

## **Unsteady single phase natural circulation flow mixing prediction using 3D thermal-hydraulic system and CFD codes**

Bousbia Salah, A.; Ceuca, S. C.; Puragliesi, R.; Mukin, R.; Grahn, A.; Kliem, S.;  
Vlassenbroeck, J.; Austregesilo, H.;

Originally published:

September 2018

**Nuclear Technology 203(2018), 293-314**

DOI: <https://doi.org/10.1080/00295450.2018.1461517>

Perma-Link to Publication Repository of HZDR:

<https://www.hzdr.de/publications/Publ-24415>

Release of the secondary publication  
on the basis of the German Copyright Law § 38 Section 4.

# Unsteady single phase natural circulation flow mixing prediction using 3D thermal-hydraulic system and CFD codes

A. Bousbia Salah<sup>1</sup>, S. C. Ceuca<sup>2</sup>, R. Puragliesi<sup>3</sup>, R. Mukin<sup>3</sup>, A. Grahn<sup>4</sup> S. Kliem<sup>4</sup>,  
J. Vlassenbroeck<sup>1</sup>, H. Austregesilo<sup>2</sup>

<sup>1</sup>Bel V (Subsidiary of the Belgian Federal Agency for Nuclear Control), Walcourtstraat 148, 1070 Brussels, Belgium

<sup>2</sup>GRS Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH, Boltzmannstr. 14, 85748 Garching, Germany

<sup>3</sup>PSI Paul Scherrer Institut, 5232 Villigen, Switzerland,

<sup>4</sup>Helmholtz-Zentrum Dresden-Rossendorf e. V., PO-Box 510119, 01314 Dresden

## **Abstract:**

Advanced 3D computational tools are increasingly used to simulate complex phenomena occurring during scenarii involving operational transients and accidents in nuclear power plants. Among these scenarios, one can mention the asymmetric coolant mixing under natural circulation flow regimes. This issue motivated some detailed experimental investigations carried out within the OECD/NEA PKL projects. The aim was, besides the assessment of the mixing phenomenon in the reactor pressure vessel, to provide experimental data for computer code validations and more specifically thermal-hydraulic system codes with 3D capabilities. In the current study, the ROCOM/PKL3T2.3 experimental test is assessed using on one hand thermal-hydraulic system codes with 3D capabilities, and on the other hand CFD computational tools. The results emphasize the capabilities and the differences between the considered computational tools as well as their suitability for such purposes.

## 1. Introduction

Mixing in the reactor pressure vessel (RPV) under single phase natural circulation flow is still challenging current computational tools. On one hand, there are thermal-hydraulic system codes such as ATHLET, CATHARE and TRACE endowed with 3D capabilities that describe the 3D macroscopic phenomena occurring at large scale geometries. On the other hand, there are computational fluid dynamic (CFD) codes such as STAR-CCM+ and ANSYS-CFX with 3D capabilities that describe the 3D microscopic phenomena occurring at small scale geometries. Therefore, in order to assess the capabilities of both approaches an OECD/NEA/PKL experiment carried out in the ROCOM test facility is considered. The ROCOM T2.3<sup>1</sup> test was carried out in order to assess the in-vessel flow mixing in and to derive conclusions about the cooling efficiency of the accumulators cold water injection of the Emergency Core Cooling system (ECCS). This test was generally considered to be suitable for CFD codes. However recent studies<sup>2-7</sup> emphasized the benefit and the capabilities of the 3D thermal-hydraulic system codes in predicting complex phenomena occurring in variety of experimental scenarios. For this purpose, three thermal-hydraulic system codes (CATHARE, ATHLET and TRACE) with 3D modelling features and two CFD codes (STAR-CCM+ and ANSYS CFX) are used. The objective is to assess and compare their prediction capabilities with respect to the experimental measurement. It was observed that, notwithstanding the numerical and modelling differences in the used approaches, similar prediction capabilities of the 3D thermal-hydraulic system codes and the CFD tools are obtained. However the discrepancies with respect to the experimental data are still quite high (around 25%). Additional investigations are needed to explain their origin.

## 2. ROCOM T2.3 test and facility description

The ROCOM test facility (see [Fig.1](#)) is a 1:5 scaled geometry mockup of a four-loop nuclear reactor RPV<sup>8, 8a</sup>. The facility was built in order to investigate the coolant mixing phenomenon in the RPV downcomer and the core inlet zones, as well as the thermal stratification phenomenon that may take place in the connecting legs. For this purpose advanced instrumentation that delivers high resolution measurement of the mixing phenomenon was installed. The downcomer sensors consist of two concentric grids at the inner and outer sides of the downcomer walls.

Each measurement plane consists of 64 azimuthal, and 29 measuring positions over the downcomer height (see Fig.1). On the other hand, the core inlet wire mesh sensor is equipped with 193 measurement points located at the entry position of each core assembly channel. In addition, temperature stratification can also be measured through sensors located in 216 measurement points distributed over the cold leg cross section<sup>8b</sup>.

The RPV of the ROCOM facility is filled with demineralized water at atmospheric temperature and pressure conditions. The desired water density can be changed by injecting an adequate amount of sugar or ethanol according to the test requirements. In this way the fluid relative density could be changed<sup>9</sup> from a value of 0.96 to 1.2.

The objective of this ROCOM T2.3 test was to investigate the effectiveness of an asymmetric emergency core cooling (ECC) system injection under low pressure conditions during the core heat-up phase. This is done by measuring the flow mixing in the downcomer and in the core lower plenum. At the start of the test (SOT), zero volumetric flow rate condition was set for all the four loops (see Table 1). The transient starts by injecting water with higher density (simulated by adding dissolved sugar) in loop-1 according to the flow rate history shown in Fig.2. This curve was obtained from a PKL test that addressed a decay heat removal system failure under mid-loop operation and cold shut-down conditions with ECC-injection from loop-1 accumulator<sup>1</sup>.

The mixing in the RPV downcomer and the core inlet plenum is then measured via the dedicated sensors according to the following formula:

$$MS(\theta_i, r_i, z_i, t_j) = \frac{\sigma(r_i, \theta_i, z_i, t_j) - \sigma_0}{\sigma_{ACCU} - \sigma_0}, \quad (1)$$

MS is the mixing scalar,  $\sigma_0$  is the sensors conductivity before SOT, and  $\sigma_{ACCU}$  is the electrical conductivity of the water slug.

The wire mesh sensors measure the instantaneous local water electric conductivity  $\sigma$  and derives the corresponding density difference with a measurement error<sup>8-9</sup> of 3.5%.

### 3. Computational tools

#### 3.1 Thermal-hydraulic system codes with 3D capabilities

The use of 3D thermal-hydraulic system computational tools for simulating complex in-vessel phenomena is particularly suitable for transients occurring at macroscopic scales inside the RPV without the need to use fixed mixing matrix coefficients.

### 3.1.1 CATHARE code

CATHARE-2/V2.5\_2/mod8.1 developed by CEA, EDF, AREVA, and IRSN<sup>10</sup> is a thermal-hydraulic system code that solves the conservation laws for water and steam for a wide variety of single and two-phase flow conditions. The code has 3D vessel component capabilities aimed at representing large scale 3D effects. The internals of the vessel are represented using the porous media approach. The equations are space averaged over the 3D mesh using the porosity P defined as the following:

$$P_v = \frac{V_{mesh} - V_{structures}}{V_{mesh}} = \frac{V_{fluid}}{V_{mesh}} \quad (2)$$

Where:

$V_{mesh}$  represents the 3D mesh volume.

$V_{structures}$  represents the volume occupied by the RPV structure inside the 3D mesh volume.

$V_{fluid}$  represents the volume occupied by fluid inside the 3D mesh volume.

The adopted CATHARE nodalization for the current study is a full 3D vessel model with boundary conditions imposed at the vessel loop leg connecting nozzles. The current ROCOM nodalization is built-up based upon a validated model used for simulating static ROCOM test conditions<sup>2</sup>. As shown in Fig.3, the vessel is divided using 12 radial, 32 azimuthal, and 40 axial nodes. The first 9 internal radial meshes are chosen to cover the sensor positions at the core inlet plenum. Two radial nodes were dedicated for the downcomer zone in order to simulate the inner and outer downcomer sensors. In the axial direction 29 meshes were chosen to cope with 29 axial wire mesh sensors. The remaining 11 axial nodes were chosen in order to get a good representability of the hemispherical downcomer shape using cartesian approach (see Fig.3).

In the azimuthal direction 32 nodes are chosen. In this configuration, each azimuthal node lumps two downcomer sensor positions. In addition each of the 8 RPV nozzles (cold and hot leg) connections are represented by 2 azimuthal nodes (see Fig.3).

### 3.1.2 ATHLET code

The German thermal-hydraulic system analysis code ATHLET 3.1A<sup>11</sup> (Analysis of Thermal-hydraulics of Leaks and Transients), is continuously developed by the Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) for the analysis of the whole spectrum of operational transients, design-basis accidents and beyond design-basis accidents without core degradation, anticipated in nuclear facilities, particularly for light water reactors<sup>3</sup>. The thermo-fluid-dynamic module is based on a two-fluid model with fully separated balance equations for liquid and vapour, while a five equation model with a mixture momentum equation and a full range drift-flux formulation for the calculation of the relative velocity between phases is also available.

ATHLET provides a classical one-dimensional flow model with a pseudo-multi-dimensional capabilities where the one-dimensional model equations are applied separately to each coordinate direction of a multidimensional numerical grid, and an enhanced model with a genuine multidimensional set of thermal-hydraulic conservation equations, for a better and a more realistic representation of the complex flow phenomena<sup>3</sup>. This approach comprises the three-dimensional momentum equations implemented in both Cartesian as well as cylindrical coordinates. A simplified description of the ATHLET's three flow models can be given in terms of the convective part of the phase separated liquid momentum balance equation, presented in equation (Eq.3), where the index *liq* stands for the liquid phase,  $\rho$  - the density,  $\mathbf{w}$  - the phase velocity vector and  $p$  - the pressure.

$$\rho_{liq} \frac{\partial}{\partial t} (\mathbf{w}_{liq}) + \rho_{liq} (\mathbf{w}_{liq} \cdot \nabla) \mathbf{w}_{liq} + grad(p) = \mathbf{RHS}_{liq} \quad (3)$$

The term labelled RHS comprises contributions due to external forces, fluid internal forces and phase change. The convective term, i.e. the second term on the left hand side of equation (Eq.3), can be modelled by the three different approaches in ATHLET as presented in Table 2.

A detailed description of the convective term discretisation for each of the flow modules and its implementation in the system analysis code can be found in ATHLET related documentations<sup>3</sup>.

For the simulation of the ROCOM experiment T2.3 the downcomer (DC) region of the RPV consisted of sixteen azimuthal distributed control volumes (CV) and an axial nodalization of thirteen nodes. The numerical grid of the lower plenum (LP) is composed of an inner and an outer part. The inner part contains two rings and one central region.

The outer part geometrically approximates the hemispherical shape of the vessel by elongating the DC grid. The curved outer grid facilitates the guidance of the flow from the DC to the lower part of the LP. Fig.4a shows a schematic representation of the multidimensional nodalization of the LP.

The sieve drum mounted in the LP of the ROCOM facility is modelled in ATHLET by an increase of the local form loss coefficient between the outer and the inner LP rings.

The complex geometrical set-up of the lower core plate was considered in the ATHLET model of the ROCOM facility. The core was divided into 33 parallel hydraulic channels arranged in two rings around the central channel. Each channel has an axial resolution of five computational cells. A schematic drawing of the 33 core channels with an exemplary assignment of the 193 fuel assemblies together with the sixteen azimuthal DC nodes, is presented in [Fig.4b](#).

The hereby employed nodalization follows the mesh strategy adopted by GRS for the simulation of large-scale PWR together with the newly developed multidimensional flow model applied in the RPV. The development of a ROCOM dedicated mesh with a very high spatial resolution is not the goal of this work, but rather to assess the capabilities of ATHLET and its multidimensional flow module for an asymmetrical flow transient within the RPV.

### **3.1.3 TRACE code**

The system code TRACE<sup>12</sup> (TRAC/RELAP Advanced Computational Engine) was developed by the U.S. Nuclear Regulatory Commission (NRC) to model thermal-hydraulic behavior during postulated accidents or operation conditions. It solves six field equations (conservation of mass, momentum and energy) for two-phase flow (liquid and vapor) in one and/or three dimensions together with one and/or two-dimensional heat conduction model for heat structures.

To address the coolant mixing phenomenon in the ROCOM facility a 3D vessel component of TRACE was used for the representation of the RPV. The discretization is based upon a nodalization having 12 axial, 5 radial and 24 azimuthal nodes (see [Fig.6](#)). It includes the downcomer, lower plenum, core, core outlet, upper plenum and RPV-inlet and outlet pipes. For each of the 3D-volume elements the main thermal-hydraulic parameters for each direction such as hydraulic diameter, flow area, heated diameter are derived from the detailed CAD model of the ROCOM facility. The cold and hot legs are modeled using PIPE components, and FILL and BREAK components are used to define the boundary conditions at the inlet and outlet sides respectively, (see [Fig.5](#)).

### 3.2 Computational Fluid Dynamics (CFD) codes

Computational fluid dynamics (CFD) codes are used to solve mass, momentum and energy conservation equations over a scale ranging from microscopic (smaller than the hydraulic diameter) to macroscopic dimensions. They contain empirical models for simulating turbulence, heat transfer, and multi-phase interactions. Nevertheless, they are typically suited to provide detailed information over a phenomenon in a narrow zone of a reactor system. They generally require millions of nodes and large computational time.

#### 3.2.1 STAR-CCM+

STAR-CCM+<sup>13</sup> solves for average mass, average momentum, average species transport equations and additional transport equations for turbulent quantities in each cell volume of the discretized three-dimensional domain using the state-of-the-art finite volume method. The continuous partial differential equations are spatially approximated using second-order accurate schemes: second-order upwind for the convective terms and second-order harmonic-average with cross-diffusion contribution for non-orthogonal meshes for the diffusive terms. Time discretization employs a second-order, semi-implicit method and the integration time-step is fixed to  $\Delta t = 0.005$  s. The production mesh is created with 11 subregions connected by the so-called internal non-conformal interfaces which allow to pass information from one sub-region to the neighboring one. Mesh convergence studies using steady-state solutions (corresponding to the maximum volumetric flow rate injected from the ECC system) have been performed before generating the production mesh to guarantee that the change of pressure drops and the change in total kinetic energy of the flow for the considered volume is below 4% between two consecutive spatial discretizations. The production mesh is made of 6,186,202 polyhedral cells (see Fig.7) and details for the five macro-regions, which the entire RPV domain is made of, are given in Table 3. The chosen closure models for the Reynolds stress tensor<sup>13</sup> are the realizable  $k - \epsilon$ , whereas the turbulent mass flux is approximated with the eddy-diffusivity hypothesis with turbulent Schmidt number  $Sc_t = 0.9$ . The density of the sugar-water mixture depends linearly on the sugar concentration, the molecular viscosity is treated as non-linear<sup>14-15</sup>. The Schmidt number of the mixture is set constant to  $Sc = 1.04$ . At solid surfaces no-slip condition is used for velocity. The inlet boundary condition is prescribed after deriving the velocity given in Fig.2 and assuming a flat velocity profile, whereas at the outlet, relative pressure is imposed. The initial condition in the RPV is a fluid at rest and only pure water is present in the domain. Finally an iterative algebraic multi-grid solver is used to solve the linear systems of equations with a tolerance of  $1.0^{-3}$ , while at each time step the non-normalized Root Mean Square (RMS) residuals are lower than  $1.0^{-5}$  using 10 iteration loops.



### 3.2.2 ANSYS-CFX Code

ANSYS-CFX<sup>16</sup> is a general purpose Computational Fluid Dynamics (CFD) software for three-dimensional problems. ANSYS-CFX is available for all major hardware platforms and operating systems. It is capable of simulating steady-state and transient problems, laminar and turbulent flows, heat transfer, buoyancy, and multiphase flow. It uses a coupled solver in which all hydrodynamic equations are solved as a single system. Simulations can be run in local parallel (multicore / multiprocessor computer) and distributed parallel (computer cluster) environments as well as using a combination thereof. Parallelization is achieved by partitioning the computational domain. In addition to the solver, ANSYS-CFX comprises a complete set of pre- and post-processing tools for problem set-up, including geometry and mesh generation, and data extraction and visualization of solution fields.

Fig.8 shows the computational domain of the ROCOM facility used in the present study. It is based on earlier calculations of ROCOM experiments<sup>17</sup> and on the CAD data of the facility. As compared to the CAD model, the primary loop pipes were shortened because they are either closed, or, as in the case of hot leg-1, sufficiently far away and downstream from the sensor locations. However, the cold leg-1 injection pipe is modelled. No other simplifications have been made in comparison to the original CAD model. Thus, the downcomer, the lower plenum, including the perforated drum, and upper plenum have been fully modelled as specified in the CAD data. Due to the geometric complexity of the lower plenum, its lower part up to the height of the perforated drum was meshed using tetrahedral cells, as can be seen in Fig.9. The remaining parts of the flow domain were nodalized using a block type (hexahedral) mesh. The overall number of cells amounts to 4,962,085 (2282229 tetras, 2679856 hexas).

Both non-conforming meshes are connected via a “Fluid Fluid” interface, at which interpolation of the solution fields is carried out during the simulation. The simulation uses the ANSYS-CFX “Shear Stress Transport” model of turbulence with automatic wall function and buoyancy induced turbulence, option “Production and Dissipation”, enabled. Buoyancy turbulence was also enabled due to the expected low flow velocities and the density difference between coolant and ECC water. The standard value “Medium (Intensity = 5%)” was used for the turbulence of the water injection.

The ‘‘High Resolution option’’ of CFX was chosen as the advection term differencing scheme. Time discretization of the transient problem was done using the Second Order Backward Euler differencing scheme, by definition a fully implicit time scheme. The simulation starts with an initial step of 0.001 s which was later dynamically adjusted to reach the chosen convergence criterion, a RMS residual target of 0.0001 within 10 coefficient loops. Since the CFD domain completely reproduces the geometry of the ROCOM vessel, no additional momentum sources, porous domains etc. have been introduced.

#### 4. Calculation Results

In order to simulate the ROCOM T2.3 test using the 3D thermal-hydraulic system codes, and also the ANSYS-CFX code, the experimental conditions were scaled as shown in Table 4 by preserving the dimensionless Froude number. This dimensionless number is generally used for scaling purposes under flow conditions dominated by gravitational rather than frictional forces<sup>8</sup>.

$$Fr = \sqrt{\frac{v^2 \rho}{gL \Delta\rho}} \quad (4)$$

This is achieved by keeping the experimental relative density ratio  $\Delta\rho/\rho$  since all the other parameters i.e. the velocity  $v$  and the length  $L$  do not change during the scaling process. Therefore the density of the injected water is 997.6 (kg/m<sup>3</sup>) where the chosen water density at ambient temperature is equal to 961.3 (kg/m<sup>3</sup>).

In this manner the experimental diluted sugar density difference variation is simulated using water density difference due to temperature changes. The comparative study is then carried out between the measured MS given by Eq.1 and the calculated MS derived by the following formula:

$$MS_{calculated}(r, \theta, z, t) = \frac{T_{RPV}(r, \theta, z, t) - T_{Loop2,3,4}}{(T_{Loop1} - T_{Loop2,3,4})} \quad (5)$$

where T is the water temperature.

## 4.1 Thermal-hydraulic system codes

The CATHARE, ATHLET and TRACE simulations were carried out for a transient period of 80 s. The calculation time step is imposed by the semi-implicit 3D Courant number limit solver scheme for the codes CATHARE, TRACE, while ATHLET uses a linearly implicit numerical scheme where the involved Jacobians are determined numerically using a higher order scheme obtained via an extrapolation scheme.

First, a comparative assessment focusing on a qualitative comparison for a series of chosen representative times during the transient course is presented in [Fig.10a](#), [Fig.10b](#) and [Fig.10c](#). The comparison concerns code predictions vs. experimental measurement data in the DC region of the RPV. As could be seen in [Fig.10](#), as soon as the denser liquid enters the DC region of the RPV it is transported azimuthally below the cold leg (CL) 1 inlet nozzle creating a plume stretching from CL2 to halfway between CL4.

A similar behaviour is predicted by both CATHARE and ATHLET except the fact that the simulated plume is slightly compacter in the case of the latter code (see [Fig.10](#) at  $t=9$ s). The denser liquid plume is then mainly flowing axially downwards in the LP, while two recirculation areas of denser liquid are created symmetrically to the CL1 inlet nozzle (see [Fig.10](#) at  $t=13$ s). CATHARE succeeds in predicting this particular behavior while predicting a more compact cold liquid plume flowing towards the LP of the RPV compared to the ATHLET results.

Owing to the lower azimuthal spreading predicted by ATHLET, the denser liquid reaches the LP of the RPV sooner than in the experiment. The TRACE results exhibit a compact plume form due to the limited axial node numbers.

When cold water reaches the bottom plane of the downcomer the MS started to decrease. At this point cold water started to penetrate to the RPV lower plenum and only after redistributing there, cold water returns to the downcomer and thus leads to an increase of the averaged MS in the downcomer.

Later on, one can observe that the codes predict well the phenomenology related to the formation and the establishment of the recirculation flow in the downcomer (see [Fig.10](#) at  $t=40$ s). The recirculation enhances the mixing of the descending plume with the surrounding media and leads to a progressive stratification in the downcomer (see [Fig.10](#) at  $t=40$ s).

At the core inlet, snapshots of the mixing as calculated by CATHARE code are shown in [Fig.11](#). At an early stage of the transient, the mixing front is visible in the peripheral channels close to the CL1 and CL4. Later on the mixing front reaches the core central zone. This propagation is well predicted by the CATHARE code.

However the code predicts more homogeneous mixing than the experimental one. In addition from the quantitative point of view the calculated MS remains lower than the measured one. As could be seen in Fig.10, darker color means the presence of lighter fluid compared to the experimental one. This could be better observed in the Fig.12 and Fig.13, which show the average and maximum MS in the entire DC and core lower plenum regions, respectively. Overall, the system codes predictions of the maximum and average MS in the downcomer are in reasonable agreement with the experimental data trends. However, they overestimate the coolant mixing by about 25% and thus underestimate the maximum and the average MS values. The same magnitude of the discrepancies was also observed under static ROCOM mixing experiments using the CATHARE<sup>2</sup> and TRACE<sup>6</sup> codes.

## 4.2 CFD code simulation results

### 4.2.1 STAR-CCM+

Unlike the thermal-hydraulic system codes which scaled the ROCOM T2.3 test conditions according to Table 4 scaling procedure, STAR-CCM+ allows simulating the real test conditions i.e. the mixing of pure water and water with diluted sugar solution under atmospheric conditions. Therefore the mixing scalar of the sugar-water mixture is given by the following formula:

$$MS(r_i, \theta_i, z_i, t_j) = \frac{C(r_i, \theta_i, z_i, t_j) - C_0}{C_{ACCU} - C_0}, \quad (6)$$

Where  $C(r_i, \theta_i, z_i, t_j)$  is the local concentration at the centroid of the cell  $i = 1, \dots, N$  at time  $t_j$ ,  $C_{ACCU}$  (kg/m<sup>3</sup>) is the concentration of sugar of the mixture injected from the ECC injection system and  $C_0 = 0$  (kg/m<sup>3</sup>) is the initial concentration of sugar in entire RPV volume.

The MS is calculated at the precise location of each wire-mesh sensor. The MS field in the downcomer is shown at four different times ( $t = 9, 13, 20, 40$  s) using the unwrapped view of the downcomer (outer section) as well as the map of the 193 channels of the core inlet (see snapshots in Fig.15 at  $t = 22, 26, 40, 80$  s).

In the downcomer the first appearance of the sugar-water mixture is delayed if compared to the experimental measurements. The first MS local maximum is reached at about  $t \approx 15$  s similarly as in the experiment (see Fig. 12a), however, the average value of the MS is significantly lower than in the ROCOM facility (see Fig 12b). From  $15 \leq t \leq 30$  s the solution seems to oscillate around a constant value. The MS oscillations are caused by the detachment of large eddies from the descending plume. After the eddies separates from the plume, they start to lose momentum while remaining in the zone covered by the sensors for longer time than the theoretical travel time of the undisturbed plume. As soon as these large eddies leave the sensor zone the spatial averaged MS decreases again until a new large structure is formed.

In the downcomer it is possible to follow the dynamics of two large structures that are formed after the impingement of the jet coming from CL1 on the core barrel and the formation of a downward plume that start to oscillate. As the time advances the large eddies mix with the downcomer water and diffuse in large areas. The plume instead does not diffuse in the same manner. Indeed its azimuthal width tends to decrease with the distance from the nozzle and the concentration, even if diminishes, remains rather high.

At the core inlet it is possible to recognize some presence of denser water only after  $t > 20$ s. In particular, the mixing front is visible in the peripheral channels close to the CL1 and CL4 (see Fig.15). This trend is also predicted by the thermal-hydraulic codes (see CATHARE snapshots in Fig.11). During the first part of the transient, the plume does not deviate from its downward motion path. This is mainly due to effect of the gravitational force that opposes resistance to the suction in core allowing only rather small deflections of the flow due to pressure (the core barrel however is an obstacle that can deviate the flow in the upward direction too).

On the other side of the RPV, since the large part of the vertical momentum has been already lost, the suction effect is dominant. Later in the transient this asymmetry will not be visible because of the stratification in the lower plenum and downcomer which will help in decreasing substantially the density difference between the plume and the surrounding fluid, i.e. diminishing the gravity force acting on the fluid.

From the quantitative point of view, STAR-CCM+ shows good prediction of the maximal value of the MS in the downcomer (see Fig.12a). The latter is significantly underestimated by all the considered thermal-hydraulic system codes. On the other hand the downcomer average MS throughout the transient is in close agreement with that predicted by the thermal hydraulic system codes considered (see Fig.12b). In Fig.13, the evolution of the spatial averaged MS at the core inlet region is shown. It can be seen that STAR-CCM+ shows a delayed arrival of the front of the denser mixture when compared to experiments and to the thermal-hydraulic system codes solutions (Better agreement with experimental data is obtained by the CATHARE, ATHLET and TRACE codes). The latter can be related to the used turbulence model. However, sensitivity to turbulence models goes beyond the scope of the present paper<sup>15</sup>.

#### 4.2.2 ANSYS-CFX

Unlike the STAR-CCM+ case, the ANSYS-CFX<sup>17</sup> evaluates the MS according to Eq. 5 and the scaling approach used by the thermal-hydraulic system codes (see Table 4). The MS values were extracted at the node positions of the wire-mesh conductivity measurement of the experimental facility. The simulation was run in local parallel mode on 36 AMD Opteron CPU cores (1.4 GHz) with the same number of domain partitions. The simulated problem time extended about 10 s beyond the transient time span. The total problem time of 88.7 s was accomplished after 5 days and 4:25 hours.

Fig.16 and Fig.17 show snapshots of the mixing scalar distribution in the unwrapped downcomer and in the core inlet level. Both figures put experimental and simulated results in direct comparison. Similarly to the STAR-CCM+ result, the maximum value of the MS in the downcomer is delayed as compared to the experiment (Fig.12a). For ANSYS-CFX this delay is somewhat larger than for STAR-CCM+ and the maximum values are lower. They are in the range of the system-code results. The MS map in Fig.17 clearly shows the time delay between the experimental and the simulated distributions in the downcomer. The simulation reproduces the separation of the main plume into two large eddy structures leading to the azimuthal dispersion of the injected water in loop-1. However, in the experiment, dispersion of the concentration front is much stronger than in the simulation. The fluctuations of the maximum MS value can be observed as in the STAR-CCM+ case (Fig. 12a).

The average MS trend is similar to the STAR-CCM+ and the thermal-hydraulic system codes curves up to  $t=20$  s, displaying a local maximum at  $t = 15$  s. After  $t = 20$  s, the average MS value of the ANSYS-CFX simulation starts to fall below the other curves (Fig. 12b).

As can be seen in Fig.13, while the CFD results show a similar qualitative behaviour, the ANSYS-CFX curve is somewhat closer to experimental curve than the STAR-CCM+ curve. Between  $t = 20$  s and  $t = 25$  s, the simulated average value of the MS is about the same as in the experiment, but starts to grow more slowly after this stage and approaches the ATHLET curve (Fig.13b). At later times of the transient, both CFD simulations tend to underestimate the mixing scalar. The distribution maps in Fig.17 show that the injected water reaches the peripheral zone of the core before its central part. While the peripheral channels are fed with injected water mostly under the effect of direct suction from the downcomer into the core, the central part is more affected by the plume reaching the inlet plane only after its reversal at the bottom of the lower plenum. In contrast to the experiment, the MS is more evenly distributed around the core circumference in the ANSYS-CFX simulation. In the experiment, the injected water from loop-1 first reaches the core at the opposite side between the loop-3 and 4 positions. However, the experimental inhomogeneous distribution at the core lower plenum diminishes at later stages of the transient. Also, the plotted distributions confirm the generally lower mixing scalar values observed in the simulation.

### **4.3 Qualitative and Quantitative assesment**

The simulation of the ROCOM T2.3 test were carried out using 3D themal-hydraulic system codes and CFD approches. All the considered computational tools provide more or less the similar results notwithstanding the differences in their numerical techniques.

Actually, a sensitivity assement on the impact of the nodalization scheme details of the 3D thermalhydraulic codes shows limited improvement as it is the case for the CATHARE code when the azimuthal node number is doubled (see Fig.18 and Fig.19 and Table 5).

On the other hand, as shown in Fig.13, the thermal-hydraulic system and CFD codes predictions of the maximum and the average MS in the core lower plenum. One can observe that both approaches underpredict the experimental data by more or less the same error (i.e. 25%). However, the thermal-hydraulic system codes overestimate the MS at the core inlet in the early part of the transient. This is not the case of the CFD predictions. Later, numerical diffusion smoothes out the MS in the system giving maximum and average values predictions lower than the experimental data. It can be also observed on Fig.13a that CFD codes show a delayed arrival of the cold plume at the core inlet zone when compared to experiments and to the thermal-hydraulic system codes solutions. This difference is related to the impact of the used turbulence model and also to the presence of local vortices that are not predicted by the coarse 3D thermal hydraulic solution. Nevertheless this does not impact significantly the quality of the predictions; the 3D thermal-hydraulic codes provide better predictions of the average value of the MS and the maximal value of the MS at the core inlet while the CFD codes provides better predictions of the maximal MS value in the downcomer.

On the other hand, when using the 3D thermal-hydraulic system code, limited CPU time and thousands of nodes are required to reach the same level of accuracy as the CFD codes..

Concerning the used scaling approach it seems that the scaling based on the conservation of the Froude number is justified for the current application since the calculated MS using (Eq.5) (based on equivalent fluid and equivalent density variation), by ATHLET, CATHARE, TRACE and ANSYS-CFX and using (Eq.6) (based on real fluid and density variation) by STAR-CCM+ provides practically the same results and discrepancy with respect to experimental data.

On the other hand, the observed discrepancies seem to be mainly due to measurement uncertainty even though contradictory results are observed. On one hand good prediction of the maximal value of the MS is predicted by STAR-CCM+ (see Fig.12a) but less accuracy is observed for the average value of the MS (Fig.12b). Indeed, the sensors measure the water conductivity with an uncertainty of 3.5%. This thermal conductivity is afterwards translated into density difference. This could induce a source of error since a density variation of 1.0% may lead to a temperature difference of about 10 K.



## **5. Conclusion**

In the current study, 3D thermal-hydraulic system and CFD codes features are assessed against the ROCOM/PKL-3T2.3 test. The pursued goal was to evaluate and compare different codes having different numerical approaches in predicting the in-vessel mixing phenomenon under asymmetric single phase natural circulation flow regime. In general, it was observed that the main phenomena occurring during the experiment are well reproduced by all the considered codes. It is also worth to notice that the 3D thermal-hydraulic system and CFD codes provide similar prediction results. This could be explained by the fact that the ROCOM T2.3 experiment was carried out under conditions in which the gravitational motion of the descending plume and the establishment of large mixing recirculation vortices in the downcomer is governed by macroscopic phenomena taking place in a relatively large scale geometry. However, from the quantitative point of view additional investigation and developmental work should be done in order to improve their prediction capabilities.

Finally, the outcomes of the current study confirm the capabilities of 3D thermal-hydraulic system and CFD codes in simulating the mixing phenomena occurring under natural circulation flow regimes at the RPV scale.

## **ACKNOWLEDGMENTS**

This paper contains findings that were produced within the OECD/NEA PKL-3 projects. The authors are grateful to the PKL-3 MB members and more particularly to the ROCOM test facility team at Helmholtz Zentrum Dresden-Rossendorf (HZDR).

The development and the assessment of ATHLET are sponsored by the German Federal Ministry for Economic Affairs and Energy.

The STAR-CCM+ and TRACE analyses were partly founded by the Swiss Federal Nuclear Safety Inspectorate ENSI within the framework of the STARS project (<http://stars.web.psi.ch>).

## **NOMENCLATURE**

3D – Three dimensional

CFD - Computational fluid dynamic

DC - Downcomer

CL – Cold leg

HL – Hot leg

LP – Lower plenum

MS – Mixing scalar

RPV – Reactor pressure vessel



## References

- [1] S. KLIEM, R. FRANZ, OECD PKL3 Project – Final report on the ROCOM tests. HZDR\FWO\2016\01, (2016)..
- [2] A. BOUSBIA SALAH, J. VLASSEN BROECK, Assessment of the CATHARE 3D capabilities in predicting the temperature mixing under asymmetric buoyant driven flow conditions, Nucl. Eng. Des, 265, 469, (2013).
- [3] P-J. SCHOEFFEL, H-V. HRISTOV, G. LERCHL, Towards Multidimensional Thermalhydraulic Simulations with the System Code ATHLET - Proceedings of 45th Annual Meeting on Nuclear Technology 6 - 8 May 2014, Frankfurt am Main, Germany, (2014).
- [4] P. MAZGAJ, J-L. VACHER, Comparison of CATHARE results with the experimental results of cold leg intermediate break LOCA obtained during ROSA-2/LSTF Test 7, Proceedings of ICAPP 2015 May 03-06, Nice, France, (2015).
- [5] S. CARNEVALI, P. BAZIN, Validation of CATHARE code on the 3D ROSA-LSTF pressure vessel, NURETH-16 August 30-September 4, 2015, Hyatt Regency Chicago, USA, (2015).
- [6] J. KURKI, Modelling of ROCOM mixing Test 2.2 with TRACE v5.0 Patch 3, NUREG/IA-0454, (2015).
- [7] P. PANDAZIS, S-C. CEUCA, P-J. SCHOEFFEL, H-V. HRISTOV, Investigation of the multidimensional flow mixing phenomena in the reactor pressuriser vessel with the system code ATHLET - Proceedings of NURETH-16 August 30-September 4, 2015, Chicago, USA, (2015).
- [8] S. KLIEM, R. FRANZ, OECD PKL2 Project – Final report on the ROCOM tests. HZD\FWO\2012\03, (2012).
- [8a] R. HERTLEIN, K. UMMINGER, S. KLIEM, H.-M. PRASSER, T. HOEHNE, F-P. WEISS, Experimental and numerical investigation of boron dilution transients in pressurized water reactors“, Nucl. Technology, 141, 88, (2003).
- [8b] S. KLIEM, H.-M. PRASSER, T. SUEHNEL, F-P. WEISS, A. HANSEN, Experimental determination of the boron concentration distribution in the primary circuit of a PWR after a postulated cold leg small break loss-of-coolant-accident with cold leg safety injection, Nucl. Eng. Des, 238, 1788, (2008).
- [9] U. ROHDE, T. HOEHNE, S. KLIEM, B. HEMSTROEM, Fluid mixing and flow distribution in the reactor circuit - Computational fluid dynamics code validation. Nucl. Eng. Des., 237, 1639, (2007).
- [10] G. LAVIALLE, CATHARE2\_V2.5\_2mod8.1, EN/CAD/DER/SSTH/LDLD/EM/NT/ 2010-033/A, (2010).

- [11] H. AUSTREGESILO, C. BALS, A. HORA, G. LERCHL, P. ROMSTEDT , P. SCHÖFFEL, D. VON DER CRON, F. WEYERMANN, ATHLET Mod 3.1 Cycle A - Models and Methods, Gesellschaft für Anlagen und Reaktorsicherheit (GRS) mbH, GRS-P-1, Vol. 4, Rev. 4, (2016).
- [12] USNRC, "TRACE V5.0 Theory manual," US NRC, (2010).
- [13] CD-Adapco, USER GUIDE STAR-CCM+ Version 9.06, (2013).
- [14] R. PURAGLIESI, O. ZERKAK, A. PAUTZ, Assessment of CFD URANS models for buoyancy driven mixing flows based on ROCOM experiments, Proceedings of Int. Top. Meetg. Nuclear Thermal-Hydraulics, Operation and Safety, NUTHOS-10 2014 Dec. 14-18, Okinawa Japan, (2014).
- [15] R. PURAGLIESI, O. ZERKAK, A. PAUTZ, Influence of URANS turbulence models on in-vessel flow mixing during cold leg accumulator injection, Proceedings of Int. Top. Meetg. Nuclear Thermal-Hydraulics, Operation and Safety, NUTHOS-11 2016 Oct. 9-13, Gyeongju South Korea, (2016).
- [16] ANSYS CFX web page: <<http://www.ansys.com/products/fluid-dynamics/cfx/>>.
- [17] T. HOEHNE, S. KLIEM, U. ROHDE, F-P. WEISS, Buoyancy driven coolant mixing studies of natural circulation flows at the ROCOM test facility using ANSYS CFX, Nucl. Eng. Des, 238(8), 1987, (2008).