

CATHARE-TRANSAT COUPLING FOR THE PREDICTION OF BORON DILUTION IN THE ROCOM TEST FACILITY

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Abstract

This contribution aims to introduce a coupled CFD/system code approach for the simulation of single and multiphase thermal-hydraulics flows in complex component-scale (mesoscale) configurations. The co-simulation approach involves the multiphase CFD code TransAT and the safety analysis system code CATHARE. It is tested against data from the Rossendorf Coolant Mixing Model (ROCOM), an experiment performed to benchmark the phenomena associated with boron dilution in PWRs, including most important details for coolant mixing.

The CFD simulations with TransAT allow capturing the details of the 3D flow in the RPV while CATHARE provides the correct boundary conditions for the velocities and boron concentrations. A semi-implicit coupling scheme ensures continuity of the fluxes and pressure fields. The implementation was validated on basic test problems, including the double T-junction mixing problem of Bertolotto et al. (*Annals of Nuclear Energy*, 36, 2009). The results compared favorably with those obtained with a coupled CFX—TRACE code.

Keywords: CFD, system code, coupling, boron, co-simulation, ROCOM

1 INTRODUCTION

There is a clear incentive in coupling between simulation tools, when each is suited for a specific task but none is sufficient to address the whole problem. The complementary capabilities between CFD and system codes have long been advocated in the context of nuclear accident scenarios studies, in particular when 3D flows, mixing or phase-change play an important role.

This contribution is an effort to use the multiphase CFD code TransAT, developed by ASCOMP, concurrently with the Plant system code Cathare, developed by CEA. The goal of this work is to demonstrate that the coupled system of TransAT and Cathare can be used to simulate boron mixing in the RPV, as in ROCOM benchmark test case [1].

In the approach presented here, the flow system could involve one or two fluids, convective and conductive heat transfer in solids, and phase-change heat transfer. The CFD approach is based on the so-called Immersed Surfaces Technology (IST), whereby solid bodies contained in the system are defined using a solid level set function to describe their surfaces, transcending conventional unstructured and body-fitted grids (BFC). In a typical two-phase flow, the material properties of the fluids and the solid are segregated based on the gas-liquid and solid Level-Set functions. The technique helps solve conjugate heat transfer problems without resorting to explicit gas-liquid and fluid-solid jump conditions. The strategy used for the thermal-hydraulic coupling is described in Section 2. We then present results from two validation studies, with data from the ROCOM test facility in Section 3 and with data from a double T-junction test case in Section 4. The outlook and future works are discussed in Section 5.

2 COUPLING STRATEGY

This section discusses the development, implementation and testing of a coupling technique that provides the flexibility of the generic coupling paradigm and the numerical stability of a semi-implicit numerical scheme.

There are several criteria that need to be considered in the development of a hydrodynamic coupling paradigm. The most important criterion is that the methodology must conserve mass and energy. A desirable feature of the coupling algorithm is that the coupled code system should not be characterized by more restrictive stability limits than any of its constitutive programs.

When the computational cost of a complete CFD simulation is too large, a coupling strategy may be advantageous. The computational domain is split and only the regions that require a full 3D description are simulated with a CFD code. In the remaining parts of the domain the simulation is performed with the less computationally expensive system code.

In the case where both codes are mass conservative, the conservation of mass for the coupled simulation depends on the continuity of the mass flux across the coupling boundary. This means that the mass fluxes computed on either sides of the coupling boundary have to be equal. Similarly conservation of energy requires continuity of the heat flux across the coupling boundary. Continuity of the pressure field results from a force balance on the coupling boundary. Based on the Thesis of Pagan [3], the thermal-hydraulic coupling is achieved by exchanging mass flow rate and pressure at the coupling interface between TransAT and Cathare:

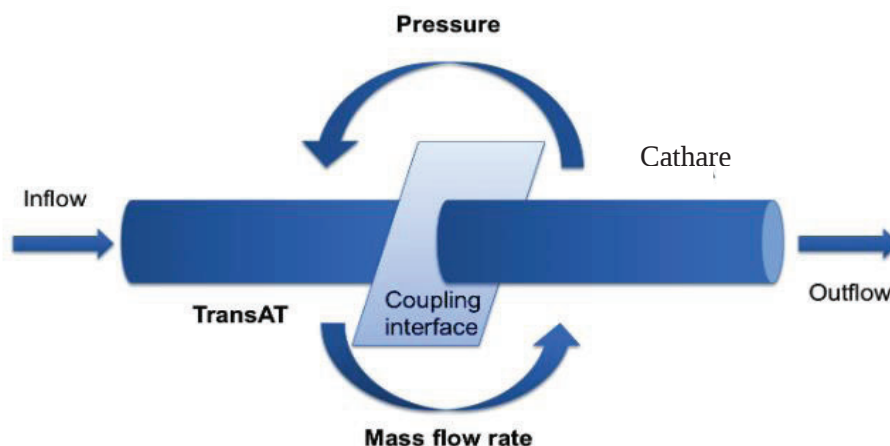


Figure 1: data exchange between TransAT and Cathare

In the examples below, TransAT has been chosen as the code to simulate the upstream part of the domain with respect to the coupling interface, whereas Cathare simulates the downstream part. This can be considered the simplest setup in relation to the variables exchanged, i.e. the mass flow rate from TransAT to Cathare, and the pressure from Cathare to TransAT. In effect, the data exchange of these variables seems reasonably easy, since the mass flow rate can be computed as the integral over the 2D surface in TransAT, whereas the 1D pressure received from Cathare can be set as a constant value over the coupling boundary on TransAT side. Assuming that TransAT receives $P_1 = P_0 + \varepsilon$, where ε is a small perturbation, and sensitivity dP/dQ , then following an iterative method, the algorithm finds out a point (P^*, Q^*) such that the distance between this point and the Cathare sensitivity curve is smaller than a certain tolerance, as shown in Figure 2.

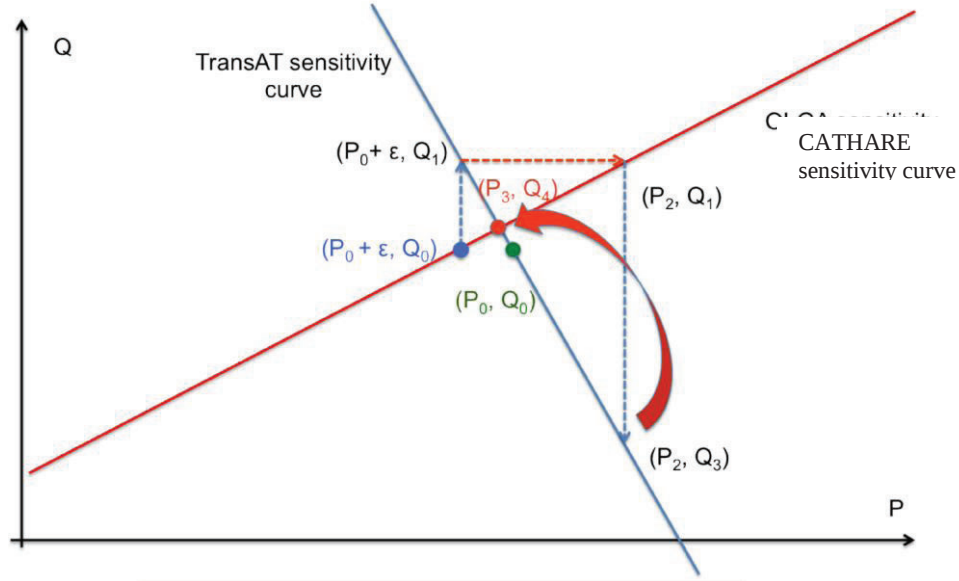


Figure 2: iterative method to satisfy coupling constraint

The extension to multi-phase cases is straightforward: an iterative scheme is used to find the pressure P^* and mass flow Q_i^* (for phase i) such that the following constraint is reached:

$$\left| \frac{P^* - \left(P_0 + \sum_{i=1}^n \frac{\partial P}{\partial Q_i} \bigg|_C (Q_i^* - Q_{i,0}) \right)}{P_0} \right| < \delta ,$$

where P_0 is the pressure received from Cathare and $Q_{i,0}$ is the mass flow of phase i (vapor or water) leaving TransAT domain across the coupling boundary, and $\partial P / \partial Q_i$ is the sensitivity parameter received from Cathare. The coupled system is controlled by a supervisor function written in C++. The ICoCo coupling interface is used for the exchange of information between Cathare and the supervisor. TransAT uses its own built-in coupling interface to exchange information with the supervisor.

3 ROCOM BENCHMARK

The implementation of the coupling between TransAT and Cathare is tested on the ROCOM benchmark test case for steady-state conditions, as described in [1]. The case has already been simulated by the group with no coupling, but conventionally by setting BC's [3]

1.1 Simulation setup

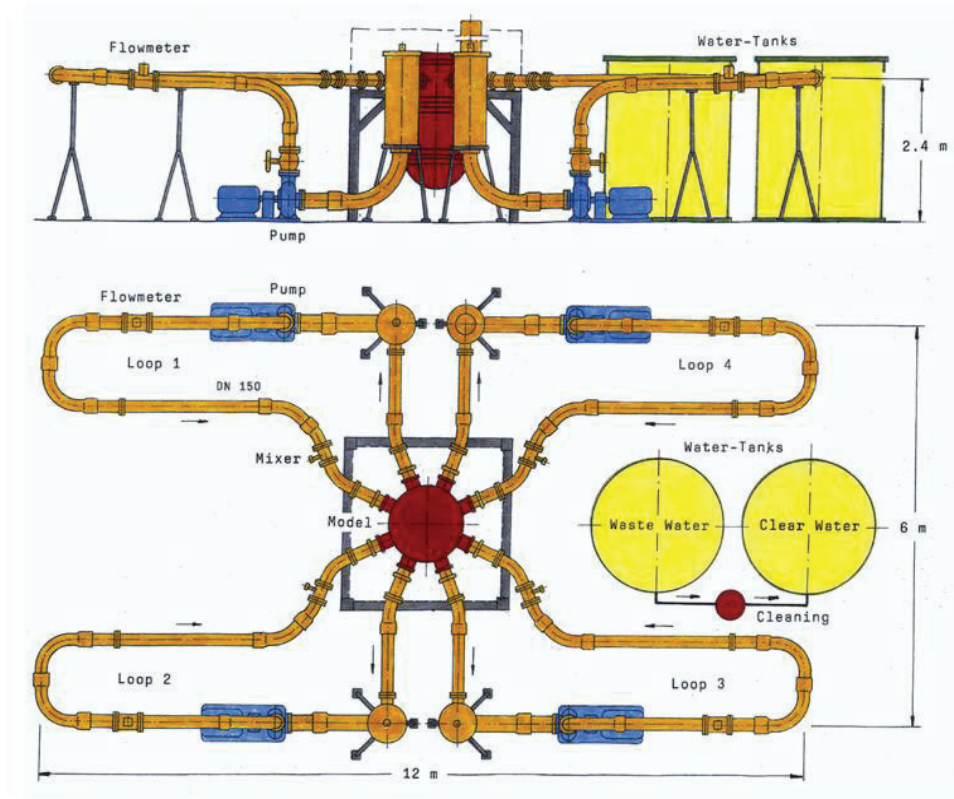


Figure 3: ROCOM test facility -A 1:5 scaled model of the PWR KONVOI

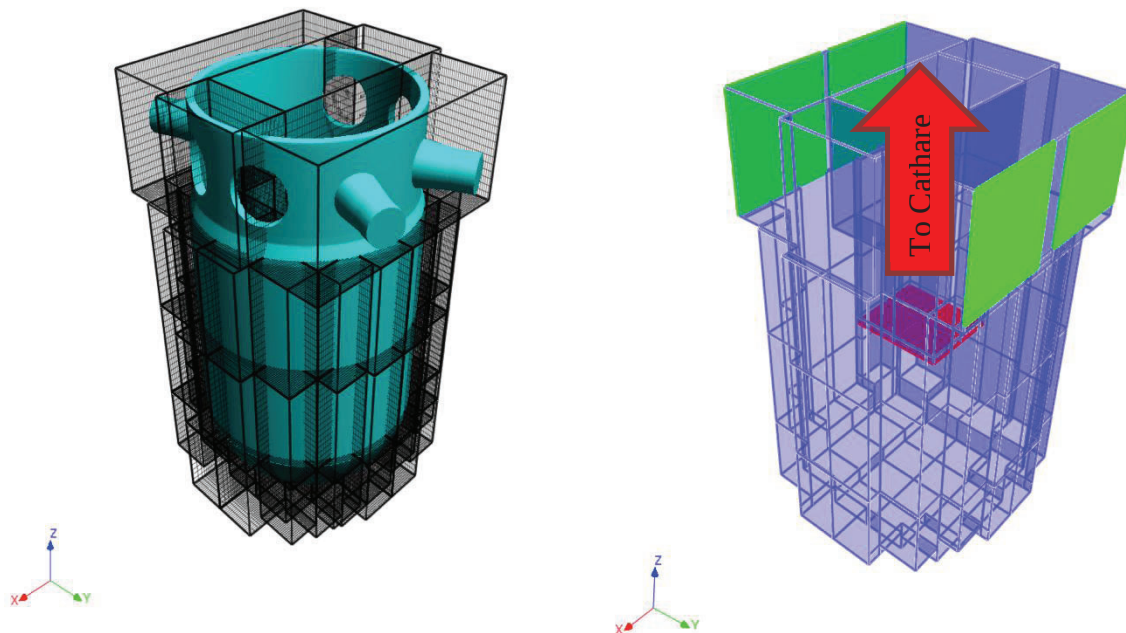


Figure 4: RPV - Setup in TransAT

Item	Unit	Value
Inlet nozzle diameter	mm	15
Inner diameter of pressure vessel	mm	1000
Height of the pressure vessel	mm	~2400
Width of the downcomer	mm	63
Water Temperature	K	293.15
Inlet velocity	m/s	2.91
Reynolds number in the inlet nozzle	----	4.4E5

Table 1: configuration value for ROCOM test case

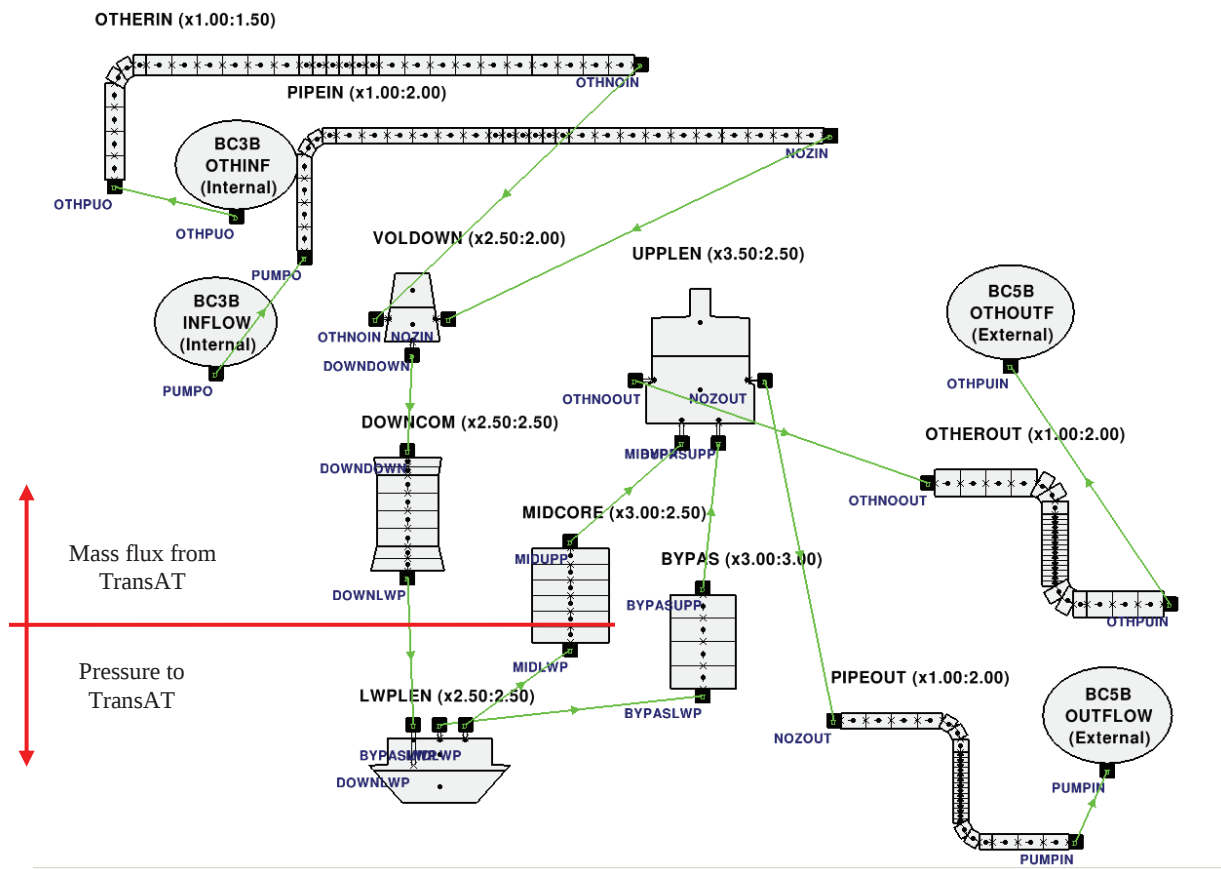


Figure 5: Setup in Cathare

The flow in the RPV is simulated with TransAT, as shown in Figure 4. On the left, the fluid domain is shown in blue - everything else is solid (“inverted” view). A Cartesian non-uniform mesh is created using multiple blocks, with a total of 709,215 cells. On the right, the inlet boundaries, indicated by green surfaces, are prescribed with velocity of 2.91m/s. The outlet/coupling boundary, which interfaces with Cathare, is indicated by a red surface and is located horizontally at the middle of the core.

As shown in Figure 5, two loops are set up in Cathare, one of them has a weight of 3. The core is modeled by an axial component, with the red line indicating where the coupling interface is located. For boundary conditions, the inlet velocity is set to 2.91 m/s and the outlet pressure to 101325 Pa. The ultimate goal is to simulate the whole pipe system with Cathare and the “reactor” with TransAT. However, currently only one coupling interface is implemented. The part downstream of the coupling interface is simulated with the imposed mass flux from TransAT while the upstream part only helps in Cathare’s initialization and becomes irrelevant in the coupled simulation.

1.2 Simulation results

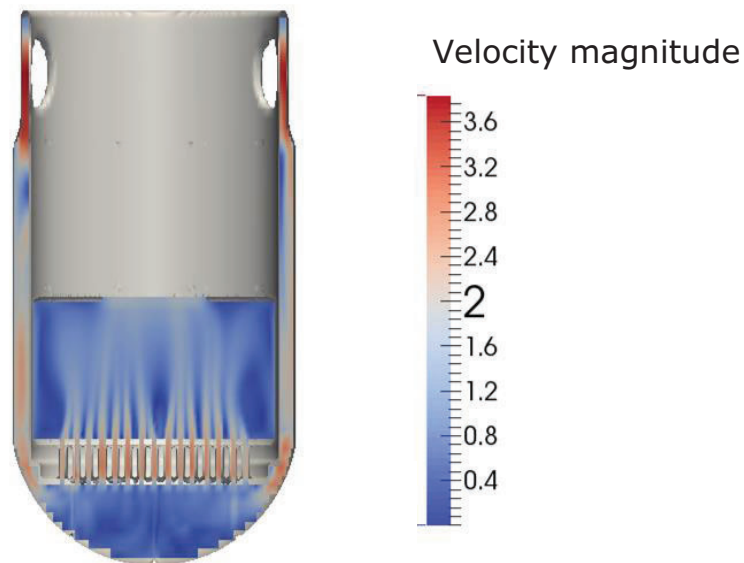


Figure 6: Magnitude of the velocity field in the RPV, as simulated by TransAT

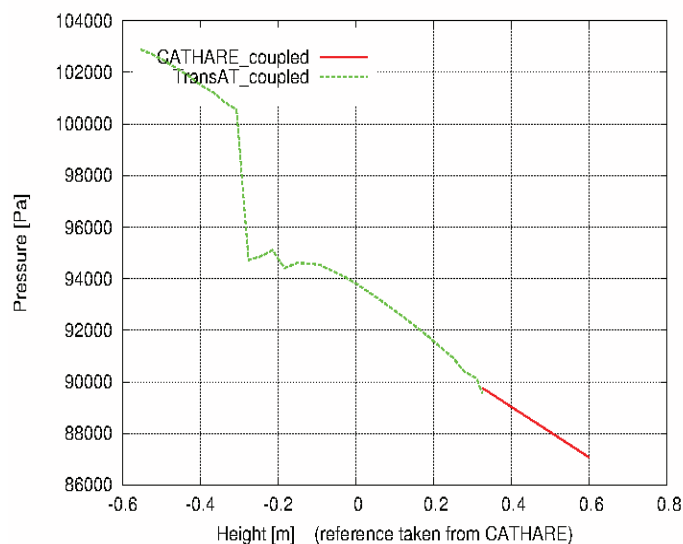


Figure 7: Pressure along a line crossing the coupling boundary

Figure 6 shows the flow velocity in the RPV at quasi steady state, as simulated by TransAT with outlet boundary condition dictated by Cathare. Figure 7 shows the pressure plotted from the bottom of lower plenum along a line parallel to the Z-axis and traversing the coupling boundary. The sudden drop and fluctuation correspond to the support plate where the flow passes 193 holes with a diameter of $d = 20$ mm. The figure shows that pressure is continuous across the coupling boundary, up to the tolerance of the numerical scheme.

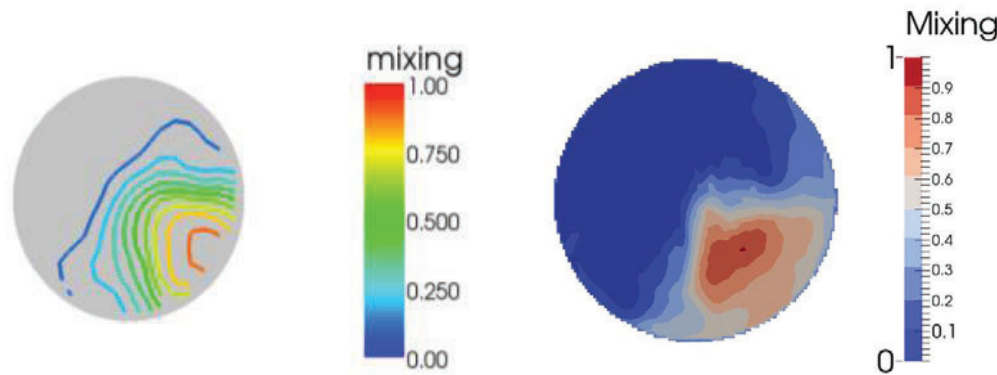


Figure 8: normalized concentration of the mixing component (boron).
Left: experiment, right: coupled TransAT-Cathare simulation.

The maximum mixing scalar in the simulation is 0.933 against 0.94 in the experiment. In the simulation result, the maximum appears closer to the center of the circle than in the experiment. The area of maximum concentration is also slightly underestimated compared to the experiment. Several factors can explain these discrepancies:

- **Coarse mesh:** The mesh has a minimum cell size of 7mm in x and y direction and 22mm in the z direction, which is not sufficiently refined in some critical regions, such as the upper downcomer, the support plate and the perforated drum.
- **Outlet geometry:** Since a horizontal plane intersects with not only the core, but also the downcomer, blocks are used to confine the coupling boundary within the core. They shape the outlet into a rectangular instead of a circle. This might have affected the fluid field.
- **Inlet profile:** The flow profile at inlet nozzle is unknown. Here it is selected as TransAT turbulent profile. In later simulation, long legs will be added to the inlets in order to let the flow fully develop.
- **Diffusivity:** The diffusivity of scalar concentration is set arbitrarily and does not match the one for salt.
- **Measurement method:** To save computational resources, the simulation is terminated at time roughly equals to 10s; while in the experiment[1], measurements are carried out after a quasi steady state has been reached, and the data is averaged over a time interval from 8.5s to 13s.

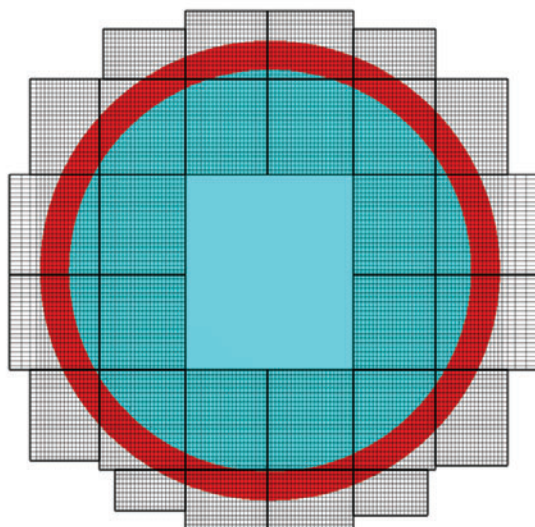


Figure 9: mesh in TransAT at the coupling boundary (cross-section)

The pressure and mass flow rates at the coupling boundary between Cathare and TransAT are continuous, which shows that the mass and momentum conservation constraints that are at the heart of the semi-implicit coupling scheme have been correctly implemented.

The results for the tracer concentration compare qualitatively well with the experimental data and are sufficient to show that the boundary conditions for the CFD calculations were correctly enforced, as provided by Cathare. More accurate results would have required a significantly finer mesh to better resolve the geometry in the downcomer, leading to expensive 3D simulations.

4 DOUBLE T-JUNCTION TEST CASE

To further validate the implementation of the TransAT/Cathare coupling, we simulate the injection of a passive scalar into a double T-junction. For comparison purposes we use the same setup as that in Bertolotto et al. [4], where a co-simulation between CFX and Trace was performed. The setup and parameter values are shown in Figure 10 and Table 2, respectively.

1.3 Simulation setup

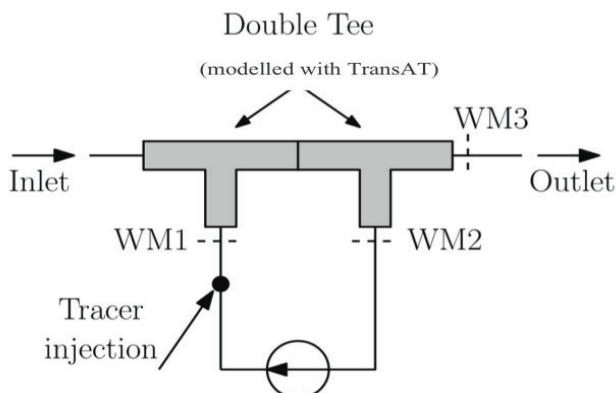


Figure 10: double T-junction setup (same as [4])

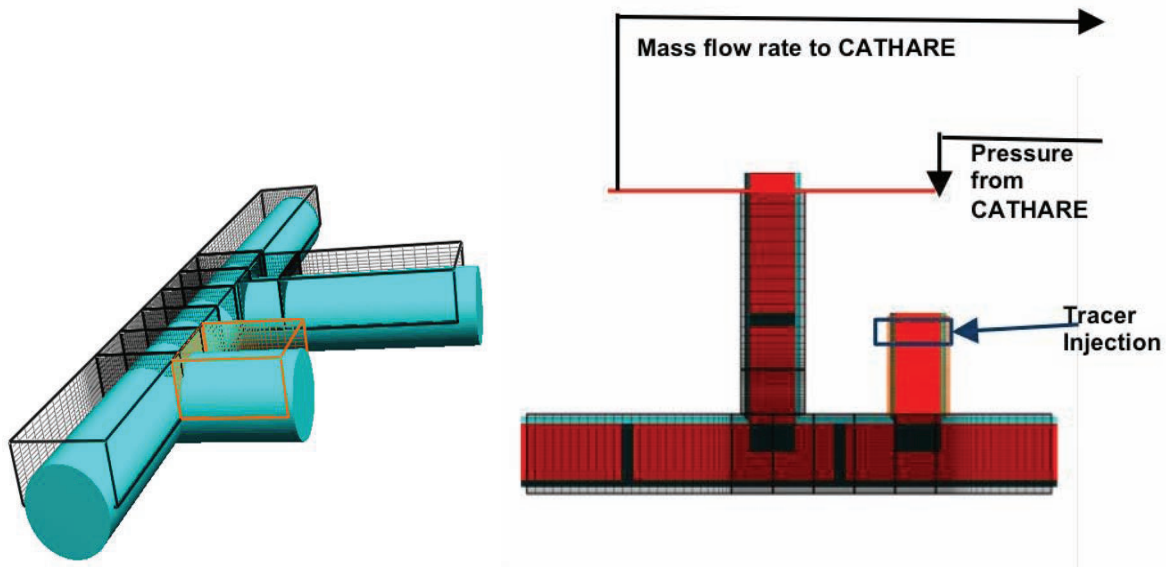


Figure 11: simulation setup in TransAT

The double T-junction is simulated in TransAT, with geometry as shown in Figure 11. The fluid is represented in blue and everything else is solid. Since the flow field is symmetric in the z-direction, to save computation efforts, only the upper half is simulated. The computation domain totals 144,816 cells.

Item	Unit	Value
Pipe inner Diameter	m	0.05
Distance between centers of side branches	m	0.13
Inlet volume flow rate	l/min	80
Outlet pressure	bar	1
Side loop length	m	5.0
Distance between pump and inlet of side loop	m	2.5

Table 2: configuration values for double T-junction test case

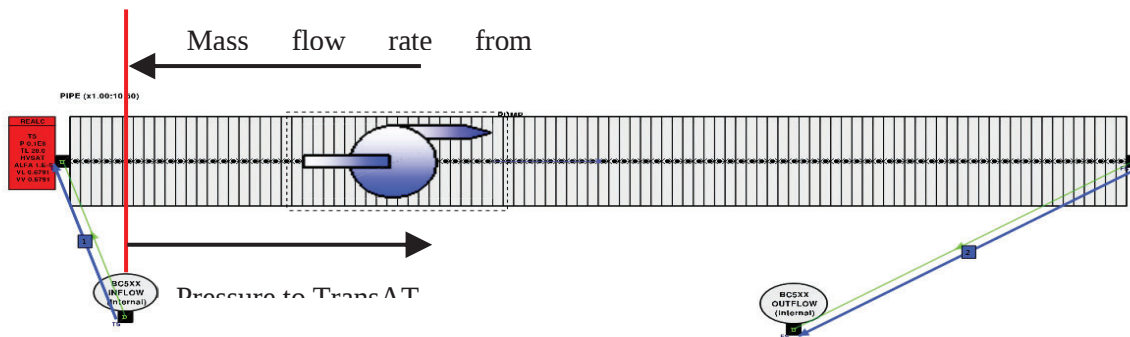


Figure 12: simulation setup in Cathare

One coupling interface is set at the outlet to side loop. The injection of the tracer is done at the beginning of simulation, by user-defined functions. The inflow velocity profile in TransAT has been set to constant. The Abe-Kondoh-Nagano Low Reynolds $k-\epsilon$ model is used.

The side loop is simulated in Cathare, using a pipe element with a pump, as shown in Figure 12. Mass flow rate (only used for pre-coupling initialization) is prescribed at inflow and pressure at outflow boundaries, and the coupling interface is set at an inner scalar point which acts as an inlet mass flux boundary in the coupled simulation.

1.4 Results

Only one coupling interface between TransAT and Cathare can currently be activated. Therefore, we stop the simulation when the tracer injected at WM1 has been advected through the loop once. Figure 13 shows the magnitude of the velocity field in the CFD domain of the coupled simulation. The overall flow field matches qualitatively the solution given in [4] for a coupled simulation using CFX and Trace. Recirculation vortices in particular have been well captured. The maximum velocity magnitude, however, is slightly overestimated compared to CFX-Trace simulation, but no judgement can be made at this point.

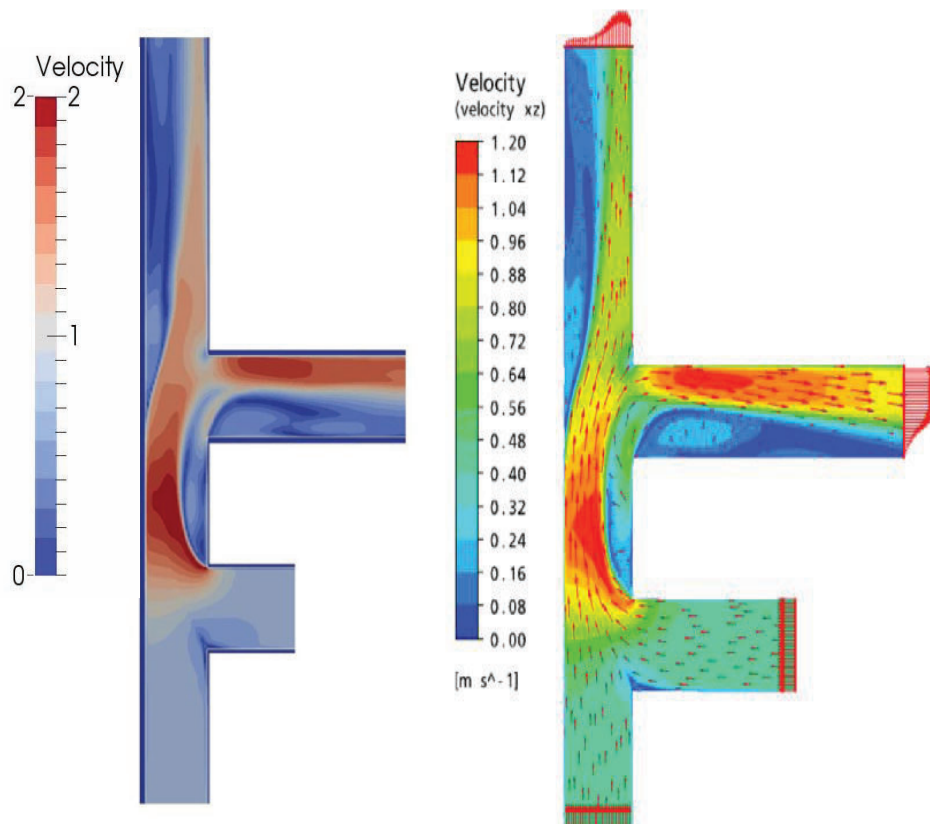


Figure 13: Velocity field in the 3D domain. Left : TransAT/Cathare simulation;
Right : CFX/Trace simulation (reproduced from [4]).

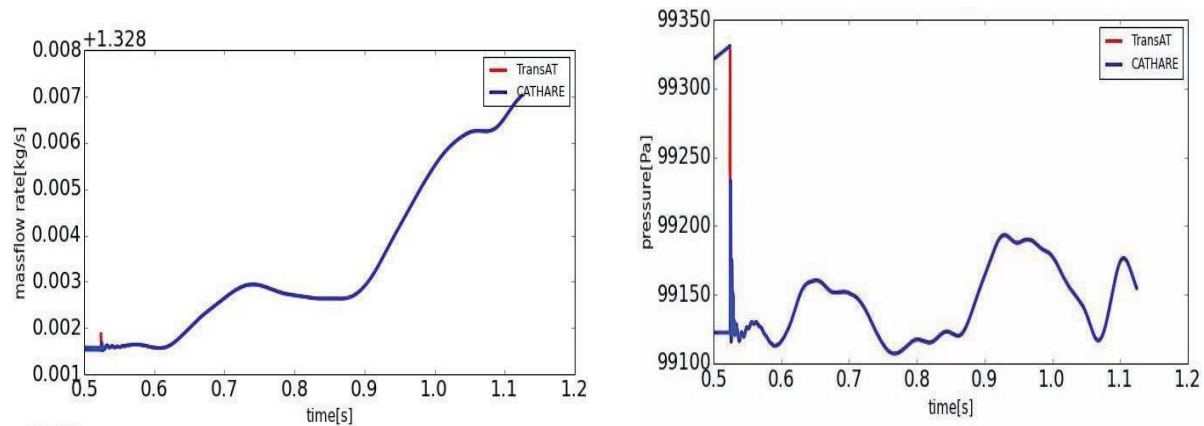


Figure 14: Mass flow rate and pressure in the two codes at the coupling boundary

As expected, the mass flow rates and pressures are identical in both codes at the coupling boundary (see Figure 14), up to a small tolerance built in the semi-implicit coupling scheme. The fact that pressure curve is oscillating and mass flow rate keeps increasing indicate that the simulation has not yet reached steady state.

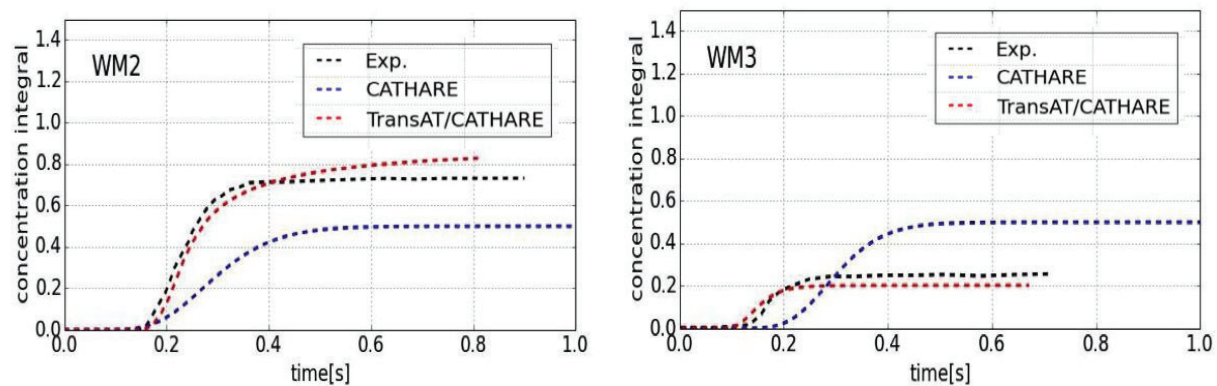


Figure 15: Cumulative integral of the tracer concentration. Left: WM2, right: WM3.

Figure 15 shows the cumulative sums of the tracer concentration at positions WM2 and WM3 in the T-Junction. Results from the TransAT-Cathare coupled simulation are close to the experimental data. If Cathare is used alone (blue curve), the amount of tracer that goes straight to the outlet (WM3) is significantly over-predicted whereas that which loops back (WM2) is under-predicted. A similar behavior was reported in the CFX-Trace coupled simulation [4]. This highlights the fact that some flow features are inherently 3D and not captured by system codes. TransAT-Cathare coupled simulation shows good agreement with experiment data and the CFX/Trace simulation, while Cathare alone cannot capture the details of splitting. This again stresses the added value of using CFD in some critical regions of the hydraulic network. Due to the fact that only one coupling interface is implemented in this simulation, the side branches do not behave like a loop, which does not match with the real situation. Multi-boundary coupling needs to be considered in the next steps to validate the coupled simulation on all regions.

5 CONCLUSION

The coupling interface between the CFD code TransAT and the system thermal hydraulic code Cathare was tested. Two numerical benchmarks were performed, based on the ROCOM test case and double T-Junction, respectively. It has been demonstrated that the coupled system TransAT-Cathare can be used to simulate scalar mixing in realistic scenarios. Although results for ROCOM were compared at steady state, the simulation itself was transient. We are thus confident that the methodology presented here would be adequate for coupled unsteady thermal-hydraulic simulations. A more thorough analysis is the object of ongoing work. The current implementation only allows for one coupling boundary condition. A more generic implementation that allows several coupling boundaries has now been successfully developed, and is under validation process. The coupling algorithm will be extended to other US-NRC codes like RELAP and TRACE.

6 ACKNOWLEDGEMENTS

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7 REFERENCES

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