Prediction of Complex Thermal-Hydraulic Phenomena Supplemented by Uncertainty Analysis with Advanced Multiscale Approaches for the TALL - 3D T01 Experiment

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Abstract: The thermal-hydraulic (TH) system code ATHLET was coupled with the commercial 3D computational fluid dynamics (CFD) software package ANSYS CFX to improve ATHLET simulation capabilities for flows with pronounced 3D phenomena such as flow mixing and thermal stratification. Within the FP7 European project THINS (Thermal Hydraulics of Innovative Nuclear Systems), validation activities for coupled thermal-hydraulic codes are being carried out. The TALL-3D experimental facility, operated by KTH Royal Institute of Technology in Stockholm, is designed for thermal-hydraulic experiments with lead-bismuth eutectic (LBE) coolant at natural and forced circulation conditions. No tests have been performed up to now. GRS carried out pre-test simulations with ATHLET – ANSYS CFX for the TALL-3D experiment T01, while KTH scientists perform these analyses with the coupled code RELAP5/STAR CCM+. In the experiment T01 the main circulation pump is stopped, which leads to interesting thermal-hydraulic transient with local 3D phenomena. In this paper, the TALL-3D behavior during T01 is analyzed and the results of the coupled pre-test calculations, performed by GRS (ATHLET-ANSYS CFX) and KTH (RELAP5/STAR CCM+) are directly compared. Moreover, this work is supplemented by uncertainty and sensitivity analysis for the T01 experiment, carried out at the Technische Universitaet Muenchen.

Keywords: Gen IV, Liquid Metal Flow, Phenomena Modelling, Uncertainty and Sensitivity Analysis

1. INTRODUCTION

In specific nuclear reactor transients and accidents like boron dilution, main steam line break or pressurized thermal shock, three-dimensional coolant mixing and stratification phenomena play an important role and might have a remarkable impact on transient results. Unfortunately, such phenomena cannot be predicted correctly by system codes, based on 1D lumped parameter approach. To overcome this limitation, these numerical tools are coupled with modern CFD programs, which are capable to predict 3D flow behavior in complex geometries and can provide detailed distributions of the physical quantities in space and time. In a coupled 1D-3D numerical analysis, the CFD code simulates only the regions with complex 3D effects, while the rest of the facility is calculated with the 1D system code [1,2].

Within the European project THINS, research activities for the development and validation of advanced multi-scale simulation tools for Gen IV reactors are being carried out. Different approaches have been developed and implemented by GRS and KTH for the coupling of the system codes ATHLET and RELAP5 with the 3D CFD programs ANSYS CFX and STAR CCM+, respectively. In order to validate the newly developed coupled 1D-3D tools, dedicated thermal-hydraulic experiments are performed in Sweden. The TALL-3D thermal hydraulic loop is an integral, two-circuit, well instrumented, 7 m high experimental facility, operated by KTH (Fig. 1, left). The primary circuit consists of three vertical legs, filled with LBE. One heater is installed in the leftmost, main heater (MH) leg, and another one in the middle, 3D test section leg. A heat exchanger (HX) is placed in the upper part of the rightmost leg. The 3D test section, which is domain of complex 3D effects and

source for challenging thermal-hydraulic feedback to the rest of the loop is shown in Fig. 2 (right) [3]. Inside the test section pool, there is a metal plate which prevents the liquid metal leaving the test section pool without extensive mixing with the heated fluid inside. This LBE mixing is well pronounced at forced circulation conditions. At natural circulation conditions, stratification occurs in the test section pool, which is enhanced by the heated upper part of the pool wall. In one of the specified experiments, T01, the main circulation pump is stopped. This leads to interesting thermal-hydraulic transient with local 3D phenomena like LBE mixing and stratification affecting the overall loop behavior.

All parameters, which are used for modeling of complex experiments including initial and boundary conditions as well as physical models, might be source of uncertainty. Such uncertainty can significantly impair the quality of code validation process. Both a sensitivity analysis (SA) for the identification of the most influential input uncertain parameters and a uncertainty analysis (UA) for the determination of the range of variability of output variables due to the uncertainty of input parameters are important for a good understanding of model properties and eventually for validation of the codes. Based on the methodology developed by GRS [4,5], TUM performed UA and SA of the TALL-3D experiment T01.

In this paper, the TALL-3D behavior during T01 is analyzed and the results of the coupled pre-test calculations performed at GRS (ATHLET-ANSYS CFX) and KTH (RELAP5/STAR CCM+) are directly compared. Emphasis is given to the understanding of the thermal-hydraulic behavior of the TALL-3D facility during test T01. In a next step, the results from the supplementing uncertainty and sensitivity analyses are discussed.

2. SHORT DESCRIPTION OF THE TALL-3D FACILITY MODELING WITH ATHLET-ANSYS CFX AND RELAP/STAR-CCM+

2.1. Modeling of TALL-3D with ATHLET-ANSYS CFX

Since the TALL-3D test section pool has a rotational symmetry, it was decided to generate a 2D CAD model of the test section [6]. This model served as an input for the ICEM CFD software, which has been used to prepare a 2D hexahedral grid. Then, the 2D grid was revolved to 1° rotational symmetry sector of the test section. In this way, a real 3D CFD mesh was generated and used for the simulations. Grid sensitivity studies were performed, resulting in a final mesh with 48.000 elements (Fig. 2). The mesh quality is very good with a minimum orthogonally angle of 88°, an expansion factor of 4 and a maximum aspect ratio of 465.

For the correct modeling of the buoyant LBE flows in the TALL-3D test section, buoyancy terms in the momentum equation and in the production terms of the turbulence model equations have been included. In the calculations, the SST turbulence model has been used [7]. In the transient CFD and coupled simulations, Second Order Backward Euler transient scheme was selected, while for the numerical transport of the quantities (velocity, temperature, etc.) through the solution domain, a High Resolution advection scheme was used [8]. An adaptive time stepping scheme (time step sizes between 0.1 and 0.5 s) was used in all coupled simulations.

Four priority chains (flow paths) were used for the simulation of the whole experimental facility with ATHLET. These describe the primary and secondary circuit of the facility. Figure 3 shows the coupled ATHLET-ANSYS CFX model (here shown with a symmetry plane of a full model of the 3D test section).

2.2. Modeling of TALL-3D with RELAP/STAR-CCM+

Both STAR CCM+ and ANSYS CFX domains comprise of pool-type section with part of inlet and outlet pipes [3]. The 2D axisymmetric mesh consists of 74.661 polyhedral cells (see Fig. 4, left). The outlet and inlet pipes are modeled with 25 prism layers and the rest of the domain is modeled with 15

layers on the wall. Inlet mass flow rate and temperature were defined at the inlet boundary and pressure was defined at the outlet. In transient simulations, unsteady implicit time integration scheme is used with second order temporal discretization. Segregated solver with second order upwind convection scheme is used for the flow [9]. Density as a polynomial function of temperature is used as the equation of state. Mixed convection turbulence inside the 3D test section is predicted using a Realizable K-Epsilon turbulence model with Buoyancy Driven Two Layer formulation developed by Xu et al. [10].

The corresponding RELAP5 nodalization of TALL-3D geometry can be seen in Figure 4 (right picture). The model consists of pipe structures connected together by single junctions and time-dependent junctions. Time-dependent volumes are used for expansion tank and secondary side inlet and outlet. The main heater (MH) is simulated as a pipe with flow area comparable to the flow area in the annulus at the facility.



Fig. 1: TALL-3D facility







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2.3. Transient Test T01 and Boundary Conditions

Since no measured data are available, only specified data and boundary conditions have been used for the developed simulation models. Later, experimental data from the steady state TALL-3D commissioning tests will be used for fine calibration of the coupled models. In the test case selection process, emphasis was put on transients with strong 3D effects in the 3D test section. It is expected, that these will have an impact on the whole TALL-3D facility. Their simulation requires the application of advanced coupled codes like ATHLET-ANSYS CFX and RELAP5/STAR-CCM+. Pressure and temperature will be measured at different locations in the facility. This data will be then used for the validation of both programs.

The planned transient test case "Test T01 – Forced to natural circulation with both heaters always switched on" was selected for comparison of the two simulations. This test case represents a loss of flow transient in the facility. It starts from a steady state forced convection with a specified mass flow rate of 4.77 kg/s in the HX leg. This mass flow rate is not distributed evenly in the rest of the primary circuit – 2.84 kg/s are expected to flow through the MH leg, and 1.93 kg/s through the 3D test section leg. The temperature at the 3D test section inlet is 563 K, while 488 K are specified at the inlet of the secondary circuit (secondary mass flow rate: 4.0 kg/s). During the whole transient, both, the main and the 3D test section heaters are in operation at 5 kW power each. At time 120 s, the electromagnetic pump is switched off. The simulation time of this transient test was specified to be approx. 1500 s.

2.4. Analysis and Comparison of the Simulation Results

With the specified boundary conditions, three calculations have been performed – two at GRS (ATHLET stand alone and coupled simulation with ATHLET-ANSYS CFX) and one coupled at KTH (RELAP5/STAR-CCM+).

The electromagnetic pump was tripped at 120 s simulation time with a run down time of one second, which leads to a rapid mass flow rate decrease in all three primary legs. Within ten seconds, the LBE mass flow rate in the HX leg drops from 4.77 kg/s to 0.5 kg/s and then stabilizes at about 0.75 kg/s in all three calculations. Due to the LBE density distribution in the primary circuit and the difference between the geodetic heights of both heaters (lower part of the facility) and the HX (upper part of the facility), natural LBE circulation occurs in the primary circuit of the TALL-3D loop immediately after the pump trip. In this early phase of the transient, a mass flow increase in the MH leg is observed (Fig. 5), while the mass flow rate in the 3D test section leg decreases further (Fig. 6).

Because of the intensive natural circulation in the MH leg, less LBE flows in the 3D test section leg. In the stand alone ATHLET calculation, the LBE flow even reverses for approx. 90 s, while in the RELAP5/STAR CCM+ calculation the flow reversal occurs with a delay of 45 s and lasts 45 s. In the coupled ATHLET-ANSYS CFX simulation, the LBE flow decreases to 0.06 kg/s, but does not reverse. This imbalance of the LBE flow distribution in the primary circuit occurs, although both heaters are kept operated at 5 kW power each. The reason for this imbalance is related to the different volumes of the MH pipe and the 3D test section pool. Since the volume of the MH pipe (4.92E-4 m³) is significantly smaller than the one of the 3D test section pool (141.37E-4 m³), LBE is heated more rapidly in the MH (up to 640-650 K, see first temperature peaks around 160 s in Fig. 7), and its outlet temperature increases faster than the temperature at the outlet of the test section outlet pipe (Fig. 8). The heated LBE is lighter (lower density) and rises faster in the MH pipe. This enhances the natural circulation in this leg, while at the same time it impedes the LBE circulation in the 3D leg.



The temperature at the test section outlet (Fig. 8) in the ATHLET-ANSYS CFX simulation starts to increase 40 s after pump trip and, in the ATHLET simulation, after 90 s. The reason for the faster temperature increase in the coupled simulation is the positive LBE flow through the 3D test section leg. It is eventually enhanced by more intensive heating in this calculation, since wall structures are not present in the current ANSYS CFX model. In ATHLET, the heater power of 5 kW is applied to the test section wall, which is 6.75 mm thick, while in the coupled simulations a heat flux corresponding to 5 kW power is applied directly to the fluid. In this way, the specific heat capacity of the test section stainless steel wall is neglected in the coupled simulation. This leads to a constant heat flux during the whole ATHLET-ANSYS CFX simulation and to higher temperatures. This phenomenon enhances the natural circulation in the 3D test section leg and hinders flow reversal there.

Figure 9 shows the LBE temperature distribution in the 3D test section at forced circulation just before the initiation of the pump trip, calculated with ATHLET-ANSYS CFX (left) and ATHLET (right). The test section pool (0.2 m high) is represented in ATHLET as a 1D pipe with 20 nodes. Since the heater is installed around the upper half of the test section pool wall, only the nodes in this part are actually heated, while the ones below the heater are still filled with cold LBE ($T_{LBE}=T_{inlet}$). In this way, for the steady state of TALL-3D (pump is running, heaters at nominal power), a 1D system code like ATHLET or RELAP5 will predict stratification in the test section (see Fig. 9, right). In the coupled calculation, a large swirl develops in the CFD domain. The cold LBE first hits the plate and then moves to the side pool wall, taking the heat away from it and transporting it to the center and the bottom part of the pool. As a result, a mixed flow pattern in the 3D test section pool is observed. The mean LBE temperature in the vicinity of the bottom plate is approx. 578 K (Fig. 9, left), while the 1D approach of ATHLET predicts 563 K cold and stratified LBE at the same location (Fig. 9, right).

Fig. 9: Temperature distribution in the 3D pool



Figure 10 shows the evolution of the LBE temperature at the inlet of the test section inlet pipe. After pump trip, the LBE flows slowly through the primary HX tube at natural circulation conditions. It is better cooled down by the cold secondary side, which is kept at constant mass flow rate of 4.0 kg/s and 488 K LBE temperature. Approximately 110 s after pump trip, the LBE temperature in the RELAP5/STAR-CCM+ simulation increases suddenly, because of the flow reversal in Fig. 6. Since the 3D pool is well mixed, warm LBE from the bottom part of the test section pool (temperature distribution in STAR-CCM+ very similar to the one in Fig. 9, left) flows back to the test section inlet pipe. Although ATHLET predicts also a flow reversal (Fig. 6), this temperature increase is not present. The temperature at the bottom of the pool is the same as the one in the inlet pipe, due to the "artificial" stratification. In the ATHLET-ANSYS CFX simulation no temperature increase is observed, because LBE flow does not reverse at all. Approximately 110 s after pump trip, the cold LBE reaches the inlet of the test section, and the temperature calculated by ATHLET-ANSYS CFX starts to decrease.

Figures 11 and 12 show the temperature distribution in the 3D test section before the initiation of the transient and at its end, approx. 1500 s after pump trip. At high LBE velocities the test section is mixed, while at low velocities and heaters switched on, buoyancy effects play an important role. At natural circulation conditions, thermal stratification establishes in the CFD domain. Cold and heavy LBE stratifies at the bottom of the test section, while lighter, hot LBE can be found in the upper half of the test section pool.



Fig. 10: Temperature at the test section inlet



Fig. 11: T_{LBE} distribution at forced convection Fig. 12: T_{LBE} distribution at natural convection

A good overall agreement between the ATHLET stand-alone and the coupled RELAP5/STAR CCM+ calculation results can be observed. The occurrence of the main thermal-hydraulic phenomena in time is almost identical. The small differences in the temperatures might be explained with the different heat transfer correlations for LBE implemented in ATHLET and RELAP5. Moreover, two different simulation approaches are used in these calculations - the 1D (ATHLET) and the 1D-3D approach (RELAP5/STAR CCM+). It is surprising to observe such good agreement between the 1D and the more sophisticated 1D-3D RELAP5/STAR CCM+ simulation approach. ATHLET-ANSYS CFX results differ from the results of the other two calculations, but are still in agreement with them. The experimental data, which is expected to be available soon, will allow better analysis of the strengths and weaknesses of the different simulation approaches.

3. UNCERTAINTY AND SENSITITY ANALYSIS OF THE TALL 3D FACILITY USING ATHLET – ANSYS CFX

Once a Best-Estimate (BE) model has been designed, the influence of model input uncertainty needs to be taken into account. Uncertainty and Sensitivity Analysis is a powerful technique to help assess the sensitivity of the model to several modeling assumptions. This method provides information on the variability induced in the model output by the model input uncertainty and helps to identify the key input parameters. This information might be used to improve model accuracy and eventually to validate a model against experimental data.

3.1. Model Adaptation for Uncertainty Analysis

The variation of the input parameters applied in the scope of an Uncertainty and Sensitivity Analysis induces perturbation in the model which makes it deviate from the Best-Estimate run. These deviations can result in a system that is not stable by the start of the transient. To ensure that the state in which the system can be found at the start of the transient is actually a stable steady-state, two simple control systems (proportional-integral-derivative) have been implemented in the ATHLET TALL-3D model. The first controls the electromagnetic pump, thus ensuring that the total mass flow rate in the primary side (HX leg) is kept constant during steady-state. The second one controls the secondary LBE mass flow rate, and thus ensures power balance between primary and secondary side.

3.2. Computer Experiment

The screening analysis performed here considered 33 uncertain parameters. Due to the lack of experimental data, only uniform distributions have been applied. For all the parameters, except for the turbulent Prandtl number (No 32) and the LBE properties (No. 10 to 13), a variation of \pm 10% or \pm 5% around the best-estimate value has been specified. The pump is tripped at t = 500 s. The model input parameters values have been generated using the Simple Random Sampling Method. The Kolmogorov Goodness-of-Fit test [11] was used to check that the original distributions were respected by the sampled distributions. The sample has been checked to avoid spurious rank correlations between the parameters which were assumed independent in this work, according to [5].

The analysis was performed with a set of 153 simulations. This is the minimum number of runs which is required to compute non-parametric two-sided tolerance limits at the second order with 95% population coverage and 95% confidence level [11]. This ensures a lower conservatism of the tolerance limits against the one which would be obtained with the first order.

Considering the 33 model input parameters, this sample size ensures a critical value of the Spearman's Rank Correlation Coefficients (SRCC) lower than 20% [11]. This is more than enough, since an uncertain parameter is not considered influential if its value is below 40%.

4. NON-PARAMETRIC UNCERTAINTY ANALYSIS

In the following paragraphs the non-parametric tolerance limits (TL) are presented along with the BE run (all model input parameter values are set to their mean value). These represent the spread of the model output which can be expected due to the model input uncertainty. Over all the possible cases (there is infinity of them) and given the model input uncertainty considered here, we are 95% sure that in 95% of the cases the model output will lie within the tolerance limits.

The main results from the non-parametric uncertainty analysis are listed below:

- The uncertainty over the input parameters induces relatively small variations in terms of mass flow rate, except for the mass flow rate in the 3D leg (Fig. 13) at the early stages of the transient (at approx. 600 s, that is 100 s after the pump trip) (Fig. 14).
- The variations induced on the pressure (not represented here) are very small (less than 1000 Pa)
- Heat transfer phenomena appear to be the most influenced by the model input uncertainty. The temperatures at 3D pool inlet and outlet (Fig. 15) and their difference (Fig.16) show relatively large variations (up to 15 K).





Fig. 15: Inlet and outlet temperature 3D pool

Fig. 16: Temperature increase over the 3D pool

5. SENSITIVITY ANALYSIS

Once the model output variability has been quantified, the model input parameters which account for this variability can be identified. This part of the analysis is called Sensitivity Analysis. The latter is performed here using correlation coefficients as a measure of the strength of the relation between the model input parameter and the monitored output variable. In the following, Spearman's Rank Correlation Coefficients (SRCC) [11] were used to quantify this influence. These coefficients are calculated assuming a monotonic relation between the input and the output, and quantify the strength of this monotonic relationship. To check whether this relation actually explains most of the model output variability, the Multiple Determination Coefficient must be calculated [4] and its value provided along with the SRCC values.

5.1. Scalar Sensitivity

At each time step, ANSYS CFX was configured to provide the maximum local LBE temperature in the whole CFD domain. The maximum of these values over the whole transient can be determined per each run. Sensitivity analysis has been performed on this data.

Following model input parameters are the most influential on the maximum LBE temperature (Fig. 17):

- The initial inlet temperature (31) is positively correlated as a starting point for the transient. It is still very influential since the maximum temperature is reached shortly after the pump trip when the LBE has been virtually blocked in the pool.
- The heat capacity of LBE (13) is negatively correlated. A lower value tends to increase the difference in temperature when a given amount of power is added to the fluid.
- The power of the 3D heater (15) is obviously positively correlated.
- The turbulent Prandtl number (32) tends to reduce turbulent heat transfer and enables higher local temperature elevation.

For the time at which the maximum temperature is reached (Fig. 18), the delaying effect of the LBE heat capacity and of the heat losses through the insulation is highlighted by the positive correlation. The power of the 3D heater is negatively correlated since a high power induces faster increase of LBE temperature and faster initiation of natural circulation.



Fig. 17: SRCC observed maximum temperature





5.2. Time-Dependent Scalar Sensitivity

The multiple determination coefficient values are not represented here, but it remains close to 1 during the whole calculation. The present analysis investigates the influence of the input parameters on the mass flow rate in the 3D leg (Fig. 19).

During the steady-state phase, the pressure form loss (PFL) related terms due to the fuel pin spacers in the MH leg and the Rotamass mass flow meter and the roughness in the 3D pool are the most influential.

During the transient:

- The more power is transferred to the fluid by the 3D pool heater, the higher the density differences driving the flow. This explains the positive correlation during most of the transient.

Within the time frame 700 - 800 s, the correlation turns negative. This is due to the transition from forced to natural circulation. The 3D pool contains a large amount of LBE. When the pump is tripped, this amount of fluid is blocked in the pool and heated up, and hence energy gets accumulated in the pool. When the mass flow rate starts to increase again after 600 s simulation time, the large volume of the pool and the energy accumulated there induce thermal inertia in the system behavior. The higher the power of the 3D heater, the longer it will take the HX to remove the accumulated energy. Therefore, the outlet temperature of the pool as well as the HX temperature remain higher and the density difference remains smaller which leads to a lower mass flow rate in the 3D leg and to the negative value of the correlation coefficient.

- The value of the heat capacity influences the temperature variations where heat transfer occurs. Globally large temperature variations lead to large density differences which drive the natural circulation: hence the negative correlation during most of the transient. The same phenomenon as previously discussed for the power of the 3D heater applies here for the time frame 700 800 s.
- The turbulent Prandtl number is globally positively correlated. If its value is increased, turbulent thermal mixing is reduced which increases the outlet temperature of the 3D pool. The density difference driving the natural circulation is then increased.
- The higher the heat losses in the 3D pool, the lower the temperature increase. This reduces the density differences (inlet and outlet of the 3D pool): hence the negative correlation.



6. CONCLUSION

This paper provides comparison of the results from the first blind simulations of the TALL-3D facility, performed at GRS (ATHLET, ATHLET-ANSYS CFX) and KTH (RELAP5/STAR-CCM+). In the specified by KTH transient test T01, a pump trip is simulated and the natural circulation phenomenon for liquid metal flows is being studied. The performed simulations show, that the selected geometry of the TALL-3D facility together with the chosen boundary conditions result in a very interesting and challenging experiment. This involves complex physics including liquid metal forced and natural circulation, combined with heat transfer and 3D mixing and stratification phenomena. All three simulations show similar behavior of the main thermal-hydraulic parameters. The most important difference between ATHLET-ANSYS CFX and the other two simulations is the fact that the mass flow rate does not reverse in the 3D test section leg.

Although a very good general agreement is observed between the 1D ATHLET and the 1D-3D RELAP5/STAR-CCM+ calculations, it was shown, that the 1D simulation is not always adequate for the simulation of geometries with pronounced 3D flow effects like mixing or stratification. This reveals the need for the development and application of advanced coupled thermal-hydraulic programs such as ATHLET-ANSYS CFX and RELAP5/STAR-CCM+. Moreover, the comparison with the experimental data will allow better analysis of the strengths and weaknesses of the different simulation approaches.

The Uncertainty Analysis leads to the conclusion that most important model output variability is to be found in the heat transfer related processes which also affect the mass flow rate in the 3D leg during the transition phase.

The Sensitivity Analysis helped identifying the most influential parameters on the calculation. There are the LBE fluid properties, the power of the heaters, the turbulent Prandtl number, some of the pressure loss related terms, especially the spacer in the MH leg and the Rotamass flow meter in the 3D leg.

Influential parameters were identified for global variables (Scalar Sensitivity) which can be safety relevant. The time-dependent Sensitivity Analysis helped identifying phenomena and provided detailed information and understanding on the influence of the model input parameters on the simulation results as well as on the hierarchy of the input parameters during the three phases of the transient (forced circulation, transition phase and natural circulation).

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