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Validation of a CFD Code Star-CCM+ for Liquid Lead-Bismuth Eutectic Thermal-Hydraulics Using TALL-3D Experiment

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ABSTRACT

The engineering design, performance analysis and safety assessment of Generation IV heavy liquid metal cooled nuclear reactors calls for advanced and qualified numerical tools. These tools need to be qualified before used in decision making process. Computational Fluid Dynamics (CFD) codes provide detailed means for thermal-hydraulics analysis of pool-type nuclear reactors. This paper describes modeling of a forced to natural flow experiment in TALL-3D experimental facility using a commercial CFD code Star-CCM+. TALL-3D facility is 7 meters high LBE loop with two parallel hot legs and a cold leg. One of the hot legs accommodates the 3D test section, a cylindrical pool where the multi-dimensional flow conditions vary between thermal mixing and stratification depending on the mass flow rate and the power of the heater surrounding the pool. The pool outlet temperature which affects the natural convection flow rates in the system is governed by the flow structure in the pool. Therefore, in order to predict the dynamics of the TALL-3D facility it is crucial to resolve the flow inside the 3D test section. Specifically designed measurement instrumentation set-up provides steady state and transient data for calibration and validation of numerical models. The validity of the CFD model is assessed by comparing the computational results to experimental results.

KEYWORDS

CFD, Validation, TALL-3D, LFR

1 INTRODUCTION

In 2002, the Generation IV International Forum (GIF) selected lead-cooled fast reactor (LFR) as one of the six nuclear systems that have the potential to take the nuclear energy production to a next level in terms of sustainability, economics, safety and security [1], [2]. LFR designs, at least in Europe, utilize pool-type primary system (e.g. ELECTRA, ELSY, ETDR (ALFRED), ETPP (MYRRHA), PROLFR, ELFR [3]) with main components installed in the reactor vessel. Engineering design and performance evaluation in nominal and accident conditions of currently operating nuclear reactor fleet has been done mainly with 1D or 0D system thermal hydraulics (STH) codes [4] which are not capable of resolving the multi-dimensional flow phenomena in the primary pool of an LFR. Design and safety analysis of LFRs requires tools capable of resolving multi-dimensional thermal-hydraulic phenomena.

By today, 2D/3D Computational Fluid Dynamics (CFD) codes have reached a level where they can be utilized in analyzing essentially every system, including human-made and natural, where fluid(s) is involved. The use of CFD for nuclear reactor problems goes back to 1970’s and diverse experience has been gained over the years in different countries (see reviews in [5] and
In future, CFD codes are expected to be used more frequently in nuclear reactor thermal-hydraulics analysis that is supported by research done for two-phase CFD and for Generation IV applications ([7]–[9]). This has been possible due to rapid developments in computers, efficient and reliable numerical algorithms, high-fidelity physical models and increased availability of CFD software, particularly commercial software. However, projects managers and decision makers who use the results of CFD simulations often ask “How accurate are these fancy (and colorful) figures?” Our task in this paper is to answer the question by comparing the computational results with experimentally obtained through a well-defined procedure called validation.

This paper deals with validation of a commercial CFD software Star-CCM+ for liquid Lead-Bismuth Eutectic (LBE) flows (i.e. the coolant used in MYRRHA). The computational results are compared against experimental data from TALL-3D facility.

2 METHODOLOGY

Methodology to perform CFD code validation includes identification of physical phenomena of interest in LFRs; definition of procedures to carry out a successful validation exercise; design and construction of a dedicated experiment; and modeling and simulation of the validation tests. In following sections all abovementioned points are addressed.

2.1 Thermal-hydraulic phenomena of interest in LFRs

Table 1 lists the main single-phase thermal-hydraulic phenomena present in pool-type LFRs.

<table>
<thead>
<tr>
<th>Single phase phenomena</th>
<th>Type of model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Free shear</td>
<td>Bulk turbulence model</td>
</tr>
<tr>
<td>Wall shear</td>
<td>Wall turbulence model</td>
</tr>
<tr>
<td>Thermal mixing</td>
<td>Momentum transport (convection and diffusion)</td>
</tr>
<tr>
<td>Thermal stratification</td>
<td>Energy transport (convection and diffusion)</td>
</tr>
<tr>
<td>Jet impingement of a surface</td>
<td>Production of turbulence</td>
</tr>
<tr>
<td>Thermal inertia of structures</td>
<td>Conjugate heat transfer</td>
</tr>
<tr>
<td>Natural circulation</td>
<td>All thermal-hydraulics models integrally</td>
</tr>
</tbody>
</table>

These are the drivers of TALL-3D experimental facility design (see details in Section 2.3). It is important to note that these phenomena may have different characteristics in steady state and transient conditions meaning that models have to be tested in both cases.

2.2 Validation approach

According to AIAA [10], validation is defined as the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model. Model validation can be divided into three stages ([11], [12]) (illustrated in Fig 1):

1. Assess the model accuracy by comparing computationally and experimentally obtained results using System Response Quantities (SRQs) using a validation metric,
2. Interpolate or extrapolate the model for the intended use, and
3. Decide whether the accuracy requirement is met for the intended use of the model.
The intended use for our model is to reproduce TALL-3D behaviour. Step 1 is divided further into following steps.

1. **Definition of validation metrics.** Validation metric is a *quantitative measure* of comparison between computational and experimental SRQs. The SRQs are also input to the validation metric. SRQs used in the validation step must be selected according to the physical phenomena that a code (or its sub-models) is designed to represent.

2. **Definition of uncertain input variables.** A model requires a specific set of input data to produce the output. The type and number of input variables is determined by the model used to produce SRQs used in validation metrics. Geometry dimensions, material properties, physical model parameters, initial and boundary conditions fall into this category. An aleatory (i.e. due to randomness of a variable) or epistemic (i.e. due to lack of knowledge or missing measurements) uncertainty is attained to each of those.

3. **Quantification of uncertain input parameters and the uncertainty.** Definition of range in which we expect the value of an uncertain parameter to be (e.g. thermal conductivity is [10-15] W/m/K) depends on the knowledge we have (i.e. uncertainty). This is important for evaluating the impact of the uncertainty on the solution (i.e. sensitivity).

4. **Quantification of uncertainty in experimental measurements.** Uncertainty in experimental measurements is assessed from the accuracy and precision specifications of measurement instrumentation.

5. **Data comparison.** A difference between experimental, typically estimated mean of an SRQ and computational results is computed. This is to be done using pre-defined validation metric.

### 2.3 TALL-3D experimental facility

TALL-3D is a loop-type facility with liquid Lead Bismuth Eutectic (LBE) as operating media [14]. The goals of the facility design are to provide (i) mutual feedback between natural circulation in the loop and complex 3D mixing and stratification phenomena in the pool-type test section, (ii) a possibility to validate standalone STH and CFD codes for each subsection of the facility, (iii) sufficient number of experimental data to separate the process of input model calibration and code validation. Guidelines to design, build and operate a validation experiment described in Oberkampf and Smith (2014) [15] were followed.
The schematic of the facility is shown in the Fig 2. It incorporates the main (LBE) loop, the secondary (cooling) side and the differential pressure measurement system. The total height of the facility is about 6.5 m. The main loop consists of a sump tank, three vertical legs and two horizontal sections with two elbows and a T-junction connected to both. The distance between adjacent vertical legs axes is 0.74 m and the length of every leg is 5.83 m with inner diameter of 27.86 mm. The Main Heater (MH) leg (left) accommodates (i) a 27 kW rod-type electric heater in the lower part and (ii) an expansion tank at the top. The Heat Exchanger (HX) leg (right) has (i) a counter-current double-pipe heat exchanger placed at the top and (ii) an Electric Permanent Magnet (EPM) pump up to 5.5 kW electrical power. The 3D leg (middle) connects to the loop a pool-type 3D test section.

During normal operation the flow is directed downwards in HX leg and upwards in the MH and 3D leg. In transients, however, the flow can reverse in all legs depending on the power of the heaters and on the initial conditions. There is feature of fine tuning the hydraulic resistances in the MH and 3D legs by adjusting the flow control ball valves. It is used to reach equal mass flow rates in hot legs with equal heater powers in natural circulation conditions (making the system more susceptible to instabilities). The 3D test section is an axisymmetric cylindrical stainless steel vessel with an inlet at the bottom and an outlet at the top (see Fig 3). The upper part (two—
thirds) of the test section is equipped with a 15 kW band heater installed around the circumference to promote the development of thermal stratification in the LBE pool. Inside the test section, a circular plate is placed orthogonal to the flow path in order to enhance pool mixing by deflecting the inlet flow to periphery. The plate is attached to the ceiling of the pool with 4 fin-shape separators, which are designed to inflict minimal disturbance on the flow.

![Fig 3: TALL-3D test section and temperature measurement locations.](image)

The facility incorporates following thermal-hydraulics phenomena: free jet flow, jet impingement on a surface, jet induced recirculation in a pool, stratification development, mixing, thermal inertia of the structure, thermal conduction through the plate and turbulence.

Implemented instrumentation provides experimental data on the flow rates and LBE temperatures in main loop legs, thermal losses, thermal inertia of the structures, mixing and stratification transients in the 3D test section and flow, temperatures and boundary conditions on the secondary side.

### 2.4 Transient T01.03

In this work we analyze the T01.03 test on transient from forced to natural circulation in the TALL-3D facility. This test imitates the loss of pumping head in a reactor with multiple parallel flow paths. For example, imagine ELSY reactor where the primary flow is distributed between eight steam generator units [16]. The natural circulation regime will then develop in each leg (flow path) with a possibility of flow instabilities between them.

First, a steady state in the loop was achieved with MH of power 4972 W and 3D test section power of 5078 W. Initial mass flow rate in the HX leg was 4.793 kg/s and in the 3D leg 1.827 kg/s. At time 0 s the EPM pump was tripped while keeping the heater powers constant. After a transition period a natural circulation steady state was established in the loop. The duration of the whole transient is about 30 minutes.

Before the transient, a calibration test was performed to identify any offset in the mass flow readings. Stagnant flow was established in all the legs and flow measurements were it can be seen Fig 4 that flow meters in both, HX and 3D leg, showed 0.05 kg/s offset that was taken into account when providing mass flow as boundary condition in the transient simulation.
Fig 4: Calibration of mass flow rate in 3D test section (mfTS) and in HX (mfHX) during stagnant flow conditions.

2.5 CFD model

The CFD code used in this study is Star-CCM+ 9.04.009. Geometry was created using the 3D-CAD module within Star-CCM+. Surface and volume meshing was done also with Star-CCM+ meshing tools.

2.5.1 Geometry

Axis-symmetry of physics in 3D test section allowed using lighter 2D model (see Fig 5). In reality, certain deviation from full axis-symmetry can be expected, but it is intractable to account for in the model. The inlet/outlet pipes are 250 mm and 450 mm long, respectively. The length to diameter ratio (L/D) is about 15 with total L/D of the inlet pipe of about 40. This reduces the sensitivity of the results to the assumptions about the inlet velocity profile.

Fig 5: Topology of the test section model regions.

2.5.2 Physics

Physics continua are defined for three materials – (i) LBE; (ii) steel (heater, walls and circular inner plate); and (iii) insulation. LBE properties are implemented in Star-CCM+ as polynomial functions in temperature according to Sobolev (2010) [17]. Steel is modeled with stainless steel properties available in Star-CCM+. Insulation material is defined and implemented according to the technical data obtained from the supplier.

There is a mass flow inlet and pressure outlet for the fluid. Heat source according to the experimental value is set in the heater region. Natural convection heat transfer between the insulation and air is modeled with heat transfer coefficient of 10 W/m²/K and ambient
temperature of 30 °C. Conjugate heat transfer between regions is calculated.

A steady state solution has been reached (all residuals were below 1.0E-8) before the transient simulation was performed. In transient simulations, unsteady implicit time integration scheme is used with 2nd order temporal discretization. Time step was 0.01 s. Coupled implicit solver is used for flow and energy with 2nd order upwind convection scheme for the flow. Contribution of the secondary gradients in the diffusive flux term is modeled to account for cross-diffusion at boundaries and interior of the polyhedral cells.

Two types of turbulence models were used to predict mixed convection turbulence inside the 3D test section – (i) a Realizable $k - \epsilon$ turbulence model with Buoyancy Driven Two Layer formulation developed by Xu et al. (1998) [18] (the model is adapted to perform calculations at all y+ values), and (ii) an SST $k - \omega$ model by Menter (1994) [19] that is an improved version of the original standard $k - \omega$ model developed by Wilcox (1988) [20].

### 2.5.3 Mesh study

A mesh study with eight different meshes for fluid region is performed. Three hexahedral and five polyhedral meshes with different cells size have been tested. Ten layers of prismatic cells were used in case of polyhedral meshes to resolve better the viscous effects on the wall. On each mesh, the same steady state case has been simulated with inlet temperature of 425 K and mass flow rate of 1 kg/s. To find the mesh-converged solution, pressure loss, temperature rise and integral momentum in the pool were monitored and flow field visually evaluated. See Table 2 and Fig 6 for details.

<table>
<thead>
<tr>
<th>Type</th>
<th>Size</th>
<th>$T_{out}$ [K]</th>
<th>dP [Pa]</th>
<th>p [kg m/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polyhedral</td>
<td>3,402</td>
<td>458.76</td>
<td>94,298</td>
<td>0.6350</td>
</tr>
<tr>
<td></td>
<td>19,126</td>
<td>458.76</td>
<td>94,362</td>
<td>0.6955</td>
</tr>
<tr>
<td></td>
<td>55,328</td>
<td>458.76</td>
<td>94,299</td>
<td>0.7301</td>
</tr>
<tr>
<td></td>
<td>195,555</td>
<td>458.76</td>
<td>94,358</td>
<td>0.7082</td>
</tr>
<tr>
<td></td>
<td>210,912</td>
<td>458.75</td>
<td>94,365</td>
<td>0.7064</td>
</tr>
<tr>
<td>Hexahedral</td>
<td>4,251</td>
<td>458.76</td>
<td>94,059</td>
<td>1.1423</td>
</tr>
<tr>
<td></td>
<td>37,550</td>
<td>458.76</td>
<td>94,210</td>
<td>0.9567</td>
</tr>
<tr>
<td></td>
<td>149,700</td>
<td>458.70</td>
<td>94,180</td>
<td>0.8338</td>
</tr>
</tbody>
</table>

Fig 6: Flow fields resolved with different (polyhedral) mesh size.
Polyhedral mesh with 19,126 cells in the fluid domain (43,787 cells in total) was chosen for the transient study because it results in a very similar solution to the finest mesh case with almost ten times fewer elements (therefore allowing faster simulations). The mesh is conformal between different regions and there is layer of ten prismatic cells near the fluid wall with total thickness of 4 mm (first cell thickness 0.1 mm). The mesh is illustrated in Fig 7.

![Polyhedral mesh of TALL-3D test section](image)

**Fig 7:** Polyhedral mesh of TALL-3D test section (blue represents fluid domain).

3 RESULTS AND DISCUSSION

We hereby present the results of simulating the transient T01.03 using two different approaches for turbulence modeling, namely realizable $k-\varepsilon$ and $SST k-\omega$, side-by-side. There are three distinct phases of the transient – (i) initial steady state (forced circulation); (ii) transient phase; and (iii) final steady state (natural circulation).

The initial steady state in the pool is characterized by one large and few smaller vortices that are created by the high-momentum inlet jet (Fig 8). If in $k-\varepsilon$ case one of the vortices is distinctively larger than the others, then $SST k-\omega$ model predicts the vortices to be more of similar size. However, the mixing is as effective in both cases. Fig 9 shows the temperature gradients (i) inside the pool, on a vertical thermocouple (TC) train in the bulk flow and (ii) on TCs distributed on the outer lateral wall (between the heater and the outer lateral). There is slight underestimation of the outer lateral wall temperatures. The difference in shapes of outer lateral wall temperature curves predicted with different turbulence models is in agreement with flow structures (peaks temperatures appear between vortices).

![Initial steady state (forced circulation) flow fields](image)

**Fig 8:** Initial steady state (forced circulation) flow fields.
Fig 9: Initial steady state (forced circulation) temperature gradients along the vertical TC train and on the outer lateral wall.

Fig 10 shows the mass flow rate through the 3D test section during the transient. Since the mass flow rate is an independent variable imposed as a boundary condition it is not subjected to validation but rather illustrates the course of the transient. The experimental mass flow is corrected to account for offset and to smooth the noise in the measurements. At time 0 s when the pump is stopped flow rate rapidly drops and even reverses reaching the maximum downward flow rate of about 0.3 kg/s at around 100 s.

The reversal of the flow is a result of competition between the buoyancy forces in MH and 3D leg – when the flow slows down, the fluid heats up faster in the narrow MH section than in the bulky 3D pool and accelerates first. Low flow rates lead in the 3D leg to gradual heat up of the LBE in the 3D pool which, due to flow reversal, is detected also at the inlet (see Fig 11). At the
same time, no increase in temperature is detected at the outlet. This means that during the close-to-stagnant conditions in the 3D leg up until about 400 s the fluid in the pool is slowly heating up (confirmed also by the inner pool temperature measurements in Fig 12 and Fig 13). It is important to note that the temperatures at the bottom part of the pool do not rise and increasing difference in temperatures between different height levels in the pool implies the development of thermal stratification – the inlet jet has not enough momentum to mix the pool (see Fig 14 for bottom plate temperatures).

**Fig 11:** 3D test section inlet and outlet temperature.

After 400 s, the flow in 3D leg accelerates, causing temperatures in the pool to drop and oscillate for some time. The drop in inner pool temperatures is also due the reduction in inlet fluid temperature. The oscillatory behavior can be attributed to competition of flow in two parallel rising flow paths with similar resistance and driving forces.

**Fig 12:** Temperatures on a train of TCs in the fluid between the wall and the edge of circular inner plate.
The results show that all temperatures are predicted very accurately considering the presence of such complex flow phenomena inside the test section. In most cases the deviation between experimental and simulated curves is within 1-2 K with peak differences at about 5 K. These differences fall mostly within the range of uncertainties in thermocouple readings and uncertainties in determining the exact location of the measurement point which is not a point, but about a 1 mm long section at the tip of a thermocouple.

Final steady state flow fields and temperature gradients imply strong thermal stratification in the pool during natural circulation conditions (Fig 15 and Fig 16). By analysing the temperature gradient curves, one can see that temperature in the bulk of the fluid and on the outer wall is practically the same in the lower part of the pool. K-epsilon simulation agrees well with the experimental data, whereas SST $k - \omega$ over predicts temperature in these lower layers. This is explained by the difference in jet penetration depths into the hot stratified layers. In case of SST $k - \omega$, the jet is longer in the pool and carries therefore too much heat down to the lower
layers. In the upper part of the pool (inside the thermally stratified layers) the fluid has higher temperature than at the outer lateral wall (in contact with the heater) – this is captured well by both turbulence models. Higher temperature inside the fluid is explained by the strong buoyant wall jet that transports the heat away from the heated wall.

![Flow fields](image1.png)

**Fig 15:** Final steady state (natural circulation) flow fields.

![Temperature gradients](image2.png)

**Fig 16:** Final steady state (natural circulation) temperature gradients along the vertical TC train and outer lateral wall.

### 4 SUMMARY AND CONCLUSIONS

In this paper we have performed a validation exercise on a commercial CFD code Star-CCM+ for predicting steady state and transient LBE flows in the test section of TALL-3D, an LBE cooled facility designed to provide high quality data for validation of thermal-hydraulics analysis codes. Detailed description of the transient T01.03 is provided. The transient features phenomena of mixing, stratification, transition from forced to natural circulation.

Simulation results with two turbulence models, *realizable k – ε* and *SST k – ω*, are presented and compared against experimental results on the integral and local temperature measurements. The main difference between the two models is prediction of the jet interaction with the stratified layer. Further analysis is necessary in order to provide quantitative metrics for
comparison of the simulation results obtained with different modeling approaches and experimental data, taking into account the uncertainties in both.

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