

# An Approach to Physics Based Surrogate Model Development for Application with IDPSA

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**Abstract:** Integrated Deterministic Probabilistic Safety Assessment (IDPSA) methodology is a powerful tool for identification of failure domains when both stochastic events and physical time dependent processes are important. Computational efficiency of deterministic models is one of the limiting factors for detailed exploration of the event space. Pool type designs of Generation IV heavy liquid metal cooled reactors introduce importance of capturing intricate 3D flow phenomena in safety analysis. Specifically mixing and stratification in 3D elements can affect efficiency of passive safety systems based on natural circulation. Conventional 1D System Thermal Hydraulics (STH) codes are incapable of predicting such complex 3D phenomena. Computational Fluid Dynamics (CFD) codes are too computationally expensive to be used for simulation of the whole reactor primary coolant system. One proposed solution is code coupling where all 1D components are simulated with STH and 3D components with CFD codes. However, modeling with coupled codes is still too time consuming to be used directly in IDPSA methodologies, which require thousands of simulations. The goal of this work is to develop a computationally efficient surrogate model (SM) which captures key physics of complex thermal hydraulic phenomena in the 3D elements and can be coupled with 1D STH codes instead of CFD. TALL-3D is a lead-bismuth eutectic thermal hydraulic loop which incorporates both 1D and 3D elements. Coupled STH-CFD simulations of TALL-3D typical transients (such as transition from forced to natural circulation) are used to calibrate the surrogate model parameters. Details of current implementation and limitations of the surrogate modeling are discussed in the paper in detail.

**Keywords:** IDPSA, Dynamic PSA, Surrogate Model, TALL-3D.

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## 1. INTRODUCTION

Generation IV nuclear reactor designs often incorporate pool type configurations with passive safety features which depend on complex physical interactions and local flow conditions. Lack of operation on large scale means the pre-knowledge of such systems performance, their safety and failure modes is scarce. The IDPSA methodology is proposed in such cases for a comprehensive safety analysis. It is a powerful tool to identify failure domains when both stochastic events and physical time dependent processes are important [1]. This method relies less on expert knowledge of the system and more on the deterministic codes to explore the event space.

Several thousands of calculations need to be run for a successful analysis of a given design. Pool type nature of the designs requires a 3D simulation code to be used as 1D system codes fail to capture complex flow phenomena e.g. mixing and stratification during transient conditions. However, application of a CFD code for the full model of the reactor design is not feasible due to unreasonably long calculation time. To avoid this, approaches for coupling STH and CFD codes have been proposed, which retain accuracy as well as efficiency [2].

However, coupled STH-CFD simulations are still too computationally expensive for IDPSA applications. Here another approach is to use calculation results from a CFD code to create a physics-based Surrogate Model (SM) which would give comparable outcome. Such SM could be used coupled

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with an STH code instead of CFD. Using a surrogate model would considerably decrease the calculation time and allow IDPSA methodology to be applied more efficiently.

## 2. TALL-3D FACILITY DESCRIPTION

Both separate models, calculation codes, and coupled code approaches need to be validated against real-world experimental data. This requires complex and highly specific experimental equipment. Therefore a lead-bismuth eutectic (LBE) thermal hydraulic test facility TALL-3D was built at the Royal Institute of Technology (KTH). The loop is designed to provide experimental data for single STH, CFD and coupled STH/CFD code validation with the aim to study complex feedbacks between the 3D and system scale phenomena [3].

The layout of the facility is shown in Figure 1. The loop is composed of 3 sections: the main heater leg (left); the 3D test section leg (center); and the heat exchanger leg (right). Total height of the facility is 6980 mm whereas the height of the loop piping is 5830 mm. The width of the loop is 1480 mm. The pipes have internal diameter of 27.86 mm and outer diameter of 33.4 mm. The main heater leg contains a 25 kW rod type electrical heater which is 8.2 mm in diameter and the heated part has a length of 870 mm. An expansion tank is installed on the top of the main heater leg. The 3D leg contains a heated pool type test section in its lower part. The test section heater power is 15 kW. The heat exchanger leg contains a heat exchanger in the top part and an electromagnetic pump below it. The secondary loop utilizes DOWTHERM RP as cooling fluid and a fan is used as a secondary heat exchanger. The LBE is stored in the sump tank located at the lower left corner of the loop.

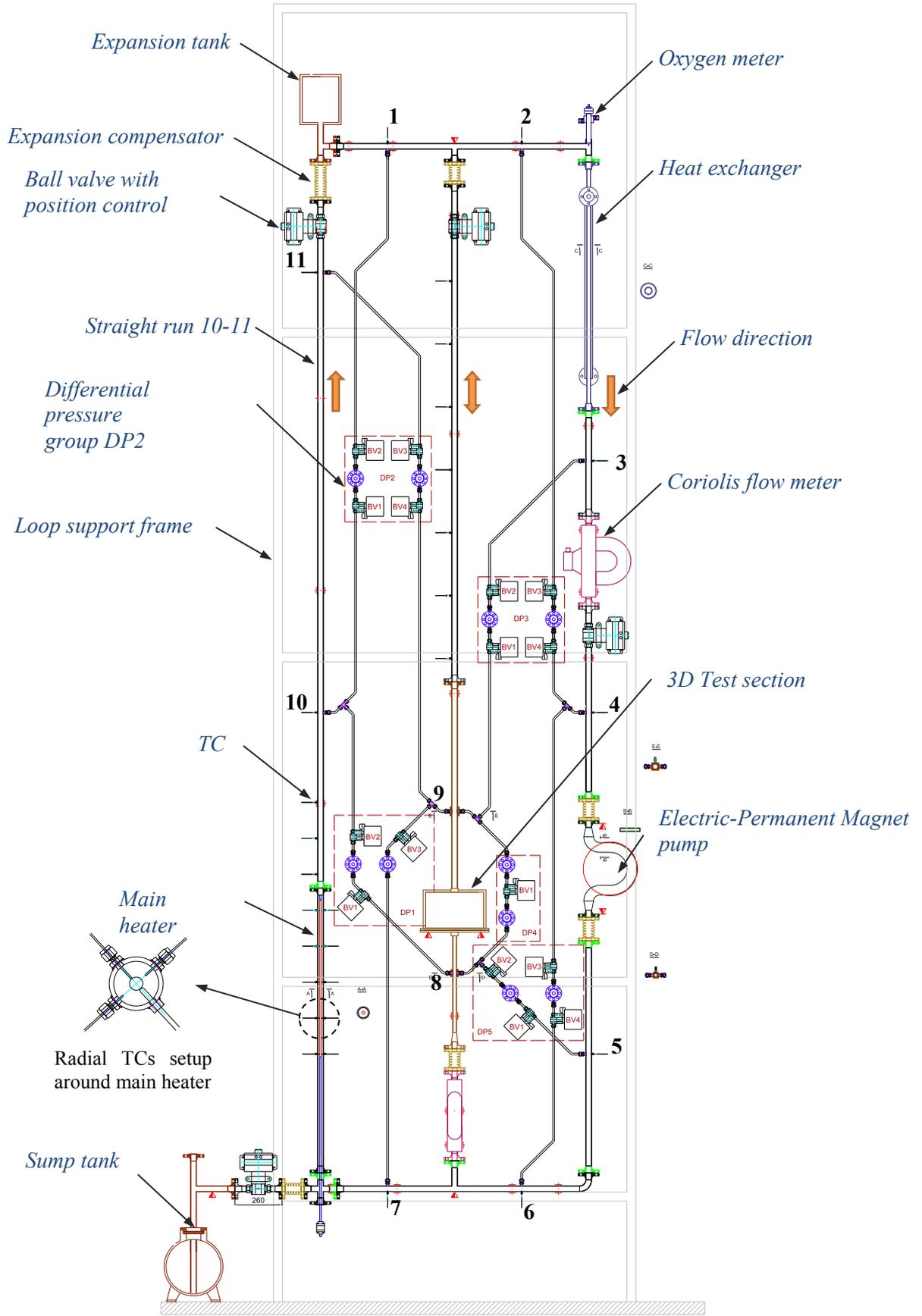
Three ball valves (one per section) are installed for fine tuning of the flow. This enables equalizing the flow rates in the main heater and 3D legs in natural circulation mode, thus allowing the mass flow rates to be brought out of balance by a relatively small effort, leading to flow oscillations in the two hot legs [3].

All parts of the facility in contact with the LBE are manufactured of SS-316L stainless steel to ensure corrosion and erosion resistance. Stainless steel is characterized by a relatively high thermal expansion coefficient, therefore the effects of thermal deformation must be considered. For this purpose TALL-3D was designed with a system of expansion joints, anchored fixation points and pipe guides to preserve the loop geometry, account for different thermal expansion of different legs, damp possible vibrations, and preserve a strict vertical position of the 3D test section.

An extensive amount of instrumentation is installed in both loop type components and the 3D test section to provide sufficient information for single STH, coupled STH/CFD code validation, and investigation of isolated physical phenomena. This includes two Coriolis flow meters on the primary loop; a five-group differential pressure measurement system, enabling measurements of total 15 differential pressures around the loop; and numerous thermocouples positioned in the flow, on the pipe walls as well as on the walls of the insulation. The instrumentation is connected to the Data Acquisition System (DAS) and is operated via a LabView interface.

Most of the facility can be represented as a 1D model since small diameter pipes have negligible 3D flow tendencies. Pool type test section in the middle leg introduces complex axisymmetric geometry and requires full three dimensional flow solution in transient conditions for correct outlet temperature estimation. This means there is a clear separation between the STH code domain and the CFD code domain for the TALL-3D facility.

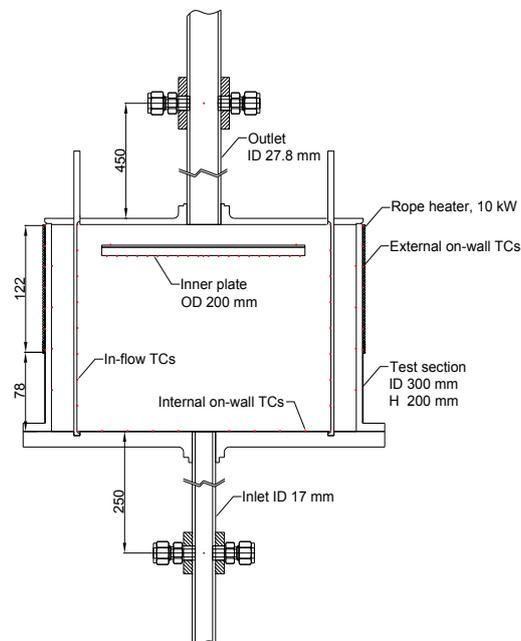
**Figure 1: Schematic view of the TALL-3D facility**



## 2.1. 3D test section

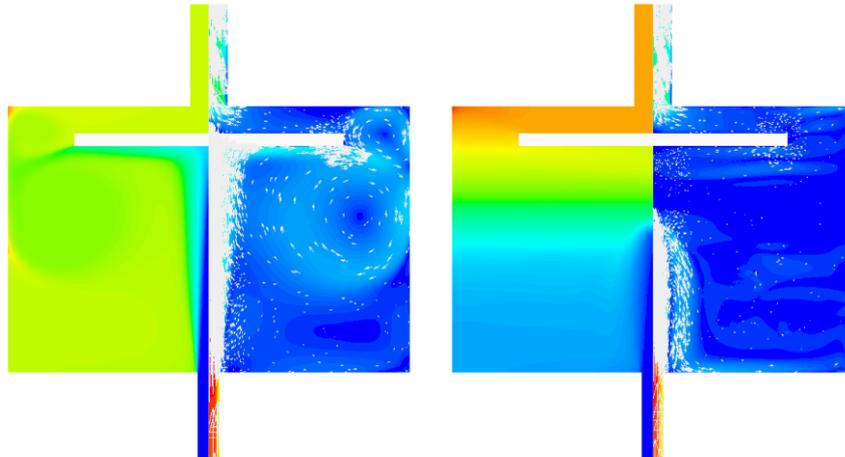
TALL-3D design incorporates a 3D test section to introduce flow conditions that cannot be properly captured by 1D STH codes. It is an axisymmetric cylindrical vessel with an outlet at the top and an inlet at the bottom. A 15 kW rope heater is installed at the upper part around the lateral wall. The heater is used to facilitate stratification development in the pool, and allows outlet flow temperatures of up to 500°C. The schematics of the test section are shown in Figure 2. Internal diameter and height of the test vessel are 300 and 200 mm respectively. A circular plate of 200 mm diameter is installed inside, orthogonal to the flow direction. The purpose of the plate is to reflect the upward LBE jet towards the walls of the vessel, thus enhancing mixing in the pool at high inlet mass flows. At low flows the jet does not penetrate all the way to the plate and stratified layer forms in the upper section of the pool. The temperature distribution is measured by thermocouples installed in-flow, and on internal and external walls of the test section.

**Figure 2: Schematics of the TALL-3D test section vessel**



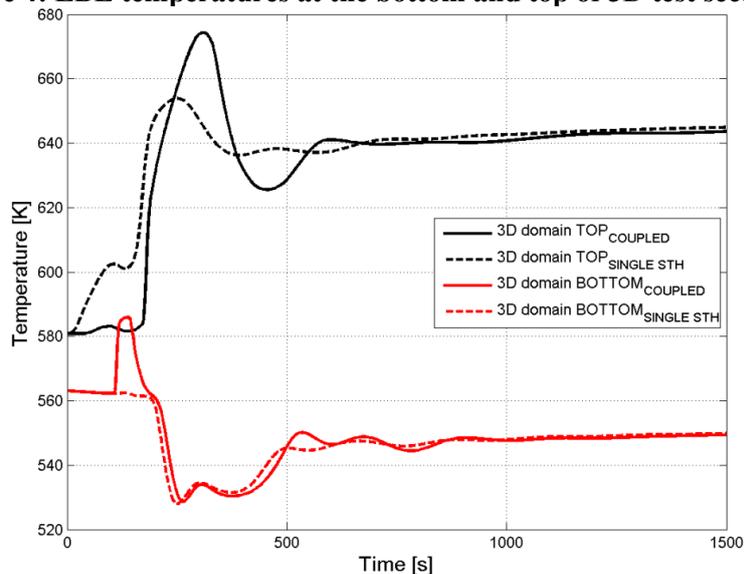
CFD analysis was performed in the 3D test section design process for choosing the proper inlet pipe diameter, test section height, heater power and geometry. The aim of the design is to ensure, that if the whole loop is close to instability in natural circulation conditions, the 3D test section would be the component responsible for 1D/3D feedbacks. Namely the pool should be mixed at high flow rates and stratified at low flow rates. The selection of parameters was done using the scaling analysis developed for buoyant jets in pool-like geometries [4]. The configuration was selected in such way that stratification is allowed to develop in the pool at flow rates up to 0.65 kg/s. Figure 3 shows the results of pre-test CDF modelling. The pool is mixed when the inlet mass flow rate is 1 kg/s and stratified when the inlet mass flow rate is 0.2 kg/s.

**Figure 3: CFD simulation results for the 3D test section. Temperature is shown on the left and velocity on the right of the pool for flow rate 1.0 kg/s and 0.2 kg/s**



The effects resulting from such 3D component introduction into the loop design were demonstrated in pre-test STH and coupled STH-CFD simulations of the TALL-3D facility. The presence of the test section causes non-linear interactions between 3D and 1D loop components, which result in oscillations, not properly resolved by single STH code, as shown in Figure 4.

**Figure 4: LBE temperatures at the bottom and top of 3D test section [2]**



### 3. SURROGATE MODEL DEVELOPMENT APPROACH

Surrogate Model (SM) is necessary when using original multi-dimensional high resolution codes becomes too computationally expensive. For example, a TALL-3D transient simulation using coupled STH-CFD approach takes several days of computing. Such approach is not suitable in the IDPSA methodology, where large numbers of calculations need to be run to identify failure domains and perform sensitivity and uncertainty analysis. Therefore we seek to develop a surrogate model to replace the CFD part in coupled calculations to decrease the computational time, and make the coupled calculation suitable for IDPSA.

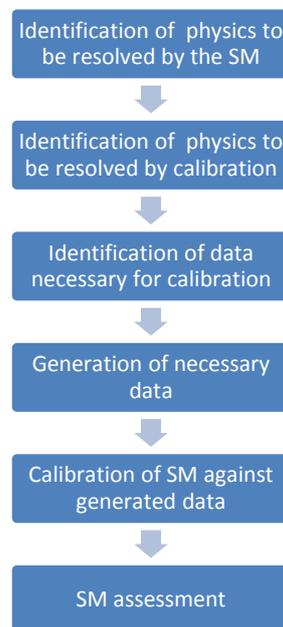
The aim of the SM is to reproduce only a limited set of results with acceptable accuracy, while disregarding the detailed modelling of the actual physical system, thus avoiding the direct

consideration of physical processes which would introduce complexity and increase computational effort (ex. solution of 3D conservation equations which leads to a CFD approach). However the SM needs to give better results than currently available models implemented in STH codes to resolve previously identified 3D effects. Thus the criterion of a successful SM development is to obtain a more accurate solution, than achievable by a single STH code, and achieve better computational performance compared to CFD or coupled STH-CFD approaches.

One of the more popular method for surrogate model development depends on an advanced approximation of a complex function which is represented by a database of full model solutions e.g. application Neural Networks (NN). However, this way no actual physics modelling is involved in the SM, and the procedure is essentially a fitting process. This approach requires large number of data calculated by the original model, so the actual gain in computational efficiency can even decline in the process of SM development and application. Furthermore, it results in a SM that cannot be assumed reliable outside of the domain of parameters covered in the database of the original model solutions, since no physical reasoning is applied to the extrapolation [5].

Our approach is to capture the most important physical phenomena in the surrogate model itself. Then, a process of calibration is applied to determine the parameters which represent the physical processes not directly modelled in the SM. Since a limited set of SM output results is desired, only few parameters need to be considered for calibration. These SM closures can be deduced by standard fitting procedures, or by more advanced application of Neural Networks. Therefore our goal is to seek for an intermediate approach in between a pure NN application and a pure analytical solution. The process can be summarized as shown in Figure 5. These steps form an iterative process, which is continued until the desired SM precision is reached.

**Figure 5: Surrogate model development procedure**



The SM should correctly reproduce the history of the system, so temporal evolution equations have to be solved explicitly. However the exchange rates in these equations are of local nature, and do not depend on history effects. Therefore they can be determined by applying empirical closures. In this work we develop the surrogate model based on pre-calculated CFD solutions. Currently an idealized CFD model is utilized, and no heat losses are considered. We believe that CFD application will give us the general form of closures, which will be later adjusted in accordance with the experimental results.

#### 4. DEVELOPMENT OF SM FOR TALL-3D

The ultimate goal of SM development for the TALL-3D test section is to couple the SM with a STH code to be used for IDPSA. The surrogate model will use the inlet mass flow, inlet temperature and pool heater power values to estimate outlet temperature of the 3D pool at given moment. This value will be used in turn in STH code in the same way as in STH-CFD coupling [2].

Four CDF transients were run to gather insight about the mixing and stratification phenomena (see Table 1). LBE temperature at the test section inlet and the test section heater power were kept constant at 425 K, and 5 kW respectively. The transition from fully mixed to fully stratified states was seen in CFD results in the decreasing mass flow rate transients, while the stratified pool was fully mixed in the increasing mass flow rate cases. The test section outlet temperature and total momentum values were monitored in CFD solution and analyzed.

**Table 1: Parameters of CFD transient cases run for mixing/stratification analysis**

Transient	Initial $\dot{m}$ (kg/s)	Final $\dot{m}$ (kg/s)	$d\dot{m}/dt$ (kg/s <sup>2</sup> )
1	1	0.2	-0.005
2	1	0.2	-0.1
3	0.2	1	0.005
4	0.2	1	0.1

The most straight-forward approach to evaluate the outlet temperature comes from a simple energy balance over the 3D test section. Assuming the LBE pool as a homogeneous control volume, the outlet temperature  $T$  can be calculated as follows:

$$\frac{d(mc_p T)}{dt} = \dot{m} \bar{c}_p (T_{in} - T) + \dot{Q}_h \quad (1)$$

Here  $m$  is the mass of LBE in the test section,  $\dot{m}$  is the mass flow,  $T_{in}$  is the inlet temperature,  $\dot{Q}_h$  is the heater power, and  $\bar{c}_p$  is the average isobaric specific heat, which can be evaluated as:

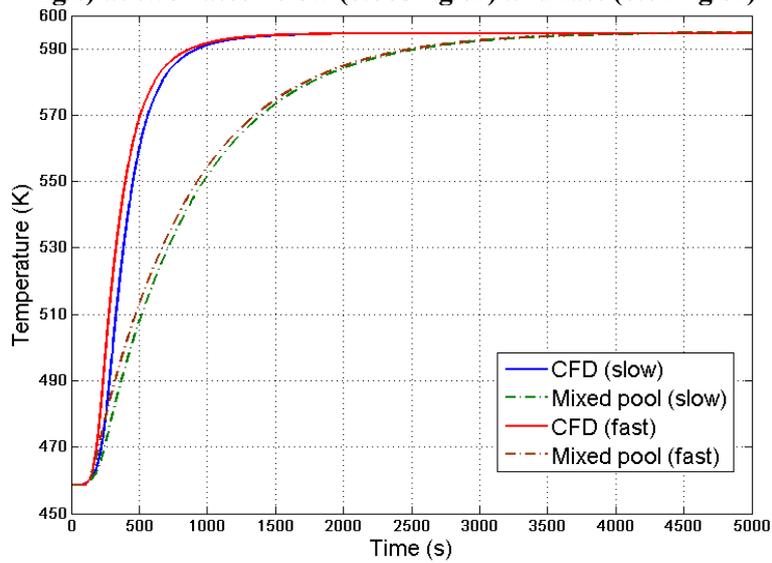
$$\bar{c}_p = \frac{1}{T - T_{in}} \int_{T_{in}}^T c_p dT' \quad (2)$$

where the isobaric specific heat correlation is given as [6]:

$$c_p = 159 - 2.72 \cdot 10^{-2} T + 7.12 \cdot 10^{-6} T^2 \quad (3)$$

Solving equation (1) gives good agreement with CFD simulation results when predicting steady state outlet temperature values. However, it fails to predict the transient behavior as shown in Figure 6, as expected. Such discrepancies are caused by 3D effects in the test section, namely the inlet jet – wall jet, and the inlet jet – stratified layer interactions. Therefore the 3D test section cannot be modelled as a homogeneous control volume.

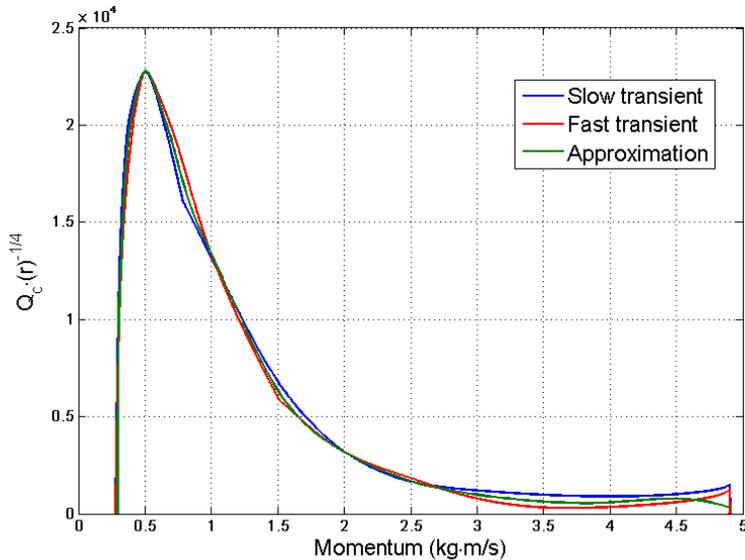
**Figure 6: Test section outlet temperature during decreasing mass flow transients (1 kg/s to 0.2 kg/s) at two rates - slow (0.005 kg/s<sup>2</sup>) and fast (0.01 kg/s<sup>2</sup>)**



Without going into detailed investigation of the 3D phenomena, the additional effects may be included in equation (1) by adding a “3D term”  $\dot{Q}_c$ , to account for the observed discrepancies:

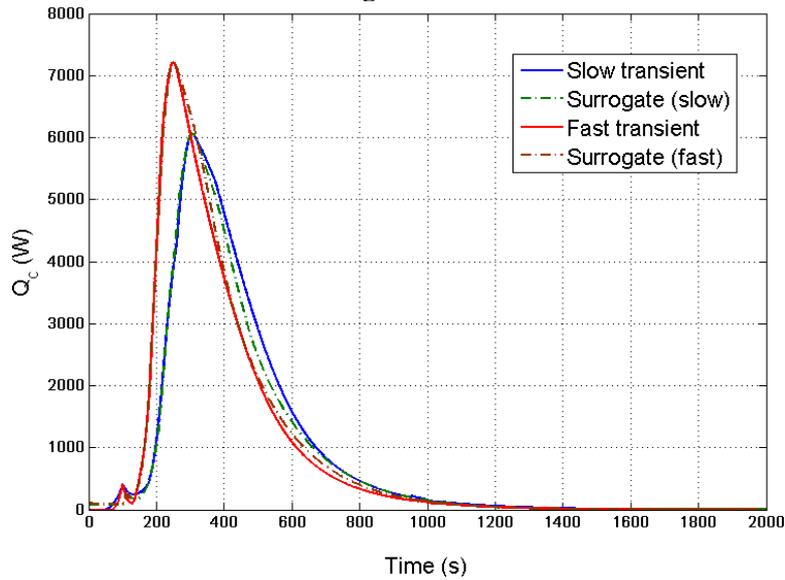
$$\frac{d(mc_p T)}{dt} = \dot{m}\bar{c}_p(T_{in} - T) + \dot{Q}_h + \dot{Q}_c \quad (4)$$

**Figure 7:  $\dot{Q}_c$  term correlation with total pool momentum for decreasing mass flow transient**



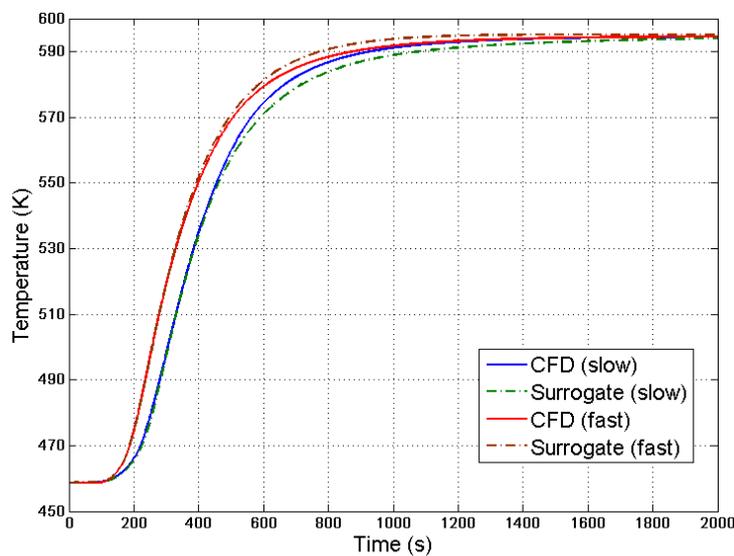
Taking the test section outlet temperature data from the CFD solution, the  $\dot{Q}_c$  term can be calculated directly from equation (4). The evolution of this term (adjusted for different rates of change of mass flow  $\dot{Q}_c r^{-1/4}$ ) during the decreasing mass flow transient (stratification development in the pool) was found to correlate with the instantaneous pool momentum values, as shown in Figure 7.

**Figure 8:  $\dot{Q}_c$  term as calculated by CFD and from the correlation with the total pool momentum for decreasing mass flow transient**



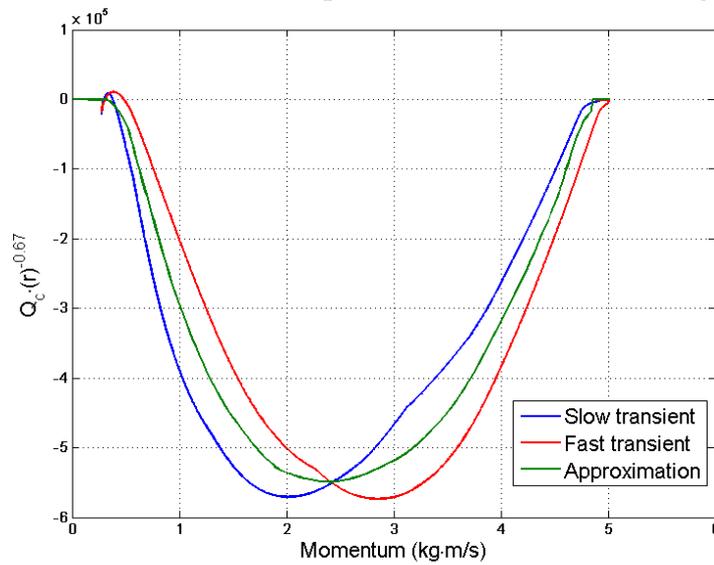
Here  $r$  denotes the rate of change of mass flow ( $dm/dt$ ). Approximating the observed trend, the  $\dot{Q}_c$  term evolution during the transient can be reproduced reasonably well, as shown in Figure 8. Substituting the reproduced  $\dot{Q}_c$  values back into eq. (4) a significant improvement over the mixed pool temperature prediction is achieved, as shown in Figure 9.

**Figure 9: Test section outlet temperature values calculated by CFD and by solving eq. (4) using the  $\dot{Q}_c$  approximation for decreasing mass flow transient**



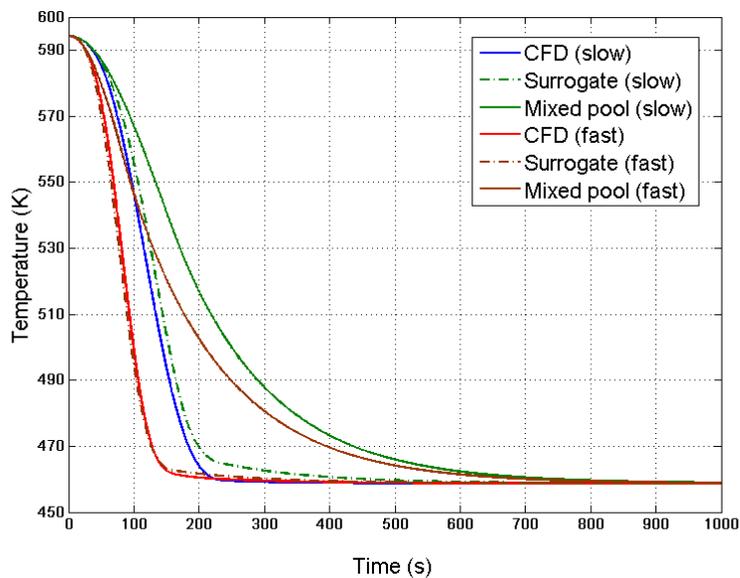
The same approach, however, does not yield a good correlation between  $\dot{Q}_c$  and pool momentum values during the increasing mass flow (mixing of the stratified pool) transient, as shown in Figure 10. The correction of the  $\dot{Q}_c$  term by  $r^{-0.67}$  allows matching the amplitude, but the pool momentum value at which the 3D effects have the highest influence seems to be dependent on the rate of change of mass flow (flow acceleration), contrary to what was found in the stratification development case.

**Figure 10:  $\dot{Q}_c$  term correlation with total pool momentum for increasing mass flow transient**



Roughly approximating the observed trend, and substituting the  $\dot{Q}_c$  values into eq. (4) results in temperature prediction as shown in Figure 11.

**Figure 11. Test section outlet temperature values calculated by CFD and by solving eq. (4) using the  $\dot{Q}_c$  approximation for increasing mass flow transient**



Better agreement could be achieved by directly interpolating the  $\dot{Q}_c$  values in the form as shown in Figure 10. This would require running CFD cases of limiting flow acceleration that could be expected in the TALL-3D loop. Furthermore, despite it was shown that 3D effects can be correlated with the pool momentum, the pool momentum itself must be calculated from the known inlet mass flow rate and flow acceleration values, for the surrogate model to be fully self-sufficient. Currently pool momentum values were taken directly from CFD calculations therefore the momentum modelling is still to be resolved. However, after identifying the relation between the 3D effects and the total pool momentum value, Neural Network approximation approach could be applied to link the  $\dot{Q}_c$  values with the pool momentum, and the pool momentum with the known parameters of LBE mass flow rate and flow acceleration.

## 6. CONCLUSION

We can conclude from the results shown in this paper that the 3D effects present in the TALL-3D test section pool can be correlated with the total momentum in the pool and that the test section outlet temperature can be predicted reasonably well in case of transient with mass flow decrease (stratification development), but further effort is needed to link pool momentum with inlet mass flow and flow acceleration. Also, further work including analysis of additional transients, confirmation of the stratification transient SM results as well as development of an approach for momentum prediction is foreseen.

## Acknowledgements

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