

PTS PREDICTION USING THE CMFD CODE TransAT: THE COSI TEST CASE

M. Labois, D. Lakehal

ASCOMP GmbH
Technoparkstrasse 1, CH-8005 Zurich, Switzerland

Abstract

The paper presents new, transient simulation results of condensing steam in the event of emergency core cooling where water is injected into the cold leg during a postulated loss-of-coolant-accident (LOCA) of a pressurized water reactor (PWR), a phenomenon known as Pressurized Thermal Shock (PTS). The model is first validated for the Lim *et al.* (1984) experiment involving a smooth to wavy turbulent, stratified steam-water flow in a 2D channel, then in 3D to predict the experimental data from COSI (EDF-CEA-AREVA). The computational framework is based on interface tracking, combined with large-scale prediction of turbulence, a new methodology known as LEIS (Large-Eddy & Interface Simulation) where super-grid or super-scale turbulence and interfaces are directly solved whereas the sub-grid or sub-scale parts are modelled. Because ergodic steady-state flow conditions are difficult to attain, recourse is made of the V-LES (instead of LES), where the flow-dependent cut-off filter is larger and independent from the grid. The computational approach is completed by a DNS-based interfacial phase-change heat transfer model built within the surface divergence (SD) theory. The original SD model is found to return better results when modified to account for scale separation, i.e. to segregate low-Re from high-Re number flow portions in the same flow. While the 2D validation results are excellent, the 3D PTS results are also good, but need to be run further before reaching statistically steady-state conditions.

1. INTRODUCTION

Emergency core cooling injection of cold water is one of the most severe scenarios of the global Pressurized Thermal Shock (PTS), referring to the occurrence of thermal loads on the reactor pressure vessel (RPV) under pressurized conditions (Lucas *et al.*, 2008). Cold water is injected into the cold leg during a hypothetical Small Break LOCA. The injected water mixes with the hot fluid present in the cold leg and the mixture flows towards the downcomer where further mixing with the ambient fluid takes place. Very steep thermal gradients may damage the structural components while the primary circuit pressurisation is partially preserved. Therefore, the transient fluid temperature must be reliably assessed to predict the thermal loads (striping) on the RPV. The coolant can be single- or two-phase flow, depending on the leak size, its location and the plant operating conditions. The PTS has been the objective of a number of international cooperative programs in the past, e.g. the OECD-ICAS as given by Sievers *et al.* (2000).

The computation of this severe scenario is now within reach of the averaged two-fluid formulation. Yao *et al.* (2005), Coste *et al.* (2008) and Coste and Lavieville (2009) solved the 3D steady-state Navier-Stokes equations within the two-fluid framework, using a modified RANS model that accounts for the production by interfacial friction. The CATHARE code was then used; but results reported in recent conferences by the same group have used the NEPTUNE-CFD code. Among the various modelling issues underlined by the CEA group and many others elsewhere, the interfacial heat and mass transfer problem constitutes a challenging one by its own. Since DNS of interfacial heat and mass transfer is still (if ever) not feasible for flows of this scale, resort should be made to interfacial modeling based on correlations. These are numerous and well documented in the literature, and are either analytically derived or based on experiments or more recently, on DNS. One of which is the so-called 'Surface Divergence SD' model, which has been found to fit real DNS data (Lakehal *et al.*, 2008a,b; Banerjee *et al.*, 2004) is now being used in two-phase flow solvers, either based on two-fluid

formulation (Tankskanen *et al.*, 2008) or ITMs, see e.g. Lakehal (2008). Because all interfacial heat transfer models are made dependent on turbulence quantities, dealing with this issue is another aspect of the large picture and needs thus to be addressed in tandem.

The first question addressed by the present contribution is whether this class of flow – including phase change- is within reach of ITMs, e.g. Level Sets. The work complements an earlier attempt to predict a simplified version of the COSI flow, presented at the second CFD4NRS workshop (Lakehal, 2008), though without comparison with the data. The present contribution reports new transient results accounting for phase change obtained using a more refined grid than used hitherto, including a new condensation heat transfer model. The second question raised here relates to turbulence, namely whether RANS approaches are suitable when used in the ITM context, and what sort of alternative strategies could one adopt instead. For the purpose, we report comparisons between URANS and V-LES results. V-LES (Speziale, 1996; Labois and Lakehal, 2010) is a sort of blending strategy between URANS and LES, best suited for high Re flows that are beyond reach of rigorous LES, in particular for two-phase flow where statistical steady-state conditions require more computational time to be reached than single-phase turbulent flow.

The model validation has been performed by reference to Lim *et al.*'s (1984) experiment involving a Steam-Water co-current STRatified flow (SWST) in a rectangular channel. The free surface could be either smooth or wavy, or in a transitional regime in the channel, based on the imposed shear. The axial decrease of the steam rate is controlled by condensation. The simulations were conducted using the TransAT CMFD code of ASCOMP. The validation results show that the original SD model (Lakehal *et al.*, 2008a,b; Banerjee *et al.*, 2004) need to be modified to account for scale separation in the flow, as suggested by Theofanous *et al.*, (1976).

2. THE PHYSICAL MODEL

2.1 The Governing Equations

In TransAT, the single-fluid equations (known as the Interface Tracking Methods context, ITM, for more details, the reader can refer to Lakehal *et al.*, 2002) for incompressible two-fluid flow with phase-change heat transfer are formulated under the form:

$$\begin{aligned}
 \frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho &= 0 \\
 \frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= -\nabla p + \nabla \cdot \mu (\nabla \mathbf{u} + \nabla^T \mathbf{u}) + F_b + F_w + F_s \\
 \frac{\partial(\rho C_p T)}{\partial t} + \nabla \cdot (\rho C_p T \mathbf{u}) &= \nabla \cdot \lambda (\nabla T) + Q
 \end{aligned} \tag{1}$$

where \mathbf{u} stands for the fluid velocity and p for the pressure, ρ is the density, μ is the viscosity, λ is the thermal conductivity, C_p is the heat capacity, and Q is the volumetric heat source. The source terms in the RHS of the momentum equation represents the body force, F_b , the wall shear, F_w , and the surface tension, F_s . Material properties are updated locally based on a phase marker field, denoting here the level-set function ϕ . Other material properties like viscosity, thermal conductivity and heat capacity are also updated in the same way. TransAT uses the so-called Immersed Surfaces Technology (IST), whereby the wall shear (F_w) appears explicitly in the equations based on the solid level-set function ϕ_s that defines solid obstacles (in addition to the gas-liquid function ϕ). The method is explained in the companion paper (Labois *et al.*, 2010). To track the interface and update material properties, a topology equation is solved for the level-set function ϕ .

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \dot{m} / \rho |\nabla \phi| \quad (2)$$

where the phase change due to heat transfer is accounted for by the source term; \dot{m} being the rate of mass transfer. In the Level Set technique (Sussmann *et al.*, 2004), the interface between immiscible fluids is represented by a continuous function ϕ , representing the distance to the interface that is set to zero on the interface, is positive on one side and negative on the other. Conceptually, Interface Tracking Methods are in principle capable of capturing the topology of interfaces and resolving accurately the interfacial boundary layers, independently from the Reynolds number. But since full DNS resolving all turbulence and interface motions is practically elusive (the grid should scale with $\sim \text{Re}^3$), one is forced to solve the flow on grids that scale with R^x , where exponent x is clearly smaller than 3, leaving the difference to diffusive-based modelling like in RANS, albeit with a clear separation between resolved and unresolved or sub-grid scales (SGS).

For turbulent interfacial flows, use should be made of the filtered form of the equations above (Liovic and Lakehal, 2007a,b). This is now known as the LEIS, short for Large Eddy & Interface Simulation, in which turbulent scales and interface deformations larger than the grid size are directly solved, whereas sub-scales are modelled. The LEIS equations and sub-grid scale models are now well known; details can be found in Lakehal (2010). Because statistically steady-state flow conditions are difficult to attain in 3D, recourse is made here of the V-LES (instead of LES), where the flow-dependent cut-off filter is larger and independent from the grid (cf. Section 2.2). Although somewhat contradictory in terms of scale separation, one actually could resort to RANS closure models to deal with turbulence as well, at the expense of affecting the degree of interface topology resolution; higher eddy viscosity levels (by use of RANS) at the interface could hamper the high-frequency surface motions, i.e. wrinkling. Be it as it may, advancing the RANS form of the above system of equation in time is referred to as URANS (Unsteady RANS).

2.2 On V-LES as an Alternative Turbulence Modeling Approach

V-LES is based on the concept of filtering a larger part of turbulent fluctuations as compared to LES (as the name clearly implies). This directly implies the use of a more elaborate sub-grid modelling strategy than a zero-equation model like in LES. The V-LES implemented in TransAT is based on the use of $k - \varepsilon$ model as a sub-filter model. The filter width is no longer related to the grid size; instead it is made proportional to a characteristics length-scale that is larger than the grid size, but necessarily smaller than the macro length-scale of the flow. Increasing the filter width beyond the largest length scales will lead to predictions similar to the output of RANS models, whereas in the limit of a small filter-width (approaching the grid size) the model predictions should tend towards those of LES. V-LES could thus be understood as a natural link between conventional LES and URANS. If the filter width is smaller than the length scale of turbulence provided by the RANS model, then larger turbulent flow structures will be able to develop during the simulation, provided that the grid resolution and simulation parameters are adequately set (in particular regarding time stepping and the order and accuracy of the time marching schemes employed). The V-LES theory as currently used has been proposed by Johansen *et al.* (2004). We will briefly present this theory; for a more detailed presentation and a discussion on the values of the model constants, the reader can refer to the paper of Johansen *et al.* (2004), or to Labois and Lakehal (2010).

The filter width is denoted as Δ in the following text. The Kolmogorov equilibrium spectrum is supposed to apply to the sub-filter flow portion, which allows writing the isotropic RMS velocity for the sub-filter flow as follows:

$$u'_\Delta = \sqrt{3/2} k_\Delta^{3/2} = \int_{k_\Delta}^{\infty} \xi(k) dk = C_k^{1/2} k_\Delta^{-1/3} \varepsilon^{1/2}, \quad (3)$$

where κ stands for the wave number and $\xi(\kappa)$ for the RMS velocity wave-number spectrum, with the constant $C_k = 1.62$ following Smith and Woodruff (1998). The cut-off wave length is related to the double filter size, i.e. $\kappa_\Delta = 2\pi / 2\delta$. The isotropic turbulent viscosity can thus be defined using

$$(u'_\Delta \cdot l) = \int_{\kappa_\Delta}^{\infty} \xi(k) \frac{\pi}{k} dk = \frac{\pi}{3} C_k^{1/2} \varepsilon^{1/3} \int_{\kappa_\Delta}^{\infty} k^{-7/3} dk = u'_\Delta \Delta / 4. \quad (4)$$

Defining the anisotropic factor $\gamma < 1$, the turbulent viscosity is rewritten as $\nu_t = \gamma u'_\Delta \Delta / 4$, so that anisotropic effects can be taken into account. In the limit of very large filter widths, the effective length scale is limited upwards by $l_{eff} = \nu_t / u'_\Delta$ which helps re-write the eddy viscosity of the filtered model as: $\nu_t = \nu_{t,RANS} f(\Delta, k, \varepsilon)$. The length-scale limiting function $f(\Delta, k, \varepsilon)$ is defined by:

$$f(\Delta, k, \varepsilon) = \begin{cases} 1 & \text{if } C_3 \Delta \varepsilon k^{3/2} \leq 1 \\ C_3 \Delta \varepsilon k^{3/2} & \text{otherwise} \end{cases} \quad (7)$$

where C_3 is a model constant introduced by Johansen et al. (2004). This function cannot be known a-priori if the entire energy spectrum is not explicitly known; thus, the simple proposal from Johansen *et al.* (2004) is used here:

$$f(\Delta, k, \varepsilon) = \min[1, C_3 \Delta \varepsilon / k^{3/2}]. \quad (8)$$

Near wall boundaries, the function is forced to be equal to unity, which means that the standard model is systematically applied in these regions. This permits the use of the standard wall-functions in the V-LES context, too. The method can also be employed under low-Re flow conditions, using either a two-layer approach based on a one-equation model or a Low-Re model. Finally, the turbulent viscosity for V-LES can be written as,

$$\nu_t = C_\mu \frac{k^2}{\varepsilon} C_3 \frac{\Delta \varepsilon}{k^{3/2}} \quad (10)$$

The difference between RANS, LES and V-LES, is that in the latter approach it is necessary to specify a filter width, which can be made proportional to a characteristics length-scale of the flow. This parameter has been the object of a systematic dependence study in Laboiss and Lakehal (2010). Apart from that, a lower bound must be set to ensure that the filtering process is compatible with the grid resolution. Practically we impose $\Delta > 1.5 \Delta_{\text{grid}}$ where $\Delta_{\text{grid}} = (\Delta x \Delta y \Delta z)^{1/3}$ in 3 dimensions.

2.3 Interfacial Heat and Mass Transfer Modelling

The task of resolving interfacial heat/mass transfer in TransAT follows two distinct routes: either the rate of mass transfer at the interface (r.h.s. term in Eq. 2) is directly determined by solving the heat balance across the interface using the relation below,

$$\dot{m}_L h_{v,L} = \lambda \nabla T|_L \cdot \vec{n}_{int} - \lambda \nabla T|_S \cdot \vec{n}_{int}$$

or resort is made to analytical or measurement and DNS-based models. The models implemented in TransAT are mainly based on DNS studies conducted by the group itself: these can be based on the surface renewal theory, under the Large-Eddy and Small-Eddy variants, as well as the Surface

Divergence mode (SD) of Banerjee *et al.* (2004), Lakehal *et al.*, (2008a,b). The models are made sensitive to various types of turbulent Reynolds numbers, the Schmidt or Prandtl number and turbulent characteristics length-scale of the flow, depending whether use is made of RANS or LES & V-LES contexts. Before applying the models for the COSI test case presented below, a validation exercise has been run first to assess the models.

Heat transfer modelling in the two-fluid modelling framework

In two-fluid models, the heat transfer rate from steam to water is defined based on the interfacial area of quality $[1/m]$, $a_i = |\nabla \alpha_L|$, the saturation temperature, T_{Sat} , and the water temperature, T_L

$$\Gamma_L = a_i h_L (T_{Sat} - T_L) \quad (11)$$

The phase-change heat transfer coefficient h_L is defined as

$$h_L = Nu_L \lambda_L / L_t; \quad \text{with} \quad Nu_L = f(Re_y, Pr_L) \quad (12)$$

where L_t is the turbulent characteristic length. Various heat transfer correlations exist in the literature, though most of which are based on experiments, e.g. the Hughes & Duffey (1999) model. Besides the fact that there exists no universal closure, the problem often encountered is the paradox as to the definition of an appropriate turbulence Reynolds number, defined in the RANS context usually by:

$$Re_y = \frac{L_t u_t}{\nu_L}; \quad \text{with} \quad L_t = C_\mu \frac{k_L^{3/2}}{\varepsilon_L} \quad \text{and} \quad u_t = C_\mu^{1/4} k_L^{1/2} \quad (13)$$

where the length and velocity scales of turbulence L_t and u_t are made proportional to k_L and ε_L , the turbulent kinetic energy (TKE) and its rate of dissipation. Further, the model holds only for turbulence equilibrium conditions (production equals dissipation), justifying assigning the standard value 0.09 to model constant C_μ . This is obviously not true very near the interface, where viscous forces dominate over turbulence (Lakehal and Reboux, 2006).

Heat transfer modelling in the ITM modelling framework (TransAT)

In the so-called Surface Divergence (SD) model of Lakehal *et al.* (2008a), the DNS-based correlation for the mass transfer rate Γ takes the following form:

$$\Gamma / u_t \equiv \dot{m} / \rho \cdot u_t = C \cdot Pr^{-1/2} \cdot f[Re_t] Re_t^m \quad (14)$$

where the model constant C depends on the liquid properties: $C = 0.35$ for $Pr = 1$, and $= 0.45$ for $Pr \gg 1$). The difference between the SD and the so-called ‘Small-Eddy’ and ‘Large-Eddy’ models of Lamont and Scott (1970) and Fortescue and Pearson (1967), is the presence of the function between brackets in Eq. (14), known as the surface-divergence function. This has previously been modelled using DNS data for both passive scalar transfers (Banerjee *et al.*, 2004), and recently for active condensing flow (Lakehal *et al.*, 2008a) and takes the form:

$$f[Re_t] = \left[0.3 \left(2.83 Re_t^{3/4} - 2.14 Re_t^{2/3} \right) \right]^{1/4} \quad (15)$$

In the so-called ‘Small-Eddy’ models, exponent ‘ m ’ in (14) is set to -0.25 , while in the ‘Large-Eddy’ variant, ‘ m ’ is set equal to -0.5 ; in both models the surface divergence function (15) is set to unity. In recent models (Coste and Lavieville, 2009), ‘ m ’ was even set equal to $-1/8$.

The ‘SD Scale-Adaptive’ model implemented in TransAT borrows the ‘two-regime’ idea from Theofanous *et al.*, (1976), and blends the exponent ‘ m ’ in (14) between -1/4 and -1/2 based on the turbulent Reynolds number. The question of selecting the right turbulent Reynolds number is posed in the ITM context, too, though, albeit the concept provides a wider degree of freedom compared to the two-fluid model which compromises the determination of near-interface turbulence properties because of interface smearing. In TransAT, the turbulence Reynolds number can be defined in various ways, depending on the turbulence model employed and the nature of the flow:

$$\text{Re}_t = \frac{k^2}{\nu \varepsilon}; \quad \text{Re}_y = \frac{|\Phi| \sqrt{k}}{\nu}; \quad y^+ = \frac{|\Phi| \sqrt{\tau_w / \rho}}{\nu} \quad (16)$$

The first form of Reynolds number, Re_t , should be taken in the core flow of the turbulence-generating phase; with the associated turbulence scales determined using a weighted-average:

$$L_t \equiv k^2 / \varepsilon u_t, \quad \text{with} \quad u_t = \min(|u|, C_\mu^{1/4} k^{1/2}) \quad (17)$$

Alternatively, the second form could be taken, which requires the distance to the interface (straightforwardly determinable since it is the level set itself) as the length scale. The velocity scale is now made proportional to TKE. The last form invokes the shear at the interface, which can precisely be determined only using ITM’s.

3. THE NUMERICAL APPROACH

The CMFD code TransAT© developed at ASCOMP is a multi-physics, finite-volume code based on solving multi-fluid Navier-Stokes equations. The code uses structured meshes, though allowing for multiple blocks to be set together. MPI and OpenMP parallel based algorithms are used in connection with multi-blocking. The grid arrangement is collocated and can thus handle more easily curvilinear skewed grids. The solver is pressure based (Projection Type), corrected using the Karki-Patankar technique for subsonic to supersonic compressible flows. High-order time marching and convection schemes can be employed; up to third order Monotone schemes in space. Multiphase flows can be tackled using (i) interface tracking techniques for both laminar and turbulent flows (level set, VOF with interface reconstruction, and Phase Field), (ii) phase-averaged homogeneous mixture model (Algebraic Slip), and (iii) Lagrangian particle tracking (one-to-four way coupling). As to the level set, use is made of the 3rd order Quick scheme for convection, and 3rd order WENO for re-distancing. Mass conservation is enforced using global and local mass-conserving schemes (Lakehal *et al.*, 2002).

To mesh complex geometries, use is made of the Immersed Surfaces Technology (IST) developed by implemented in TransAT (Labois *et al.*, 2010). The idea is inspired from ITM’s for two-phase flows: In the IST the solid is described as the second ‘phase’ with its own thermo-mechanical properties. The technique differs substantially from the Immersed Boundaries method of Peskin, in that the jump conditions at the solid surface is implicitly accounted for, not via the 1st order penalty approach. It has the major advantage to solve conjugate heat transfer problems and flow systems with rigid body motion. In IST the solid, via its CAD file, is immersed into a cubical grid covered by a Cartesian mesh. The solid is defined by its external boundaries using the solid level set function, which like in fluid-fluid flows, it represents a distance to the wall surface; is zero at the surface, negative in the fluid and positive in the solid (Labois *et al.*, 2010). To better resolve boundary layers, IST is complemented by the BMR (block mesh refinement) technique. In BMR, additional refined sub-blocks are automatically generated around solid surfaces, with dimensions made dependent on the Reynolds and/or Grashoff number (based on the dynamic and thermal boundary layer thickness) and desired y^+ for wall treatment (low Re model, two-layer or wall functions). This combined IST/BMR method can save up to 75% grid cells in 3D, since it prevents clustering grids where unnecessary.

4. VALIDATION: THE SWST PROBLEM OF LIM et al. (1984)

The experiment used to validate the different mass transfer models (14-16) has been performed by Lim et al. (1984), involving a Steam-Water co-current STRatified flow (SWST) in a rectangular channel. The free surface could be either smooth or wavy, or in a transitional regime, based on the imposed shear. The axial decrease of the steam rate is controlled by condensation. The dimensions of the channel are 6.35 cm high, 30.48 cm wide and 160.1 cm long. At the inlet the water height is 1.59cm. The liquid temperature is 298.15 K, and the phase densities are $997 \text{ kg}\cdot\text{m}^{-3}$ and $0.5734 \text{ kg}\cdot\text{m}^{-3}$, respectively. The flow conditions considered are given in Table 1. A pressure outflow is specified, using the ambient pressure for reference. The inlet conditions for k and ϵ are rough estimates only; the sensitivity study conducted by Coste (2004) has shown that the inlet values have little impact on the flow, and this has been confirmed in our simulations, too. 2D simulations were performed using a mesh consisting of 32×130 cells, i.e. 4,160 cells. The $k-\epsilon$ turbulence model was used, together with wall functions and modified interfacial boundary conditions (Liovic and Lakehal, 2007a).

Case	\dot{m}_G (kg/s)	\dot{m}_L (kg/s)	T_g (K)	$k_L(\text{m}^2/\text{s}^2)$	$k_G(\text{m}^2/\text{s}^3)$	$\epsilon_L(\text{m}^2/\text{s}^3)$	$\epsilon_G(\text{m}^2/\text{s}^3)$
1	0.657	0.041	384.15	$2.8 \cdot 10^{-4}$	0.36	$3.9 \cdot 10^{-4}$	6.1
2	0.657	0.065	389.15	$2.8 \cdot 10^{-4}$	0.92	$3.9 \cdot 10^{-4}$	24
6	1.44	0.065	389.15	$1.3 \cdot 10^{-3}$	0.92	$4.1 \cdot 10^{-3}$	24

Table 1: Flow conditions for the test cases of Lim et al. (1984).

The system of equations (1) was solved combined with the level-set method (2) to track the free surface. Fully developed flow conditions at the inlet boundary were obtained using converged results of an early simulation without phase change. Converged profiles of the velocities and TKE were fixed at the inflow plane for the phase-change case. The simulations were performed in transient regime, with an adaptive time step lying in the range 0.0001-0.0005 seconds. The flow was established after 5 seconds, and time averages were then performed during the next 0.5 seconds of simulation time. A systematic analysis of the model was carried out by Lakehal and Labois (2010), including comparing the original SD model with the scale-adaptive variant, effect of grid resolution, etc.

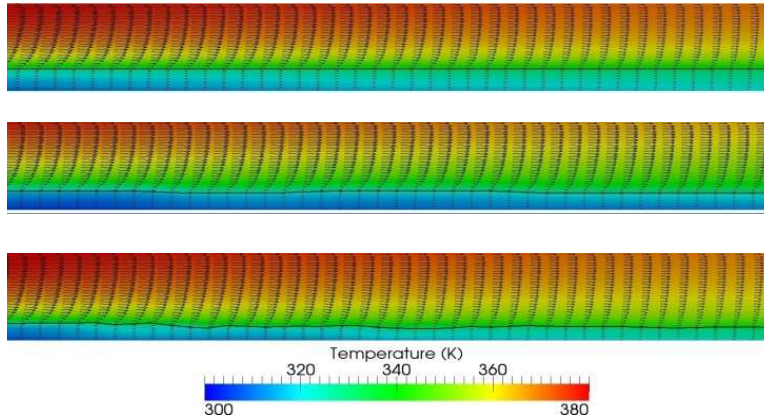


Figure 1. Flow and heat contours in the channel with TransAT.

The flow predicted by TransAT by means of level set is shown in Fig. (1), depicting the interface deformation and temperature contours for the three cases studied. The temperature gradients at the free surface seem to change with surface deformation, i.e. with the imposed gas shear and subsequent turbulence production in the core flow and near the interface.

The decay in the rate of steam along the channel is also very well predicted, in particular for Case 6 results; Case 1 and Case 2 exhibit quite similar trends. Results of steam mass flow rate along the channel shown in Figure (2) reveal the performance of the model for this class of flow, for the three cases considered, ranging from flat to wavy interface. While Case 1 and Case 2 show comparable results, the rate of steam remaining in the channel after condensation in Case 6 (wavy) is heavily reduced with increasing imposed gas shear and mass flow rate. The model can now be applied for the main problem; the COSI test case.

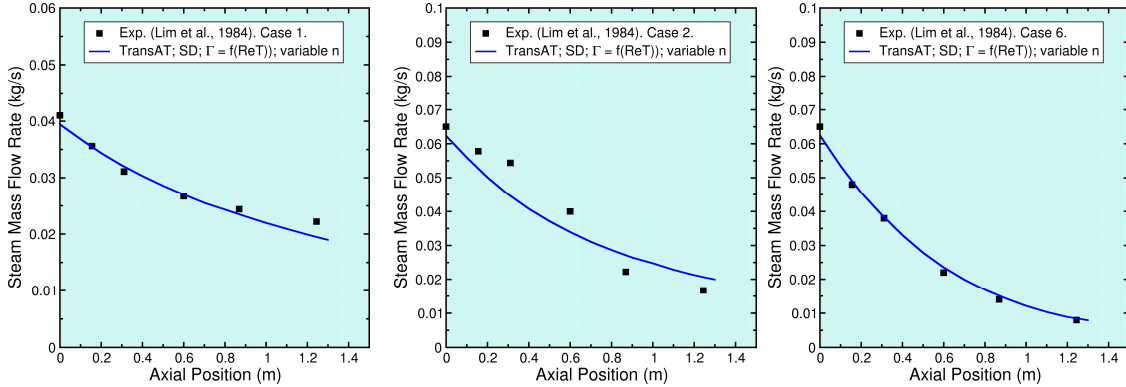


Figure 2: The Rate of steam mass flow rate along the channel with the SD-scale-adaptive eddy model.

5. PTS PREDICTION: THE COSI TEST CASE

Emergency core cooling injection of cold water is systematically associated with thermal loads on the RPV as the injected water mixes with the hot fluid in the cold leg and flows towards the downcomer. The process is necessarily three-dimensional featuring intermittent transients that can only be predicted using an unsteady approach. A steady-state approach may produce results that are in average close to the data, but will not provide a clear picture of what might be expected in reality. Further, thermal loads (stripping) are unlikely to be well predicted using a steady-state simulation, since the critical variable in this context is the fluctuating temperature, or its variance.

5.1 Problem Set-up

The COSI experiment (short for CONDensation at Safety Injections) mimics a 1/100 scale in power PWR Framatome reactor. Steam flows in a horizontal pipe representing the cold leg, in which cold water is injected from a tube located in the central part of the main pipe (Fig. 3). The main piping system is delimited by a downcomer at one end and a double elbow at the other end; a small weir is introduced to control the water level. The downcomer is composed of a vertical pipe directed towards a reservoir. The setup is equipped with global (pressure, mass flow rate) and local (temperature) measurement sensors. The COSI test N⁰ COSI-03 is used here for comparison. The coolant fluid is initially at ambient temperature, the steam is at saturation temperature. The measurement data of COSI made available to us and used here for comparison are restricted and thus cannot be disclosed in this paper; results will thus be presented in non dimensional form.

Here we have employed LEIS combining V-LES and level set (2) modified to account for phase change heat transfer using (15). The grid was generated using the IST method described thoroughly in the companion paper (Labois *et al.*, 2010), whereby a CAD file of the piping systems was embedded within a Cartesian grid. A first single-block IST grid was used here, rather coarse, consisting of 500,700 cells, with the cross section covered by 20x20 nodes. The final grid consists of 1 million cells (57x88x200) with 32x32 nodes for the pipe for capturing most of the flow details, in particular the interfacial phase change. High order schemes were employed for time and space discretization.

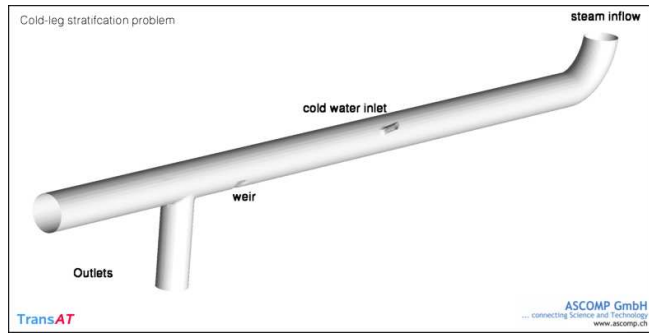


Figure 3: Computational domain used for meshing using IST.

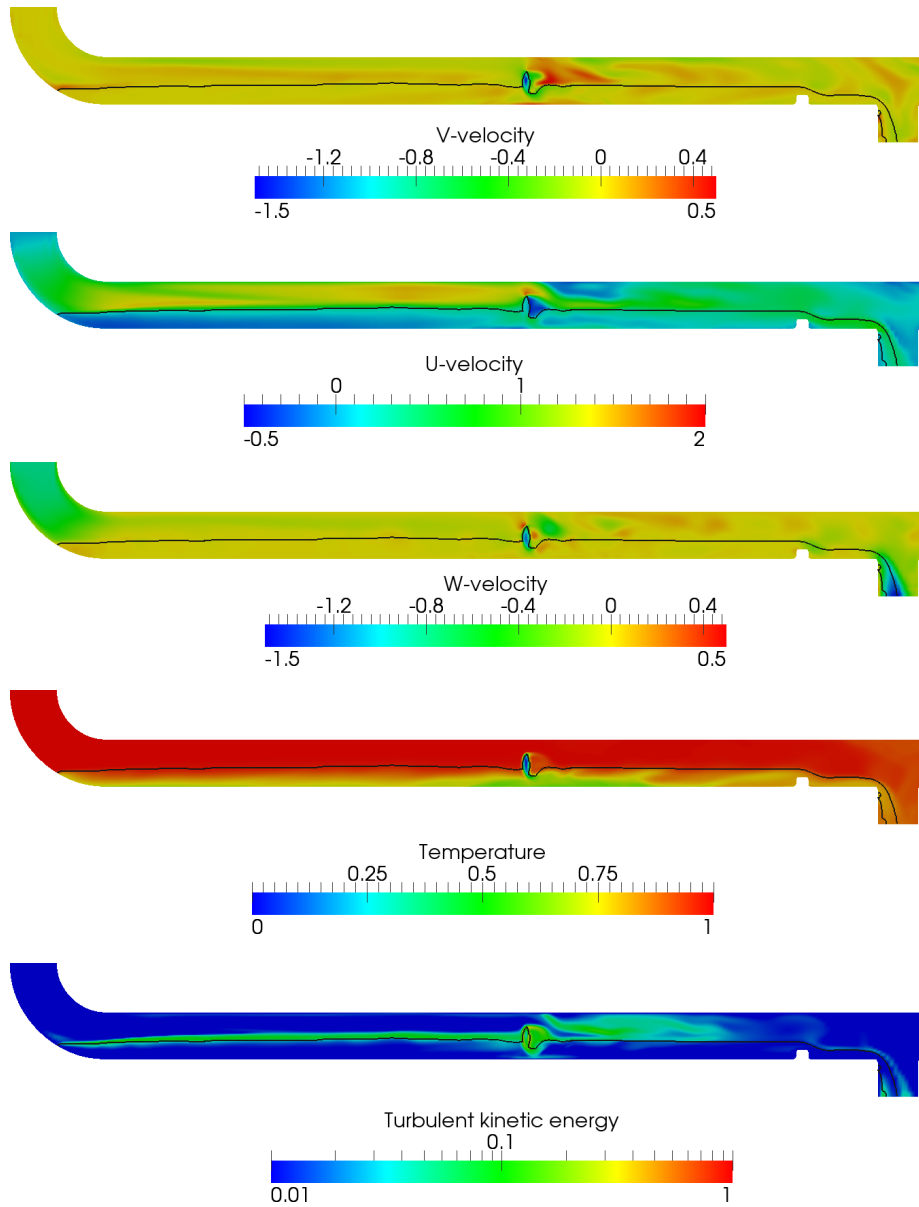


Figure 4: Steady-state surface deformations and velocity, temperature and TKE contours

5.2 Transient Results

In this section, only V-LES simulation results are discussed. Qualitative flow features are depicted in Figure 4, showing the interface deformations subsequent to coolant-jet impingement on the surface of the hot water flowing in the cold leg, coloured with the velocity (3 components), temperature and TKE fields as the mixes downstream towards the downcomer. The deformations of the sheared surface are most intense in the region below injection; the subsequent waves that form travel in the flow direction up to the wire level. The velocity contours suggest that the flow is populated with scales of various lengths. The quality of the simulation is not comparable to LES, but the flow picture is definitely more comprehensive from what might be expected from a RANS simulation (results not shown here). While the flow shows a sort of steady-state convergence in the upstream injection portion, it clearly suggests that more time steps are needed to achieve similar ergodic conditions at the downstream injection. This is particularly true when looking at the temperature contours shown in the 4th panel. TKE contours depicted in the lowest panel suggest that turbulence is generated at the interface at the gas-side due to interfacial friction, but more intensively around the jet and downstream. This suggest that most of the condensation occurs indeed in these zones, which is well confirmed when looking at the 3D snapshot reported in Fig. 5, depicting the contours of the rate of steam condensation.

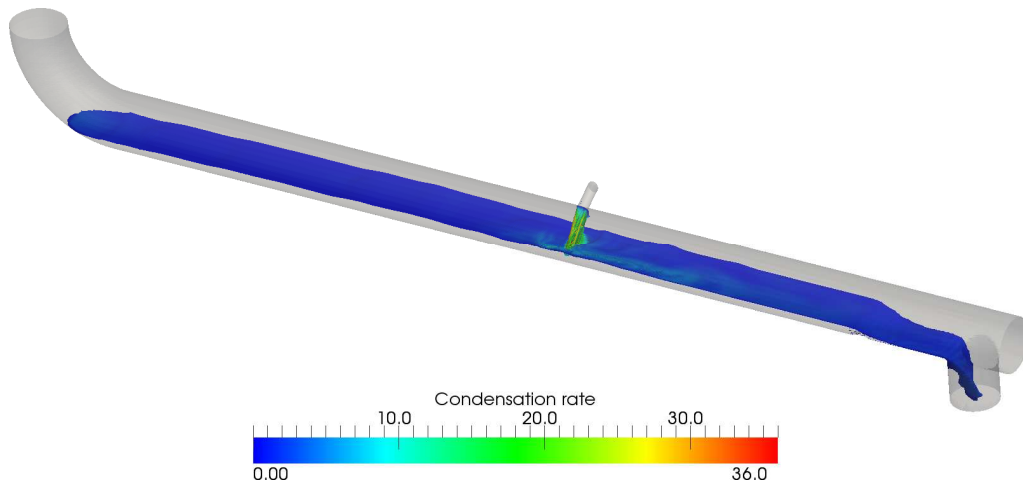


Figure 5: Instantaneous surface deformations and steam condensation rate contours

Figure 6 depicts several cross-flow planes inside the cold leg, showing time-averaged secondary velocity vectors and magnitude, interface level, condensation rate and temperature contours. The images start from left to right with flow direction: the first panels depict the flow prior to injection; the second one depicts the flow at injection level; the 3rd and 4th panels depict the flow downstream injection. The second panel depicts the time-average (the instantaneous pictures show more vigorous deformations) water level in the leg subsequent to coolant injection. The jet penetrates there quite deep and thus lowering quite substantially the temperature of the water by about 50%, judging from the temperature contour panel at the right. The temperature contours show that the cooling along the leg occurs on the side, not at the centre, even when analysed under time-averaged conditions. Prior to injection of cold water the condensation rate is somewhat greater in the pipe than downstream the injection, where the figures show that it occurs at the interface, slightly to the side to the side injection. The heat diffuses from the steam to the water in the leg rather gradually prior to injection, and more sharply downstream. But the main conclusion is that most of condensation occurs around the coolant jet; only an average of 20% from the maximum occurs elsewhere in the pipe.

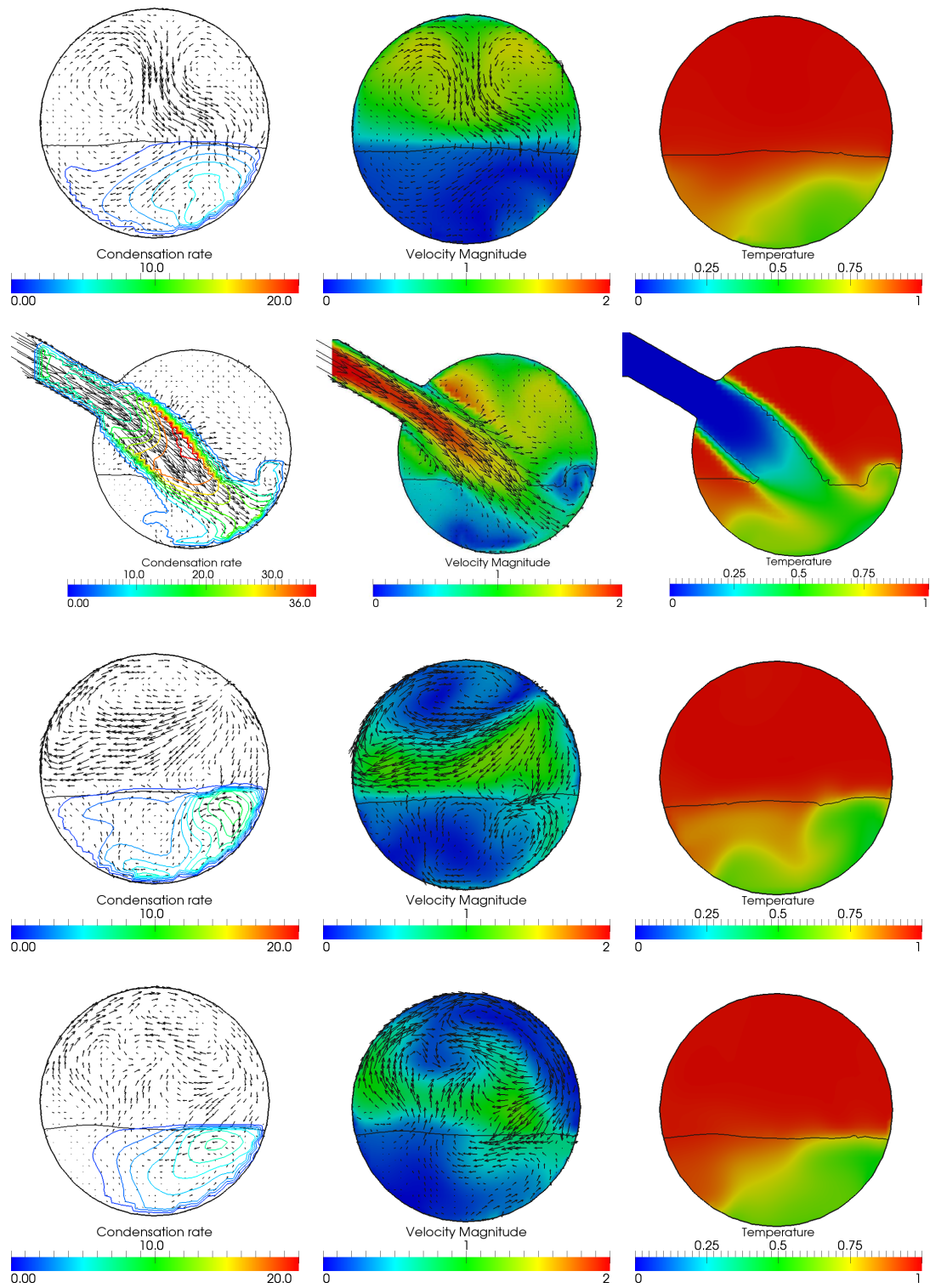


Figure 6: Instantaneous surface deformations, and contours of condensation rate velocity and temperature

5.3 Time Averaged Results

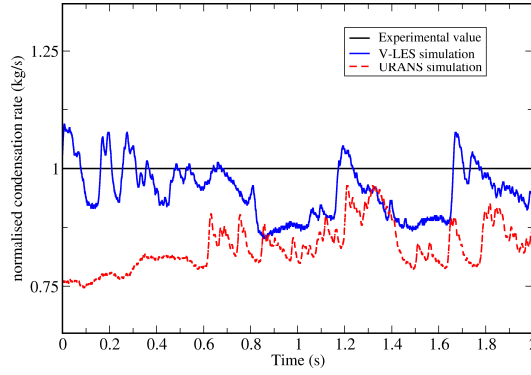


Figure 7: Time evolution of condensing steam rate: URANS and VLES vs. experiment

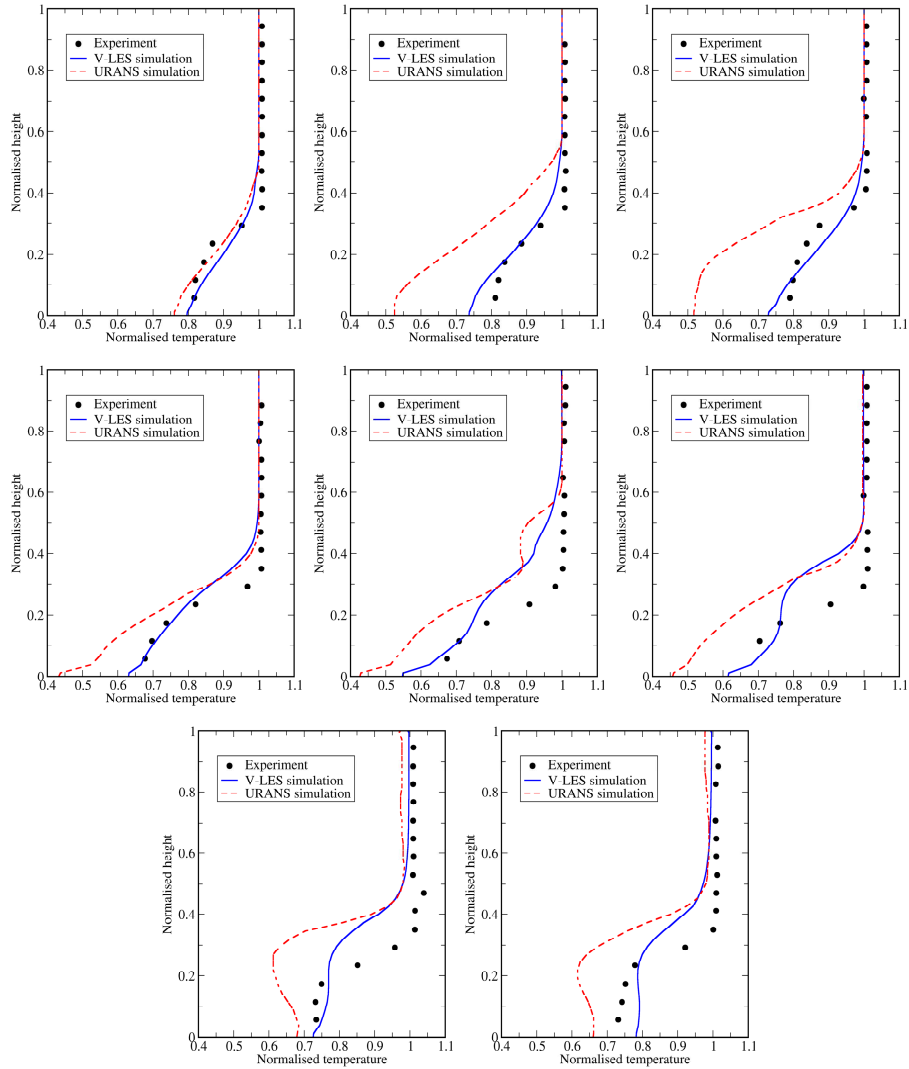


Figure 8: Time-average temperature profiles at various locations across the cold leg

Time averaged results discussed in this section were obtained by URANS and V-LES simulations. The results of steam condensation rate (normalised by the experimental value) are discussed in the context of Fig. 7. URANS simulations deliver a globally averaged quantity of condensing steam that is 10-20% less than the experiment, which is a good result. Better results are obtained with V-LES; oscillating between -10 to +7% around the mean data. This result is excellent when considered from the time-evolution aspect of the problem indeed; however, the time needed for heat to diffuse from the steam to water is as discussed previously not enough to reach statistical flow conditions, even if the rate of mass transfer is well predicted. The signals depicted in the figure suggests that the flow actually experiences strong transients returning r.m.s. magnitudes for the condensing steam rate of about 5% in URANS against ~ 10-12% in V-LES. This is one of the many advantages of this sort of unsteady large-scale simulations, in particular V-LES. Full LES simulations would have required more CPU time and storage resources. Time averaged normalized temperature profiles obtained by URANS and V-LES simulations are compared to the data in Fig. 8. The locations presented in the figure are: $x/D = -0.885; -300; -0.210; -0.05; +0.065; +0.145; +0.370$, from left to right, and from top to bottom. The temperature of the steam is overall well predicted, both using URANS and V-LES. The difficulty is clearly observed for the interfacial region where the steep temperature gradient visible from the experiments is not well captured, most probably because of lack of statistics for V-LES. At most of the locations V-LES results are better than URANS, showing in particular that the temperature in the water is not well mixed when use is made of RANS. The temperature values are good in the water side, but the flow is still under development (results not included here).

6. CONCLUDING REMARKS

The paper describes the way computational thermal-hydraulics is migrating to more sophisticated modelling techniques, transcending the two-fluid formulation and steady-state RANS equations for turbulence by integrating interface tracking methods within the LES and V-LES framework, defined here as "LEIS". The case studies simulated in this paper illustrate well what can be done with LEIS for a class of turbulent, interfacial flows featuring phase change heat transfer. The method can be successfully combined to generate realistic transient simulations in reasonable computing times. The perspectives for extension and generalization of such strategies to a variety of thermal-hydraulics problems are real, in view of the ever-increasing computational resources. As to the computational tool employed in this investigation, namely TransAT CMFD code of ASCOMP, we have shown here that it is built with advanced physical models and innovative algorithms: (i) turbulence is treated with LES, V-LES rather than URANS, (ii) two-phase flow is dealt with using ITM's rather than two-fluid approaches, which turns out to be better for (iii) phase-change heat transfer, and (iv) the grids are treated using the Immersed Surface Technique instead of BFC and unstructured grids.

Acknowledgements

This research is financially supported by the NURISP research project of the Euratom 7th Framework Programme (GA n° 232124). The authors wish to thank CEA, EDF and AREVA for having made available the COSI data.

REFERENCES

- S. Banerjee, E. Rhodes, D.S. Scott, "Mass transfer through falling wavy liquid films in turbulent flow", *Ind. Eng. ChE Fundamentals*, 7, 22, 1968.
- P. Coste, "Computational simulation of multi-D liquid-vapor thermal shock with condensation", *Proc. ICMF04 Paper 420*, Yokohama, Japan, May 30–June 4, 2004.
- P. Coste, J. Lavieville, "A Wall function-like approach for two-phase CFD condensation modeling of the pressurized thermal shock," *Proc. NURETH 13*, Kanazawa City, Japan, 2009
- P. Coste, J. Pouvreau, J. Laviéville, M. Boucker, "A two-phase CFD approach to the PTS problem evaluated on COSI experiment", *Proc. ICONE 16*, Orlando, USA, 11-15 May, 2008.

- G.E. Fortescue, J.R.A. Pearson, “On gas absorption into a turbulent liquid”, Chem. Engr. Science. 22, 1163, 1967.
- E.D. Hughes, R.B. Duffey, “Direct contact condensation and momentum transfer in turbulent separated flow”, Int. J. Multiphase Flow. 17, 599–619, 1991.
- S.T. Johansen, J. Wu, W. Shyy, “Filtered-based unsteady RANS computations”. Int. J. Heat & Fluid Flow, 25, 10-21, 2004.
- M. Labois, C. Narayanan, D. Lakehal, “On the prediction of Boron dilution with the CMFD code TransAT: The ROCOM Test Case”, Proc. CFD4NRS 4, Washington, Sep. 2010.
- M. Labois, D. Lakehal, “Very-Large Eddy Simulation (V-LES) of the Flow across a Tube Bundle”, (*submitted*), Nucl. Eng. Design, 2010.
- D. Lakehal, M. Labois, “A level-Set based interfacial heat and mass transfer model built in TransAT”, Proc. ICMF10, Tampa, Florida, USA, May 30 - June 4, 2010.
- D. Lakehal, “LEIS for the prediction of turbulent multifluid flows for thermal hydraulics applications”, Nucl. Eng. Design, (available online: doi:10.1016/j.nucengdes.2009.11.030).
- D. Lakehal, M. Fulgosi, G. Yadigaroglu, “DNS of a condensing stratified steam-water flow”, ASME J. Heat Transfer, 130, 0215011, 2008.
- D. Lakehal, M. Fulgosi, S. Banerjee, G. Yadigaroglu, “Turbulence and heat transfer in condensing vapor-liquid flow”, Phys. Fluids, 20, 065101, 2008.
- D. Lakehal, M. Meier, M. Fulgosi, “Interface Tracking towards the direct simulation of heat and mass transfer in multiphase flows,” Int. J. Heat & Fluid Flow, 23, 242-257, 2002.
- D. Lakehal, S. Reboux, P. Liovic, “SGS turbulence modelling for the LES of interfacial gas-liquid flows”, La Houille Blanche - Revue Internationale de l'Eau, 6, 125-131, 2005.
- J.C. Lamont, D.S. Scott, “An eddy cell model of mass transfer into the surface of a turbulent liquid”, AIChE J., 15, 1215, 1970.
- I.S. Lim, R.S. Tankin, M.C. Yuen, “Condensation measurement of horizontal concurrent steam-water flow”, J. Heat Transfer, 106, 425-432, 1984.
- P. Liovic, D. Lakehal, “Interface-turbulence interactions in large-scale bubbling processes”, Int. J. Heat & Fluid Flow, 28, 127-144, 2007a.
- P. Liovic, D. Lakehal, “Multi-physics treatment in the vicinity of arbitrarily deformable fluid-fluid interfaces”, J. Comp. Physics, 222, 504-535, 2007b.
- D. Lucas *et al.*, “An overview of the PTS issue in the context of the NURESIM project”, Science & Technology of Nuclear Installations, Special Issue on CFD for Gas-Liquid Flows, available on line, (doi:10.1155/2009/583259), 1-13, 2008.
- D. Lucas, D. Bestion, “Review of the existing data basis for the validation of model for PTS”, 6th Euratom Framework Program NURESIM, Deliverable D2.1.2, (2007), Sub-Project 2.
- J. Sievers *et al.*, “Thermal-hydraulic aspects of the International Comparative Assessment Study on RPV under PTS loading (RPV PTS ICAS)”, OECD/CSNI Workshop on Advanced Thermal-Hydraulic and Neutronic Codes: Current and Future Applications, Barcelona, 2000.
- L.M Smith, S.L. Woodruff, “Renormalization-group analyzes of turbulence”. Annual Review of Fluid Mechanics 30, 275-310, 1998.
- C. Speziale, “Computing non-equilibrium turbulent flows with time-dependent RANS and VLES”, Lecture Notes in Physics, Springer Berlin/Heidelberg, 490, 123-129, 1997.
- S. Sussman, P. Smereka, S. Osher, “A Level set approach for computing incompressible two-phase flow”, J. Comp. Physics, 114, 146-161, 1994.
- V. Tanskanen, D. Lakehal, M. Puustinen, “Validation of direct contact condensation CFD models against condensation pool experiment,” Proc. CFD4NRS, Grenoble, France, Sep., 2008
- T.G. Theophanous, R.N. Houze, L.K. Brumfield, “Turbulent mass transfer at free gas-liquid interfaces, with applications to open-channel, bubble and jet flow”, Int. J. Multiphase Flow, 19, 613-623, 1976.
- W. Yao, D. Bestion, P. Coste, M. Boucker, “A 3D two-fluid modeling of stratified flow with condensation for PTS investigations”, Nuclear Technology, 152(1), 129–142, 2005.