# PRE-TEST CFD SIMULATIONS ON TOPFLOW-PTS EXPERIMENTS WITH ANSYS CFX 12.0

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**Abstract**

Pressurized Thermal Shock (PTS) has been identified as one of the most important industrial needs related to nuclear reactor safety. The PTS analysis requires the simulation of the thermal mixing of cold Emergency Core Cooling (ECC) water injected to the cold leg and flowing to the downcomer with the hot coolant, which is present in the primary circuit. The simulation of single-phase and two-phase PTS situations including e.g. stratification of the flow and direct contact condensation is a challenge for CFD methods and requires careful validation against experimental data. In the frame of the NURISP project attempts are made to improve the CFD modelling for two-phase PTS situations. For this purpose, two reference cases with and without mass transfer due the condensation were defined, which are related to the TOPLOW-PTS experiments. The present paper focuses on numerical investigations of thermal mixing process in the cold leg and the downcomer using homogeneous and inhomogeneous models for the resolution of momentum equations. Numerical simulations were performed by using the commercial CFD code ANSYS CFX 12.0.

## 1. INTRODUCTION

Pressurized Thermal Shock (PTS) has been identified as one of the most important industrial needs related to nuclear reactor safety. The PTS analysis is required to assure the integrity of the Reactor Pressure Vessel (RPV) throughout the reactor life. One important part of this analysis is the thermal hydraulic analysis. The output of the thermal hydraulic analysis is the possible pressure and temperature fields experienced by the structural parts of the cold leg and especially of the RPV. Such data are applied as the input data for further structural analyses. Several scenarios that describe what could occur in Small Break Loss Of Coolant Accidents (SB-LOCA) result in an Emergency Core Cooling (ECC) water injection into the cold leg of a Pressurized Water Reactor (PWR). The cold water mixes there with the hot coolant, which is present in the primary circuit. The mixture flows to the downcomer where further mixing of the fluids takes place. Single-phase as well as two-phase PTS situations have to be considered. In case of two-phase PTS situations the water level in the RPV has dropped down to or below the height position of the cold leg nozzle, which leads to a partially filled or totally uncovered cold leg. Pressurized Thermal Shock implies the occurrence of thermal loads on the Reactor Pressure Vessel wall. In order to predict thermal gradients in the structural components of the Reactor Pressure Vessel (RPV) wall, knowledge of transient temperature distribution in the downcomer is needed. The prediction of the temperature distribution requires reliable Computational Fluid Dynamic simulations. The CFD models should be able to model the complex mixing processes taking place in the cold leg and the downcomer of the reactor pressure vessel (IAEA, 2001; Lucas et al., 2009a,b).

Although, there are a number of experiments available where flow phenomena are investigated as separate effects (see for instance Bonetto et al. (1993), Iguchi et al. (1998), Vallée et al. (2005), Lim et al. (1984), Ruile (1996)), there is still a need for well-instrumented experiments for validation and demonstration purposes, where experimental parameters are varied in order to investigate PTS phenomena. High resolution data are required in both space and time for the whole domain of interest. This should include local and time-dependent information on the interface between the phases, mean and fluctuations values for temperature and velocity. For this purpose, the TOPFLOW-PTS experimental program has been conceived. Its objective is to provide a well-informed experimental database for both the validation of CFD modelling of the two-phase flow in the cold leg and the downcomer and to improve the understanding of the key thermal hydraulic phenomena involved. The experimental program includes steady-state and transient tests with and without mass transfer due to condensation.

Currently available CFD tools are not able to simulate accurately all phenomena that occur in the cold leg and the downcomer during the ECC injection. Numerical simulations have already been performed with moderate success; see e.g. the contributions of Egorov (2004), Vallée (2005), Štrubelj et al. (2007) and Coste et al. (2008). In the frame of the EU project NURISP (Nuclear Reactor Integrated Simulation Project) attempts are made to improve the CFD modelling for two-phase PTS situations. For this purpose, two reference cases out of the TOPFLOW-PTS experimental programme were defined: one for steady air-water and one for steady steam-water flow. The NEPTUNE_CFD code (see Bestion et al. (2005)) as well as the ANSYS CFX (ANSYS CFX, 2009) and FLUENT (ANSYS Fluent, 2009) codes are used in the project for PTS investigations.

This paper presents the pre-test simulation results of TOPFLOW-PTS experiments by using CFD-code ANSYS CFX 12.0. The experiments are still yet to be carried out on the TOPFLOW-PTS test facility of the Forschungszentrum Dresden-Rossendorf. In the calculations, the effect of heat transfer between structures and fluid was not considered. The paper is divided in two parts. In the first part, physical models, computational domain, boundary and initial conditions, as well as numerical scheme are described. The discussion of the results will be described in the second part.

## 2. NUMERICAL SIMULATIONS

### 2.1 Mathematical Models

ANSYS CFX 12.0 has been used in order to perform pre-test simulations of two selected experiments: steady-state air/water test and steady-state steam/water test with mass transfer due to condensation. The two-phase flow can be simulated by using the homogeneous (one fluid model) or the inhomogeneous model. The homogeneous model means that a common flow field is shared by all fluids, as well as other relevant fields such as turbulence and temperature. In the inhomogeneous or two-fluid model each fluid has its own flow field and the fluids interact via interphase transfer terms. Interfacial transfers (momentum, heat and mass) are dependent on the contact surface area between the two phases. This is known as interfacial area density and it is defined by the interfacial area per unit volume. The choice between homogeneous or two-fluid model can be made on the transport equations for mass, momentum and energy, as well as the turbulence transport equations (ANSYS CFX, 2009).

In the present study, the influence of homogeneous and inhomogeneous models (as regards the resolution of momentum equation) on the temperature distribution in the cold leg and the downcomer is analyzed. Turbulence was modeled in both reference cases with homogeneous Shear Stress Transport (SST) model. This model is a combination of $k$-$\varepsilon$ and $k$-$\omega$ model and it is available with automatic wall functions. The choice of the turbulence model is taken on the basis of the personal experiences and the facts that the two-equation models offer a good compromise between complexity, accuracy and robustness (Menter, 2002). In the simulation of the air/water reference case, heat transfer was modeled by solving one energy equation for each fluid phase (homogeneous heat transfer model). For homogeneous heat transfer model, the interphase heat transfer coefficient is not modelled. It is chosen to be very large (ANSYS CFX, 2009). In the steam/water reference case steam was supposed to be isothermal. Only one energy equation for water was solved. For this reason, the use of inhomogeneous heat transfer model is needed.

Direct contact condensation (DCC) takes place in the ECC injection region of steam/water experiments and it also occurs at the free surfaces of the stratified flow. The essential closure law for DCC is the heat transfer coefficient between the liquid and the interface. Condensation phenomena depend on the turbulence in the liquid, where turbulent eddies transport the heat away from the interface. For this reason we chose to use a heat transfer correlation which is based on the surface renewal theory introduced by Hughes and Duffey (Hughes, 1991):

$$HTC_L = \frac{2}{\sqrt{\pi}} \rho_L c_{p,L} (a_L)^{1/2} \left( \frac{\varepsilon}{\mu_L / \rho_L} \right)^{1/4}, \quad (1)$$

where $\rho_L$ stands for liquid density, $c_{p,L}$ for liquid specific heat capacity at constant pressure, $a_L$ for liquid thermal diffusivity, $\mu_L$ for liquid viscosity and $\varepsilon$ for turbulence dissipation rate modeled with turbulence model.

A CFX built-in model called two resistance model has been chosen to define mass and heat transfers between the two phases. According to this model, the heat transfer processes on either side of the interface are considered separately by using two heat transfer coefficients, which are defined on each side of the interface. A zero resistance condition was set to specify heat transfer between the steam and the interface, i.e. the fluid specific heat transfer coefficient was assumed infinite. To describe phase change induced by interphase heat transfer, the ANSYS CFX thermal phase change model has been chosen. The mass flow between steam and water can be expressed, as follows:

$$m_{SL} = \frac{q_{IS} + q_{IL}}{L} \quad (2)$$

In eq. (2) $q_{IS}$ is the heat transfer between interface and steam, $q_{IL}$ the heat transfer between interface and liquid and $L$ the latent heat. The interphase mass source per unit volume was calculated by equation 3:

$$\Gamma = m_{SL} A, \quad (3)$$

where interfacial area density $A$ is calculated as $A = |\nabla \alpha|$.

## 2.2 Geometry and Mesh

The EDF CPY 900 MWe PWR was defined as the reference plant for the TOPFLOW-PTS test facility. The geometrical scale of the test facility is 1:2.5. The TOPFLOW-PTS test facility was designed in a way to simplify the configuration in order to allow better access for instrumentation and analysis of the results. According to the design of the test facility, the pump simulator, the cold leg with the ECC line, as well as the downcomer simulator were included to the CFD model (see Fig. 1). The geometrical model was generated using the CAD software Autodesk Inventor 2009.

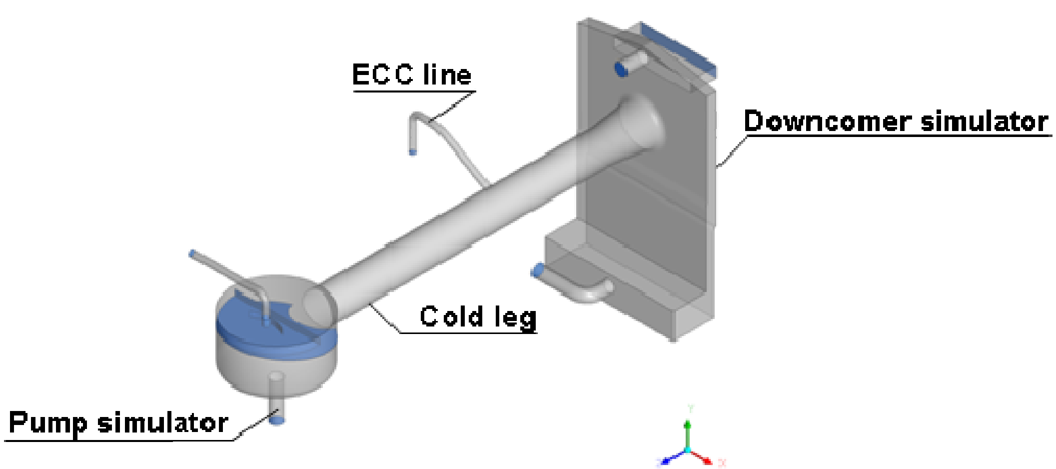


**Figure 1: CFD model of the TOPFLOW PTS test facility**

The computational mesh was generated with the ICEM CFD software. Hexa meshing was used for the whole computational domain. The mesh consisted of approximately 850,000 hexahedral elements. The averaged value of $Y^+$ was approx. 400. For the generation of the geometry and the mesh best practice guidelines were considered as far as was reasonable.

## 2.3 Boundary and Initial Conditions

**Air/Water Reference Case**:

The operating pressure in the corresponding experiment is 2.25 MPa. At this pressure the air density corresponds to the steam density at 5 MPa. In the simulation of the air/water reference case, the following boundary conditions were defined. The cold leg was 50% full of water. The mass flow rate of ECC injection, $M_{ECC}$, was 1.7 kg/s and the temperature of ECC water, $T_{ECC}$, was 40 °C (313.15 K). The mass flow rate, $M_{PS}$, and temperature, $T_{PS}$, of the pump simulator injection were 1 kg/ and 50 °C (323.15 K) respectively. All the injected water flow was withdrawn from the downcomer. The outlet water mass flow rate, $M_{DC}$, was equal to 2.7 kg/s. On the back side of the downcomer there is an opening connected to the ambient environment of the TOPFLOW vessel. An air temperature $T_{Air}$ of 44 °C (317.15 K) was set on that boundary.

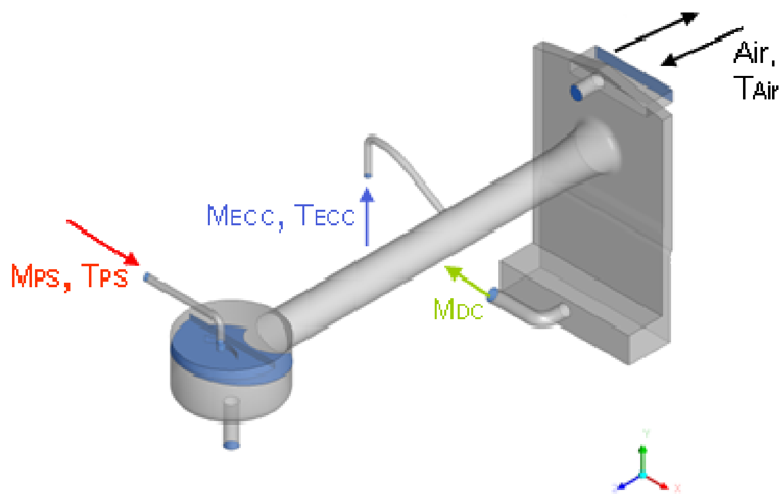


**Figure 2: Boundary and initial conditions for the air/water case**

The inlet boundaries were defined in the inlet leg to the pump simulator and in the ECC line. The outlet boundary was set in the outflow pipe at the bottom of the downcomer. The opening boundary was defined at the top of the back side of the downcomer. The boundary conditions given for the inlet boundaries were constant bulk mass flow rate, turbulence intensity (5%) and temperature. Bulk mass flow rate was set at the outlet boundary. A constant opening pressure, opening temperature and turbulence intensity (1%) were specified at the opening boundary. Due to the lack of the corresponding experimental data, the turbulence intensities at the inlet and opening boundaries were assumed on the basis of the personal experiences and the recommendations from the CFX User Manual.

A perfect mixed temperature was assumed as an initial temperature for the PTS simulator. This corresponds to a temperature of 44 °C (317.15 K). The pressure was initialised with the hydrostatic pressure. The simulation of the air/water reference test was performed with constant material properties of water and air. They are related to the temperature of 44 °C (317.15 K) and the pressure of 2.5 MPa.

**Steam/Water reference Case:**

The steam/water experiments will be carried out at a pressure of 5 MPa. The following boundary conditions were used in the pre-test simulation:

As in the case of the air-water simulation the cold leg was 50% full. The mass flow rate of ECC injection, $M_{ECC}$, was 1.7 kg/s and the temperature of ECC water, $T_{ECC}$, was 214 °C (487.15 K). The mass flow rate, $M_{PS\_in}$, and temperature, $T_{PS}$, of pump simulator injection were 1 kg/s and 263.95 °C (537.1 K), respectively. The outlet flow rate of the pump simulator, $M_{PS\_out}$, was 1 kg/s. These operating conditions were defined in the experimental test matrix in order to avoid condensation in the pump simulator. To maintain steady-state conditions, the water level in the cold leg must be kept constant. For this reason, the downcomer outlet flow rate, $M_{DC}$, was calculated as $M_{ECC}$ + $M_{Cond}$ ($M_{Cond}$=Total condensation rate). Saturated steam was supplied through a short pipe at the top of the front side of the downcomer. The steam in flow rate, $M_{Steam}$, was 0.4 kg/s. The surplus of steam left the downcomer through the opening, which is connected to the condenser. On that boundary the steam temperature was equal to the saturation temperature, which was 263.95 °C (537.1 K).

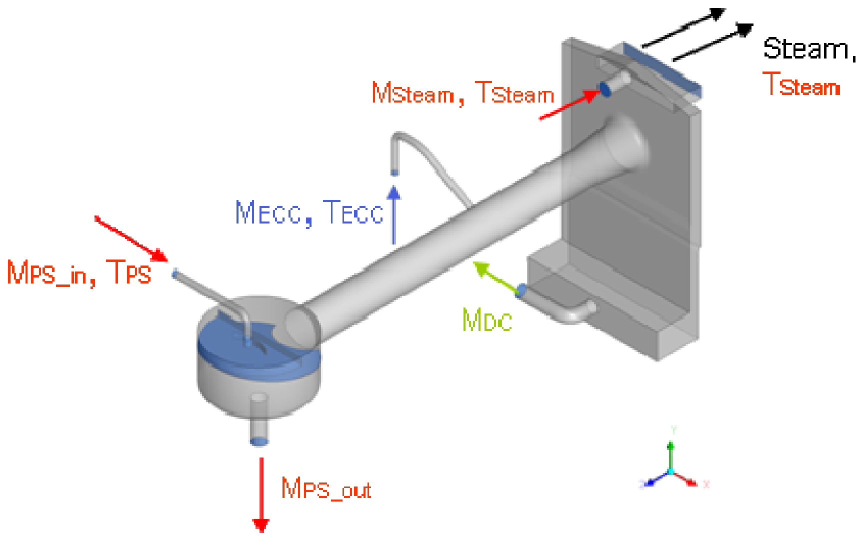


**Figure 3: Boundary and initial conditions for the steam/water case**

As an initial temperature, the saturation temperature was used. The pressure was initialised with the hydrostatic pressure. The properties of the steam and the water were assumed constant for the simulation.

The inlet boundaries were defined in the inlet leg to the pump simulator and in the ECC line. The outlet boundaries were set in the outflow pipes at the bottom of the pump simulator and the downcomer. The opening boundary was defined at the top of the back side of the downcomer. The boundary conditions given for the inlet boundaries were constant bulk mass flow rate, turbulence intensity (5%) and temperature. Bulk mass flow rate was set at both outlet boundaries. A constant opening pressure, opening temperature and turbulence intensity (1%) were specified at the opening boundary. Due to the lack of the corresponding experimental data, the turbulence intensities at the inlet and opening boundaries were assumed on the basis of the personal experiences and the recommendations from the CFX User Manual.

## 2.4 Numerical Scheme and Nodalization

ANSYS CFX is an element-based finite-volume method with first and second-order discretization schemes in space and time. It uses a coupled algebraic multigrid algorithm to solve linear systems arising from discretization. The discretization schemes and the multigrid solver are parallelized.

In both simulations the coupled volume fraction algorithm has been chosen. This option allows the implicit coupling of the discretised velocity, pressure and volume fraction equation in order to converge of calculations in fewer iteration loops. In the simulations shown below, the high-resolution discretization scheme was used to discretize the convective terms in the equations. A Second Order Backward Euler scheme was used to approximate the transient terms. A Root Mean Square (RMS) convergence criterion of 1 x $10^{-5}$ was used to ensure negligibly small iteration errors. The simulations were performed on the FZD LINUX cluster (Operating system: Linux Scientific 4.3 (64 bit), Node configuration: 2xAMD Opteron F

2220 (2.8 GHz, dual-core), 16 GB Memory). Three nodes (12 processors) were used for above mentioned transient simulations in a parallel mode with message passing protocol parallel virtual machine (PVM). The simulations took 2.5-3 months each to complete.

Quantification and separation of the error components (e.g. grid resolution, time step size, discretization method, physical models etc.) for complex 3D CFD calculations are difficult. Using finer grids, higher order discretization methods and smaller time step size can reduce discretization errors. In the current study, the simulations were performed according to the BPGs described by Menter (Menter, 2002).

## 3. RESULTS

In both reference cases transient simulations were performed. A steady-state was reached when RMS normalized values of the equation residuals became lower than $1 \times 10^{-5}$ and the fluctuations of the main physical variables (temperature, velocity, pressure etc.) at different locations in the cold leg and the downcomer were negligible. The result obtained by using homogeneous model was used as an input for the simulation with inhomogeneous model in order to save computational time.

Eight locations were selected in the cold leg and the downcomer, which present the local temperature distribution. The locations correspond to the positions of the thermocouples used in the cold leg and the downcomer (see Fig. 4). In the cold leg, the thermocouple lance LA1 is located upstream from the ECC injection point and the thermocouple lances LA2, LA4 and LA3 are located downstream from the ECC injection point. Thermocouples DCLA1, DCLA3, DCLA17 and DCLA20 are located in the downcomer.

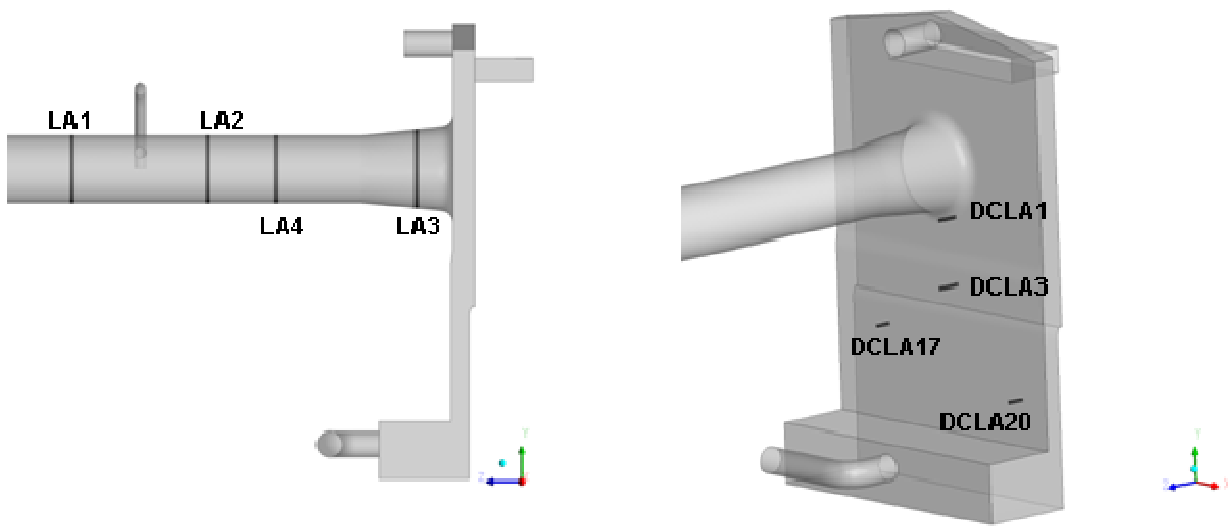


**Figure 4: Locations of the temperature profiles in the cold leg (left) and the downcomer (right)**

### 3.1 Air/Water Reference Case

**Cold Leg:**

The temperature profiles in the cold leg that were calculated for the air/water case by using both the homogeneous and inhomogeneous model are compared in Fig. 5. At LA1 (thermocouples upstream of the ECC injection), the homogeneous model predicted a considerably lower temperature gradient in the water than the inhomogeneous model. The largest temperature difference is on the bottom wall and it amounts to approximately 6 K. The air temperature predicted with homogeneous model is about approximately 2.5 K lower than it was estimated by the inhomogeneous model. At different locations in the ECC downstream direction, similar temperature profiles were obtained with both models. It is remarkable that with homogeneous model quite similar temperature profiles were calculated at the locations of thermocouples LA1 and LA2, while with two-fluid model two different temperature profiles were obtained. Downstream from the ECC injection point, the liquids are well mixed and the water temperature is approximately equal to perfect mixed temperature. It corresponds to a temperature of 44 °C (317.15 K).

Differences between both models are considerable in the area close to the ECC injection. Several causes could explain the reasons behind the variations. For example, different velocity fields were obtained by homogeneous and inhomogeneous models. Fig. 6 presents a cross-sectional contour plot of the liquid superficial velocity in the cold leg, which were obtained by using both models. The location of the plane corresponds to LA1 thermocouples. At the given location, there are two main fluxes where in one the water flows from the pump simulator to the downcomer (downstream) and in the second flux, the water flows to the pump simulator (upstream). Thus, the way the jet split differed according to the use of the homogeneous and the two-fluid model. Another explanation might be that the homogeneous model does not allow a slip velocity between the phases; therefore the entrained aspect of the phases could not be modelled.

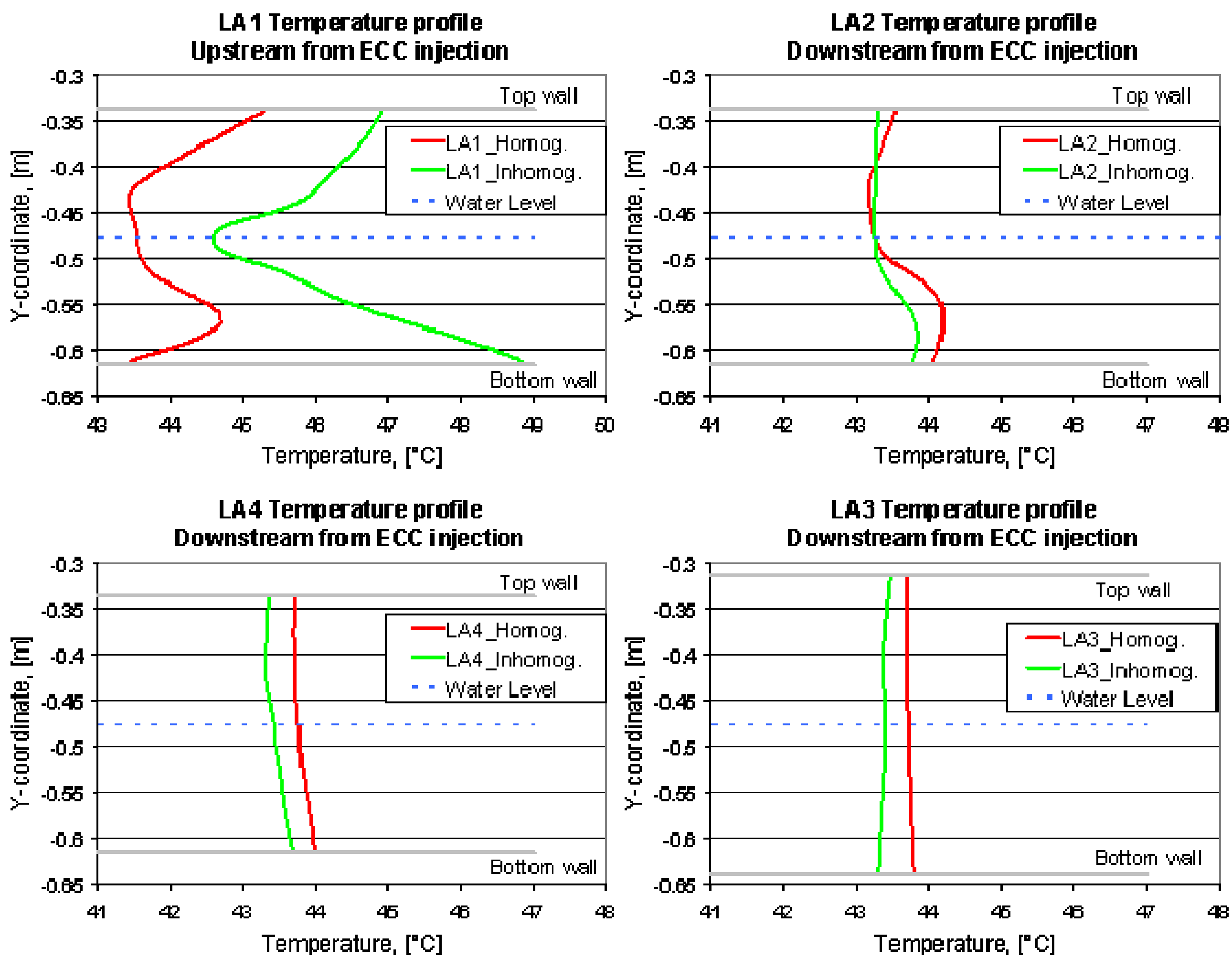


**Figure 5: Temperature profiles in the cold leg upstream and downstream from ECC injection point**

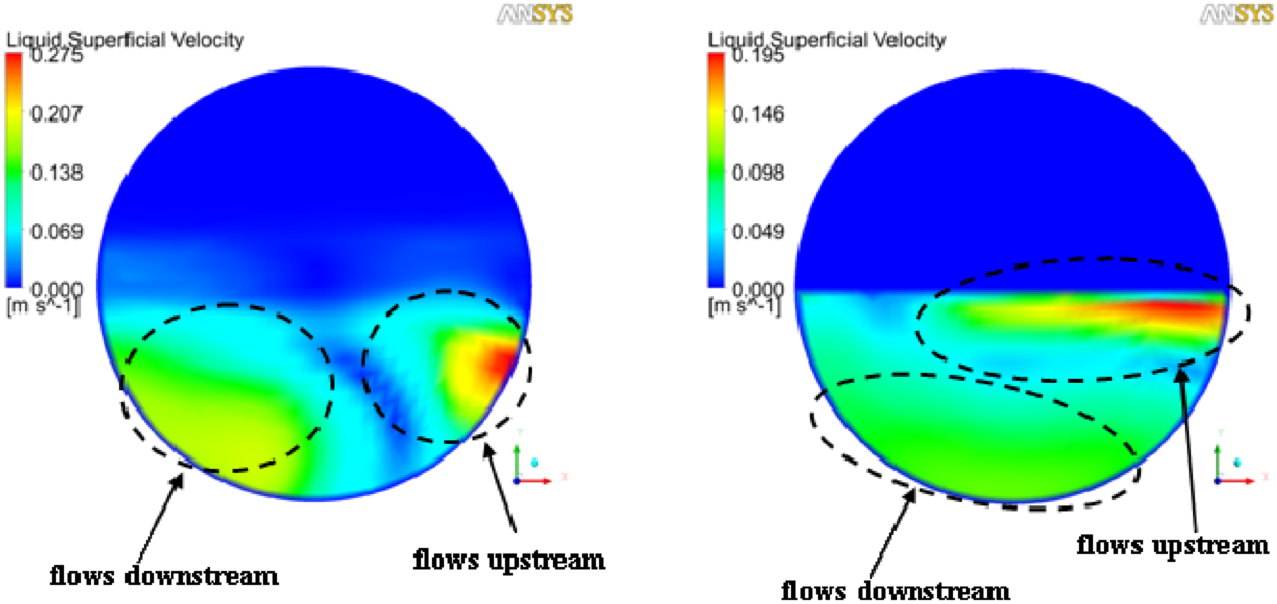


**Figure 6: Liquid superficial velocity in the whole cross-section of the cold leg (location of the plan corresponds to the location of TC LA1): left - homogeneous model, right - inhomogeneous model**

**Downcomer:**

Temperature profiles at the selected locations in the downcomer that were obtained by using homogeneous and inhomogeneous model are presented on Fig. 7. The points at Z = -0.01 m and 0.014 m are found on the back wall of the downcomer. The water temperature at all four locations is homogeneous and it is equal to perfect mixed temperature. Both the homogeneous and inhomogeneous models provided the same result; thus, it is expected that there will be no thermal stratification in the downcomer.

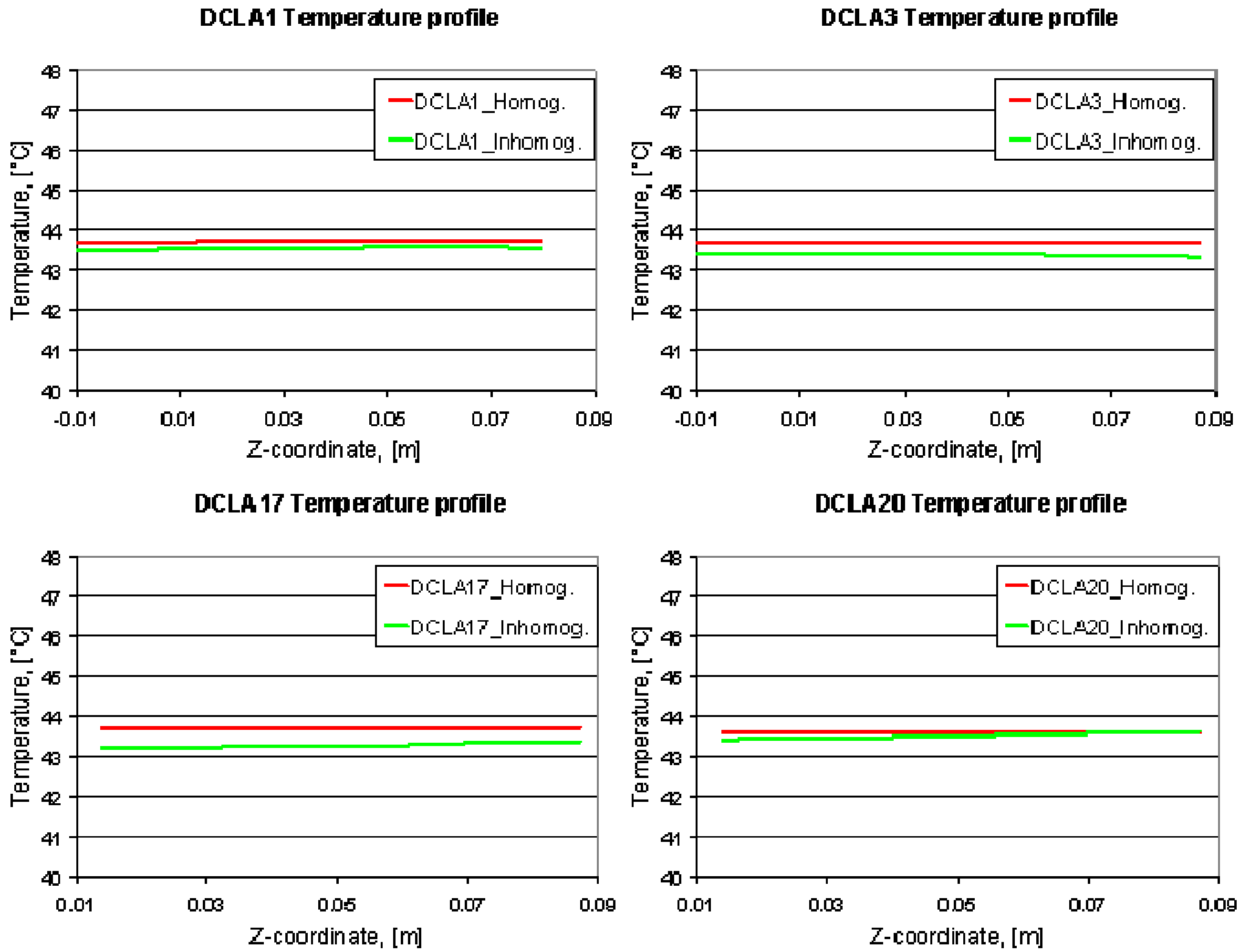


**Figure 7: Temperature profiles in the downcomer**

## 3.2 Steam/Water Reference Case

### Cold leg:

The temperature profiles in the cold leg that calculated for steam/water case by using both the homogeneous and inhomogeneous model are compared in Fig. 8. The locations of the temperature profiles are on the left hand side of Fig. 4. As in the case of the air/water simulation, the temperature profiles predicted by both models vary at the location of TC LA1. In case of homogeneous model a larger amount of ECC water was sent to the direction of the pump simulator (i.e. ECC upstream) than in case of inhomogeneous model. This can be recognized by a comparison of the bottom wall temperature of the cold leg in the area of the ECC injection (see Fig. 9). The temperature profiles in the downstream direction, calculated by both models, are quite identical. This can be explained by means of the fact that much larger condensation rates were predicted with inhomogeneous model. This is confirmed by the total (integral) condensation rate, which was 0.191 kg/s when using inhomogeneous model, while it was 0.166 kg/s in case of use of homogeneous model. These values of the total condensation rate were obtained in what was considered to have been a steady-state condition.

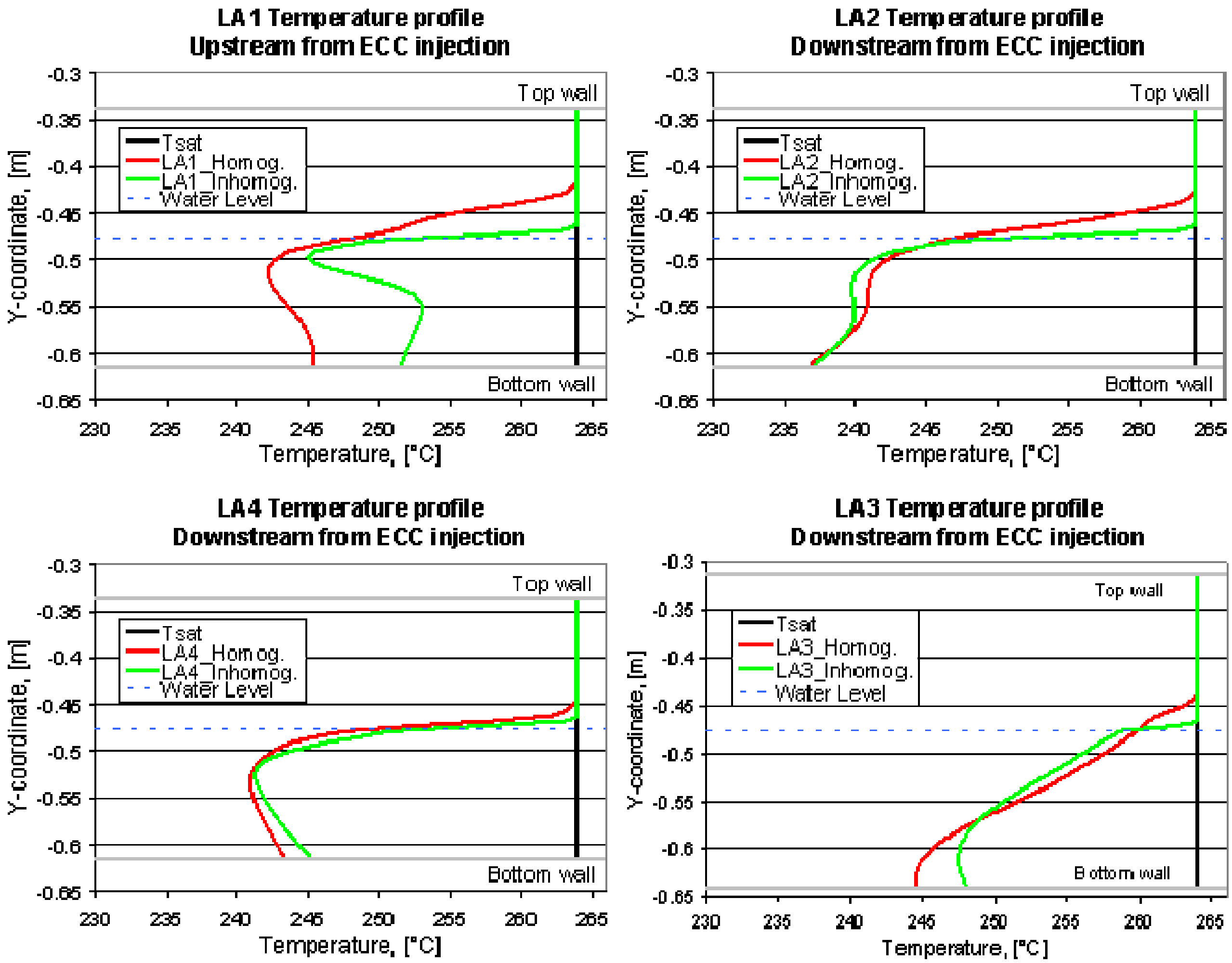


**Figure 8: Temperature profiles in the cold leg upstream and downstream from ECC injection point**

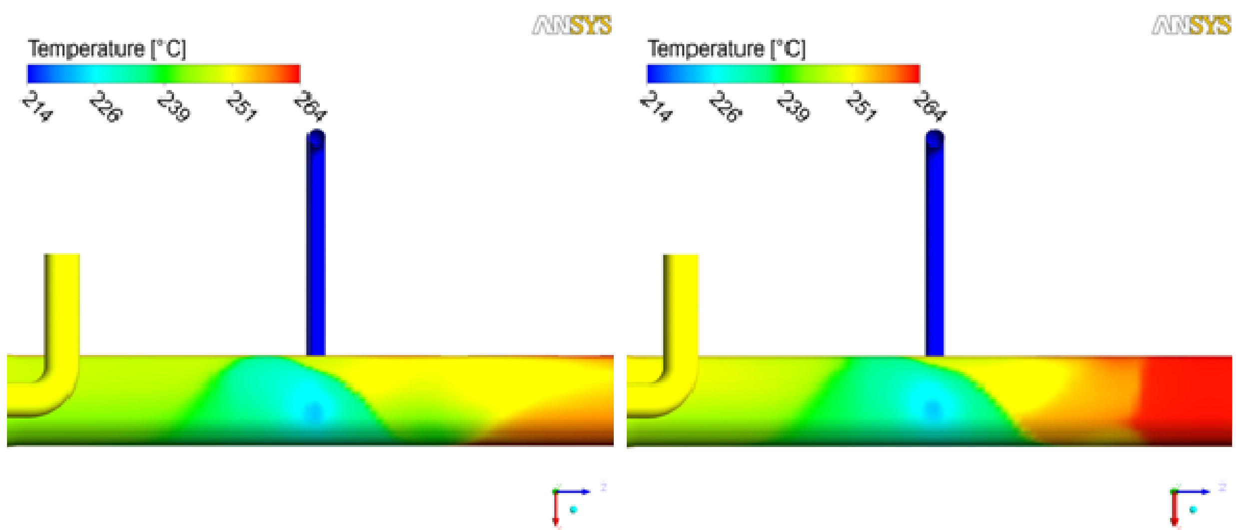


**Figure 9: Bottom wall temperature of the cold leg in ECC injection region: left - homogeneous model, right - inhomogeneous model**

Both models predicted thermal stratification in the cold leg at the entrance into the downcomer (see LA3 Temperature profile in Fig. 8), where the temperature difference in case of homogeneous and inhomogeneous model are approx. 19 K and 16 K, respectively.

**Downcomer:**

Temperature profiles at the selected locations (see the right hand side of Fig. 4) in the downcomer obtained by using homogeneous and inhomogeneous model are given in Fig. 10. The points with Z = -0.01 m and 0.014 m are found on the back wall of the downcomer.

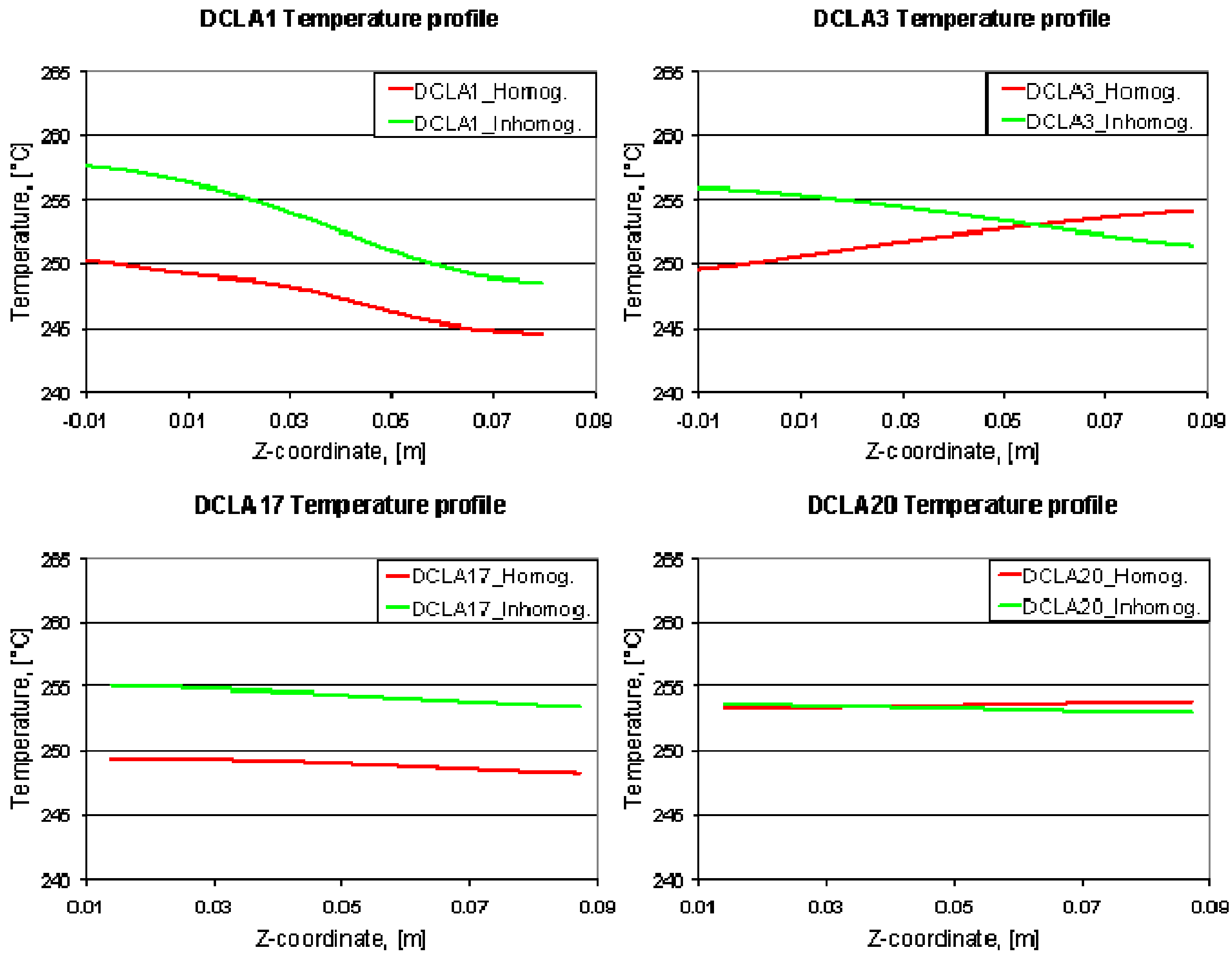


**Figure 10: Temperature profiles in the downcomer**

Based on the temperature profiles at DCLA1, DCLA3 and DCLA17, it can be observed that different results were obtained with both models. The temperature differences range is between 3 K and 8 K. The main reason for it is that both models predict different formations of the cold-water plume. In Fig. 11 we see a clearly separated, meandering plumes, which differ in the width and propagation direction. In case of homogeneous model the plume coming from the cold leg, it remains in the left part of the downcomer and flows down the side wall where it mixes with the ambient fluid. The mixing occurs in an area close to water tank at the bottom of the downcomer. The plume width is between 18 cm and 22 cm. In other case (Fig. 11, right) the plume remains mostly in the middle of the downcomer, flows vertically down. It has width, which varies between 27 cm and 33 cm. It then splits in two streams of relatively small width, which then propagate further in different directions. The lowest plume temperatures for homogeneous and two-fluid model are approximately 244 °C (517.15 K) and 247 °C (520.15 K), respectively.

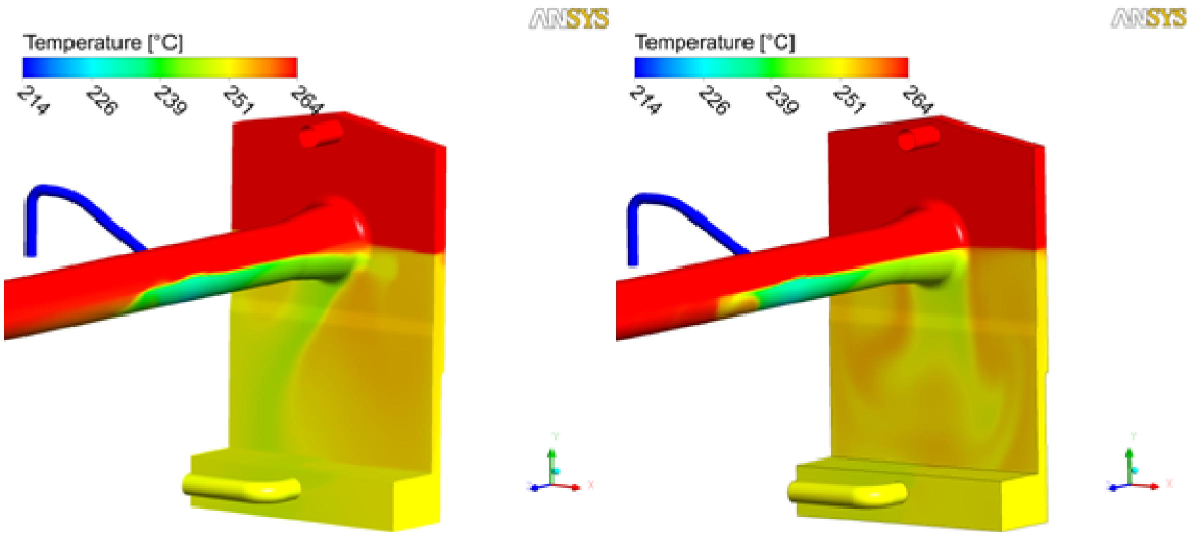


**Figure 11: Temperature of the front wall of the downcomer: left - homogeneous model, right - inhomogeneous model**

An accurate prediction of formation or lack of formation of the cold-water plume is essential for the further structural analyses and in general for the assessment of the safety aspects. Such a plume being in contact with the RPV wall for a long time cools it down. Since the cold-water plume has a relatively low temperature compared to the surrounding liquid, large thermal loads can occur on the RPV wall. The temperature difference observed in the simulation in the region of the plume is up to approximately 20 K. Note that such temperature differences in the simulation results need to be validated against the data that will be obtained from the equivalent experiments.

## 4. CONCLUSIONS

Pre-test numerical simulations of two steady-state reference tests (with air/water and steam/water) were performed by using the commercial CFD code ANSYS CFX 12.0. In the present study, the influence of homogeneous and two-fluid models of the temperature distribution in the cold leg and the downcomer was analyzed.

The simulations of the air/water reference case showed an inhomogeneous temperature distribution in the cold leg only upstream from ECC injection point. ECC downstream and at the entrance into the downcomer the homogeneous temperature due to completely mixing of the fluids was predicted, which corresponds to a temperature of approx. 44 °C (317.15 K). As a consequence of this, the temperature in the downcomer was also homogeneous and it is equal to the perfect mixed temperature. Homogeneous and inhomogeneous models provided very different results concerning the temperature distribution in the area close to the ECC injection due to different simulation of the splitting of the cold ECC water. In the simulation of the steam/water reference case we observed thermal stratification in the cold leg and the downcomer. Direct contact condensation, taking place in the cold leg and the downcomer was modelled using surface renewal theory introduced by Hughes and Duffey. The total condensation rate in the simulation with the inhomogeneous model was higher than in the simulation with the homogeneous model. The next important difference between the homogeneous and inhomogeneous model consisted in the prediction of the cold water plume formation and propagation in the downcomer. In the future work, the TOPFLOW-PTS experimental data will be used for the validation of the pre-test simulations described in this paper. Finally, it is noticed that due to the very high computational effort, the simulations with different grid sizes could not be performed.

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