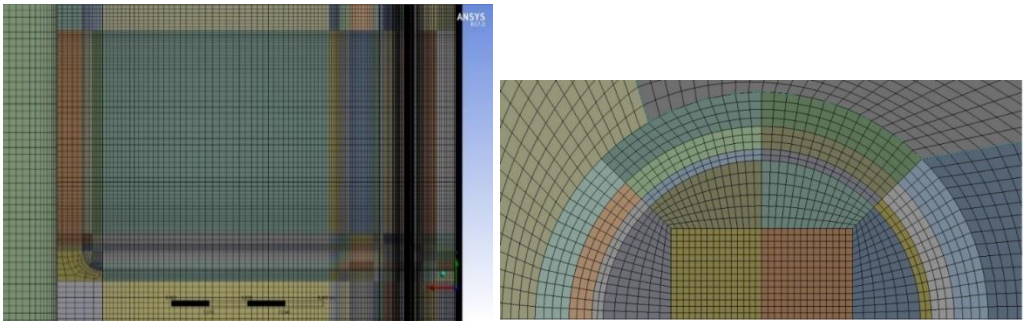

Figure 1: Mesh's symmetry, detail of the bottom region (left). Heater's internal structure, structured and conformal mesh (right)

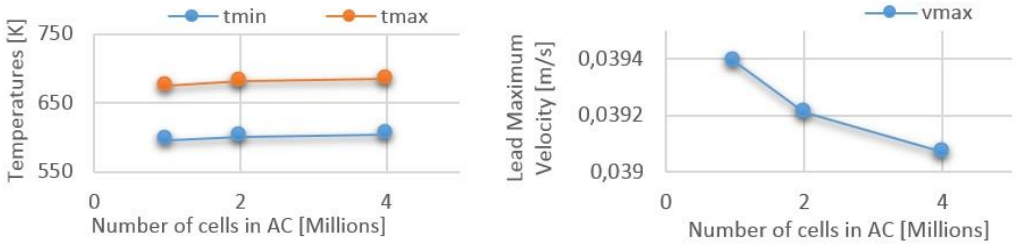

Figure 2: Grid independency study: Min, Max Temperatures and Max Velocity

A temperature difference of 3K between the finest and the medium mesh was considered acceptable and the medium mesh was chosen for further calculations. In the second step, the number of elements of the chosen mesh was doubled only in the EV. The differences in the output variables were negligible and the medium grid was confirmed. The quality of the final mesh is described using parameters contained in Table 1.

Table 1: Quality metrics for the final mesh

Maximum/Average Aspect ratio	61/5.7
Minimum/Average Orthogonal quality	0.45/0.87
Maximum Y+	4.2

3.3 Solver settings in Fluent

ANSYS FLUENT's Solidification Module can be activated only with the pressure-based solver. Consequently, the PRESTO! scheme was chosen [5] as suggested in buoyancy driven flows. For pressure-velocity coupling SIMPLE scheme was used. Physical properties suggested within the SESAME consortium were assumed [7].

The k-ε RNG turbulence model was considered as a first choice. In this model, Full Buoyancy Effects option is available, this is suggested in non-zero gravity simulations and implies the inclusion of buoyancy effects in the ε equation [5]. Enhanced Wall Treatment was selected, which means that the variables in the boundary layer are modelled numerically and not using wall functions. The maximum acceptable value of the Y+ output was set to 5. The main advantage of the RNG model is the built-in analytical formula for the local turbulent Prandtl number, that is appropriate for modelling of two fluids characterized by very different values of this variable [5]. Calculations were performed on the EV mesh (Convection BC) comparing k-ω SST and k-ε RNG results. The results are shown in Table 2.

Table 2: Results of turbulence models' comparison

Turb Model	k-ε RNG	k-ω SST
Tmin Lead [K]	613.9	614.0
Tmax Lead [K]	666.2	665.5
Max Lead Velocity [m/s]	0.050	0.055

Maximum and minimum temperatures are within 0.1% of difference between the two calculations. This result means that the different turbulence models are agreeing about the temperature field inside the liquid metal volume. On the other hand, the difference in the maximum velocity is not negligible. A difference was expected because the turbulent Prandtl number has great importance in the momentum equations and k-ω SST has no built-in formulation for it.

The solidification module [8] was set using the default mushy constant and the solidus temperature was set equal to the liquidus temperature as suggested for pure materials in [9].

3.4 CRS4's CFD model

The 3D geometrical model was built with the STAR-CCM+'s 3D-CAD modeler, according to the dimensions issued by RC-Rez. The CFD model includes the EV and the cooling air duct. The experimental vessel is formed by: solid wall, fins, main heater, thermocouple probes, obstacle, lead and argon. The heater is formed by four heating rods placed in the centre of the EV, around the central thermocouples pipe. The heating rods are simple steel cylinders with the outer diameter of 10 mm. Inside the pool there are 12 bottom pipes and 8 top pipes which host the thermocouples. In the numerical model, the pipes hosting the thermocouples have a hexagonal geometry instead of circular, for better mesh matching at the interfaces with the fluid. The argon occupies the upper part of the vessel's internal for 40 mm of height above the lead volume. The bottom of the vessel considers the 2 degrees inclination. Thanks to the central symmetry, a quarter of the domain was modelled (Figure 3).

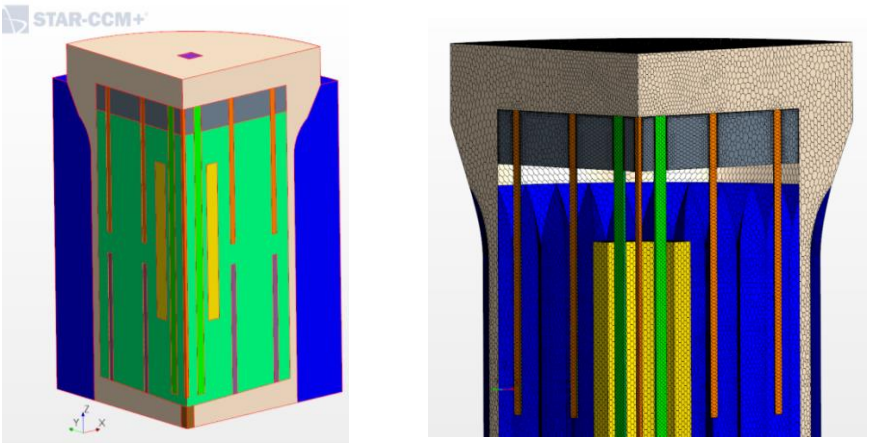

Figure 3: Geometry and mesh in the CRS4's model

Once the geometrical parts have been assigned to the regions and the interfaces between the various solids-fluids, solid-solid, fluid-fluid regions have been defined, the surface and volume mesh have been generated. The Surface Remesher and the Polyhedral Mesher where used with the surface size of 3-4 mm. For the fluid regions, the Prism Layer Mesher is added,

including 3 prism layers with the thickness of 1.5-2.5 mm. The total volume mesh representation accounts for 0.7 million of control volumes.

3.4.1 Solidification model and numerical set-up

The procedure to bring the system to the desired minimum temperature near the solidification point (601 K) is the following one:

- the heat transfer between the outlet and the inlet of the cooling air channel is measured and monitored;
- the total enthalpy of the lead is calculated;
- the volumetric heat source to be applied to the heater is determined such that to bring the system to the desired enthalpy:

$$\boldsymbol{HS = min(20\,kW, max\,(HF - 0.01 * (H - H_0)), 1kW)},$$

where
HS is the heat source,
HF is the heat flux removed by the cooling air,
H is the total enthalpy of the lead,
H_0 is the target enthalpy of the lead.

The minimum temperature of 601 K is reached for a heat source of 3.12 kW. The Volume of Fluid (VOF) model is enabled in an Eulerian multiphase configuration with lead as single phase. The Argon zone at the top of the lead is treated as a separated continuum. In the VOF framework, the Melting-Solidification model is enabled with the following settings:

- Latent heat of fusion=23070 J/kg
- Liquid temperature=600.6 K
- Solidus temperature=598.6 K
- Prandtl number=0.9

4 RESULTS

The steady state calculations have been used to find both the optimal initial and final working conditions for the experimental runs. The desired initial condition consists of two goals: a minimum temperature a few Kelvins above the freezing point and a heating power able to grant a fast transient to the freezing of the Lead volume. This means a limited power at the Heaters. A general hypothesis was assumed: during both steady state and transient calculations, only the cooling air mass flow rate must be modified to make the results easily understandable.

4.1 Steady-state results

For the initial condition, 100 % molten Lead, an air mass flow rate of 0.145 kg/s and a heating power of 3 kW were chosen. In the CRS4's model, for the same mass flow rate of the cooling air, the minimum temperature above the freezing point (601 K) is reached for a heat source of 3.12 kW. The difference in the heat source entity may be given by the geometrical difference between the two models. An interesting final state for an experimental run was found for 0.176 kg/s of cooling mass flow rate and again 3 kW of heating power: the solidification front arrives very close to the internals (heaters and obstacles) without reaching them. This allows the operators to open the vessel and to scan the solidification front. Similarly, in the CRS4's model, this condition is reached for a mass flow rate of 0.178 kg/s

and 3.12 kW. The velocity and the temperature fields are shown on the same scale in Figure 4 and Figure 5 in the case of 100% molten Lead and in Figure 6 in the case of the higher cooling air mass flow rate.

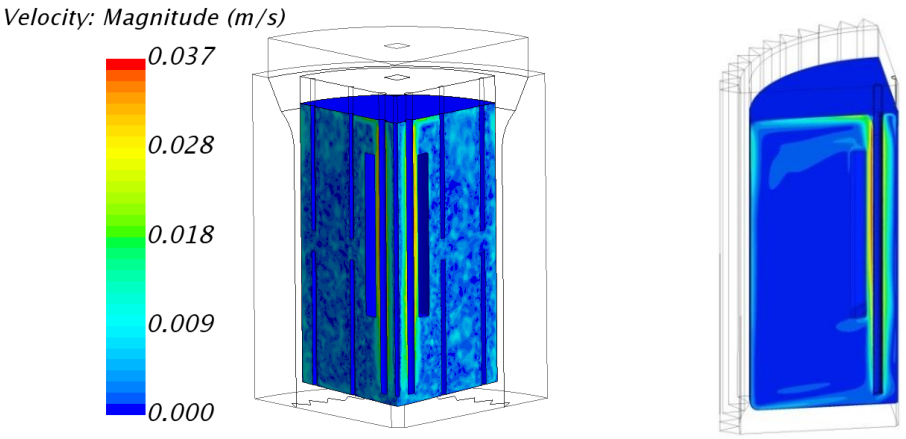

Figure 4: Velocity field: 100% molten lead in STAR-CCM+ (left) and FLUENT (right)

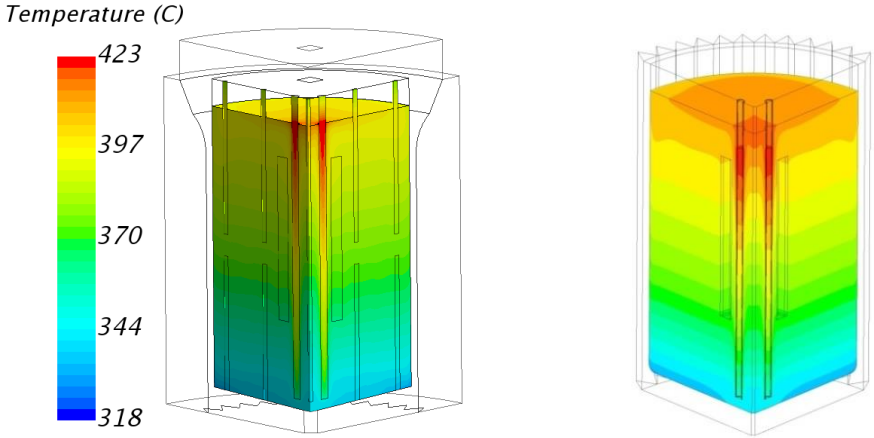

Figure 5: Temperature field: 100% molten lead in Star-ccm+ (left) and Fluent (right)

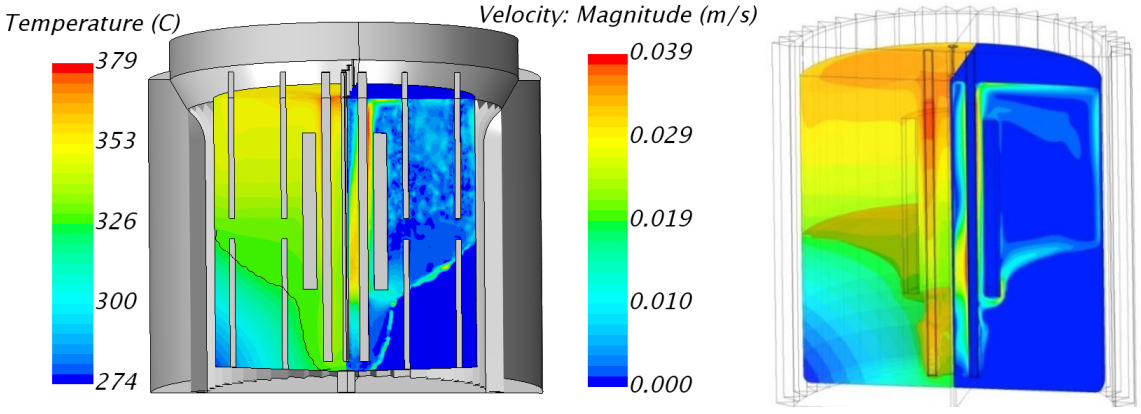

Figure 6: Temperature and velocity fields:

33% Frozen Lead –STAR-CCM+ (Left) - 42% Frozen Lead – FLUENT (Right)

The comparative results from the steady state calculations in the two models are summarized in The 33% frozen fraction has been chosen as a conservative final condition for the Phase 2 experimental run, to certainty allow the opening of the EV.

Table 3. The 33% frozen fraction has been chosen as a conservative final condition for the Phase 2 experimental run, to certainty allow the opening of the EV.

Table 3: Comparative results of the steady state calculations

	Fluent	Star-ccm+	Fluent	Star-ccm+
Air Mass Flow Rate [kg/s]	0.145	0.146	0.176	0.178
Tmax [K]	695.27	695.90	651.65	652.90
Tmin [K]	606.40	601.10	547.05	550.06
Vmax Lead [m/s]	0.0373	0.0362	0.0392	0.0398
Frozen Fraction of lead [%]	0	0	42	33

4.2 Transient results

The transient calculation was started after reaching the convergence of the initial steady state. Rather long time (260 seconds) of transient stabilization keeping the initial boundary condition was needed to obtain a stable transient calculation after it. The stabilization finishes once the residuals are showing an ordinated and harmonic behaviour. The same procedure was applied in the CRS4's model. The steps consisted in switching the steady state simulation just before the beginning of the solidification to unsteady state and initiate the solidification with a small time step (10^{-3}s), a large number of inner iterations (20) and with smaller under relaxation factors in the velocity and pressure solvers. Further on, the time step is progressively increased, until 0.1s, the inner iterations are diminished and the under relaxation factors are set to the initial default values. For the simulation of the solidification, the air cooling boundary condition is switched to the maximum reachable from the blower: 0.5 kg/s, in both models. This test was performed in order to evaluate how much time is needed to reach some specific fraction of frozen volume. The result of the transient simulation indicates that a frozen fraction of 33% (the maximum considered for the Phase 2 experimental run) is reached after 21 minutes in FLUENT and 27 minutes in STAR-CCM+.

An upper limit for the solidified volume was considered for the Phase 1 runs and was set to 67%. In the FLUENT model, this value is reached after 37 minutes while in STAR-CCM+ after 48 minutes. The curves of the solid volume fraction of lead, in litters and percentage, are shown in Figure 7. The trend of the solidification curve agrees with the curve of the heat flux removed by the cooling air which is slowly decreasing towards the thermal equilibrium. The temperature and the velocity fields and the isosurface with the solidification front at 67% are shown in Figure 8.

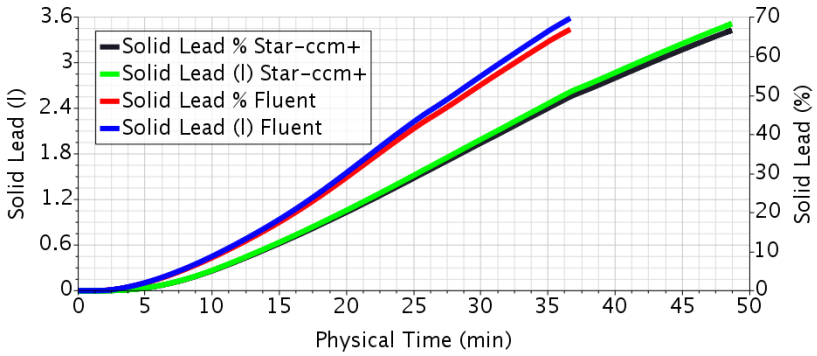

Figure 7: Frozen fraction of lead in the two models

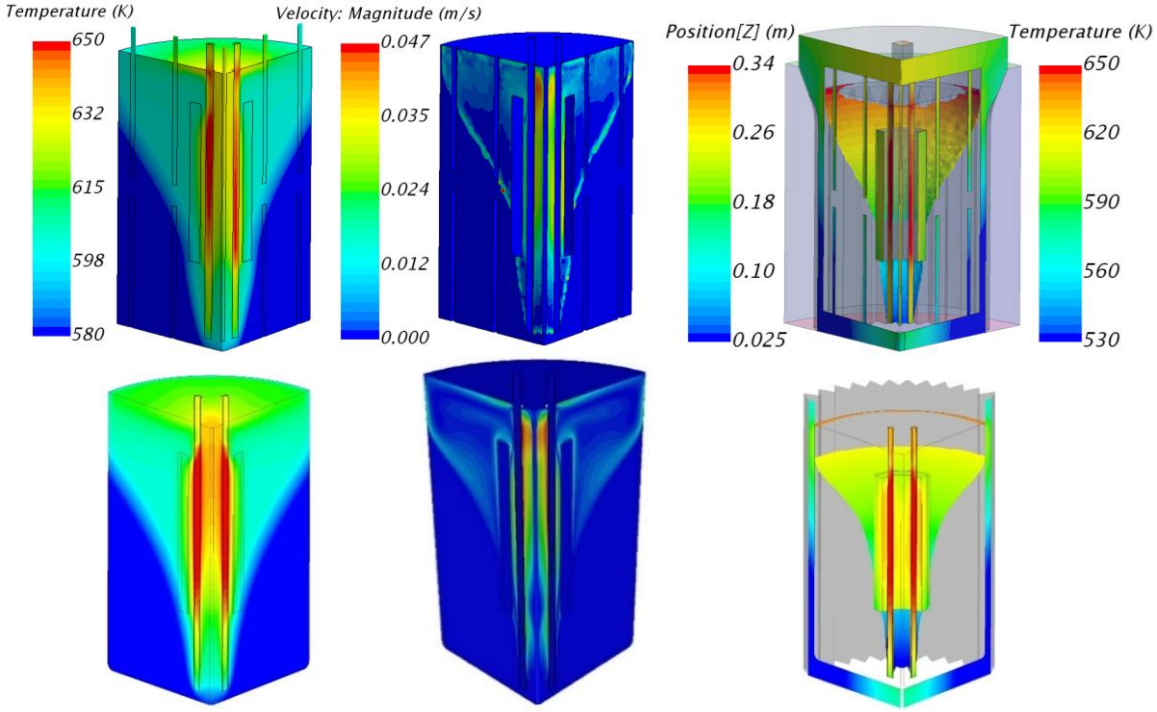

Figure 8: Temperature and velocity fields and the isosurface of the solidification front at 67% in the STAR-CCM+ model (top) and in the Fluent model (bottom)

5 CONCLUSIONS

Two computational models able to simulate the behaviour in case of solidification of the Liquid Metal Coolant inside the SESAME-stand facility were developed using Fluent and STAR-CCM+.

An agreed procedure to reach convergence in every working condition was defined between the two simulation codes. Possible initial and final steady state conditions for the experimental runs were found according to the technical needs.

A first transient simulation was successfully performed. The results in the two models are very similar in steady state while there are differences in the transient calculations (particularly the same percentage of frozen lead being reached slower in the CRS4's model).

The differences might be caused by different approaches in the geometry simplifications, mesh or by numerical uncertainties. The suitability of the codes will be

evaluated in the following stage of the SESAME project, which is focused on collection of experimental data and the codes benchmarking.

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