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NEW PERSPECTIVES IN THE SIMULATION OF PTS: FROM RANS TO VLES & LES AND FROM PHASE-AVERAGED TO INTERFACE TRACKING METHODS

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Abstract

We report recent LEIS results of steam condensation under violent turbulence and phase-change conditions in the cold leg of the COSI experiment [1], completing earlier efforts on the subject [2, 3]. The LEIS framework, short for Large-Eddy & Interface Simulation [2], is based on interface tracking methods (level set approach) combined with large-scale prediction of turbulence, where super-grid scale turbulence and interfaces are directly solved whereas the sub-scale parts are modelled. Large scale prediction of turbulence is interpreted here broadly, including either the LES or the V-LES (Very Large-Eddy Simulation) variant [4], in which the flow-dependent cut-off filter is larger and independent from the grid, in contrast to LES where it depends on the grid. The interfacial phase-change heat transfer model used is DNS-based, built on the Surface Divergence theory modified to account for high-shear flow conditions using a scale-separation approach. The model is found to return good results: VLES is superior to RANS, but LES seems to remain quite expensive to reach statistically converged results, while it delivers instantaneous local flow-events with valuable details.

Introduction

The modelling of condensation heat transfer has been of major importance in connection with nuclear reactor safety systems, in particular during postulated Pressurized Thermal Shock (PTS). Emergency core cooling (ECC) injection of cold water is one of the most severe scenarios of the global PTS in a pressurized water reactor (PWR). Cold water is injected into the cold leg during a hypothetical loss-of-coolant accident. The injected water mixes with the hot fluid present in the cold leg and 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 thermal-hydraulics transients must be reliably assessed to predict the thermal loads on the pressurized vessel. The coolant can be single- or two-phase flow, depending on the leak size, its location and the plant operating conditions. From a physics-of-fluid viewpoint, various factors play in tandem in such events and may subsequently affect the transients [5, 6]: two-phase flow dynamics, turbulent eddy motions, diffusion of non-condensable fluids and condensation at interfaces, and conjugate heat transfer.

Since Direct Numerical Simulation (DNS) of interfacial heat and mass transfer in general and Direct Contact Condensation (DCC) in particular is still (if ever) not feasible for flows of this scale, resort should be made to interfacial modelling 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 was initially developed for unsheared gas-liquid surfaces and far-field turbulence that is homogeneous and isotropic. The model has since then been first applied to coupled gas–liquid turbulence and scalar exchange across deformable surfaces [7], then to steam-water scenarios [8, 9] involving mild interfacial shear and moderate subcooling conditions. Further, 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.

We report here new results obtained using the SD-based condensation heat transfer model, but within the LES context. A qualitative comparison is made here between LES and URANS and V-LES results published recently [10]. The filter based approach [4] or V-LES [11] is shown to perform better than URANS, and is clearly best suited for high Re flows that are beyond reach of rigorous LES.

1. Model formulation

1.1 The LEIS concept

In TransAT, the single-fluid equations (or Interface Tracking Methods) for incompressible two-fluid flow with phase-change heat transfer are formulated under the form:

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \mathbf{u}\,\nabla \rho = 0 \\
&\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla.\left(\rho \mathbf{u}\mathbf{u}\right) = -\nabla p + \nabla.\,\mu\left(\nabla \mathbf{u} + \nabla^T \mathbf{u}\right) + F_b + F_w + F_s \qquad (1)\\
&\frac{\partial (\rho C p T)}{\partial t} + \nabla.\left(\rho\, CpT\,\mathbf{u}\right) = \nabla.\lambda\left(\nabla T\right) + Q
\end{aligned}$$

where **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 [12]. To track the interface and update material properties, a topology equation is solved for ϕ [13]:

$$\frac{\partial \phi}{\partial t} + \mathbf{u}\,.\nabla \phi = \dot{m} / \rho\left|\nabla \phi\right| \qquad (2)$$

where phase change heat transfer is accounted for by the source term; with $\dot{m}$ being the rate of mass transfer. In the Level Set technique [13], 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 ITMs 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 as ~ 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 momentum diffusion models, e.g. 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 [14]. 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 [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 resolution of the interface topology; higher eddy viscosity levels (by use of RANS) at the interface could hamper the high-frequency surface motions. Be it as it may, advancing the RANS form of the above system of equation in time is referred to as URANS. Since LES is still beyond reach of many practical flow problems, in particular those featuring space development, TransAT promotes the use of an alternative approach known as V-LES, short for Very-Large Eddy Simulation; see section below.

1.2 Turbulence modelling/simulation using VLES

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 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 standard RANS model, 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 U-RANS. The model for sub-scale turbulence is supposed to mimic the diffusive effect of flow motions smaller than the specified filter width. 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, depending on the grid resolution and simulation parameters (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 [10]. We will briefly present this theory; for a more detailed presentation of the model, the reader can refer to [10] and [4].

1.3 Interfacial heat/mass transfer modelling

Interfacial heat 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 or resort is made to analytical or measurement and DNS-based models. The models implemented are based on DNS studies [6, 7]: 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). The models are made sensitive to various types of turbulent Reynolds numbers Re_t, the Prandtl number Pr and turbulent characteristics length-scale of the flow, depending whether use is made of RANS or LES. In SD model, the DNS-based correlation for the interfacial heat transfer rate is determined by:

$$K / u_t \equiv \dot{m} / \rho . u_t = C . \mathrm{Pr}^n . \left[0.3 \left(2.83 \, \mathrm{Re}_t^{3/4} - 2.14 \, \mathrm{Re}_t^{2/3} \right) \right]^{1/4} \mathrm{Re}_t^m \qquad (3)$$

where the model constant C depends on the liquid properties: C = 0.35 for Pr = 1, and = 0.45 for Pr >> 1), and Pr and Re_t exponents 'n' and 'm' are governed by the surface condition and turbulence intensity. In the 'Small-Eddy' models, exponent '*m*' in (3) is set to -1/4, while in the 'Large-Eddy' variant, it is set equal to -1/2; in their original form the surface divergence function (function in brackets in Eq. 3) is set to unity. As to the Prandtl number exponent 'n', it is equal to -1/2 for free surfaces and about -2/3 for surfaces behaving like rigid walls.

The 'SD Scale-Adaptive' model implemented recently in TransAT [3] and used here borrows the 'two-regime' idea from [15], and blends the exponent '*m*' in (3) between -1/4 and -1/2 based on Re_t and the nature of the phase producing interfacial turbulence. In the original work of [15], the threshold between small eddy and large eddy is about Re_t = 500, taken in the liquid bulk considering that turbulence is generated underneath the free surface due to upwelling actions. In various industrial applications, however, turbulence could be generated at the interface due to the imposed gas-side shear, in which case the turbulence Reynolds number should be taken right at the interface, where Re_t could be ten times larger than in the core. More precisely, the model is implemented in TransAT such as '*m* = -1/2' for Re < 3'000, and '*m* = -1/4' for Re > 15'000, with a linear match between these two limits. The question of selecting the right turbulent Reynolds number is posed in the ITM context, too, albeit the concept provides a wider degree of freedom compared to the two-fluid model which compromises the determination of near-interface turbulence properties (in particular U_τ) because of interface smearing. In TransAT, the turbulence Reynolds number can be defined in various ways, depending on the model employed and the nature of the flow:

$$\mathrm{Re}_t = \frac{k^2}{\nu \varepsilon}; \quad \mathrm{Re}_y = \frac{|\Phi| \sqrt{k}}{\nu}; \quad y^+ = \frac{|\Phi| U_\tau}{\nu} \qquad (4)$$

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:

$$L_t \equiv k^2 / \varepsilon . u_t , \quad with \quad u_t = \min \left(|u| , C_\mu^{1/4} k^{1/2} \right) \qquad (5)$$

Alternatively, the second form could be taken, which requires the distance to the interface (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 (ϕ is a distance to the interface). An order of magnitude estimation of these numbers in practical applications is: $Re_t \sim 10^{2\text{-}3} \sim 10^{-3}$ Re in the bulk. At the interface, $Re_y \sim 10\ Re_t$.

2. The numerical approach in the code TransAT

2.1 General structure

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 parallel based algorithm is 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 low-Mach number 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 (1) interface tracking techniques for both laminar and turbulent flows (level set, VOF with interface reconstruction, and Phase Field), (2) phase-averaged homogeneous mixture model (Algebraic Slip), and (3) Lagrangian particle tracking (one-to-four way coupling).

2.2 IST/BMR meshing techniques

To mesh complex geometries, use is made of the Immersed Surfaces Technology (IST) developed by ASCOMP and implemented in TransAT. The underpinning idea is inspired from Interface Tracking techniques for two-phase flows: the solid is described as the second ‘phase’ with its own thermo-mechanical properties. The technique differs substantially from the Immersed Boundaries method, in that the jump condition at the solid surface is implicitly accounted for, not via the penalty approach. It has the major advantage to solve conjugate heat transfer problems. The solid is first immersed into a cubical grid covered by a Cartesian mesh. The solid is defined by its external boundaries using the solid level set function. Like in fluid-fluid flows, this function represents a distance to the wall surface; is zero at the surface, negative in the fluid and positive in the solid. The treatment of viscous shear at the solid surfaces is handled very much the same way as in all CFD codes. To better resolve boundary layers, IST is complemented by the BMR (block mesh refinement) technique, where additional refined sub-blocks are automatically generated around solid surfaces, with dimensions made dependent on the Reynolds number (based on the boundary layer thickness) and desired y^+ for wall treatment (low Re model or wall functions). This IST/BMR method can save up to 75% grid cells in 3D, since it prevents clustering grids where unnecessary.

3. PTS in the COSI experiment

3.1 Problem setup

The COSI experiment (short for COndensation at Safety Injections) mimics a 1/100 scale in power PWR Framatome reactor [1]. 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. 1). 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 N^0 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.

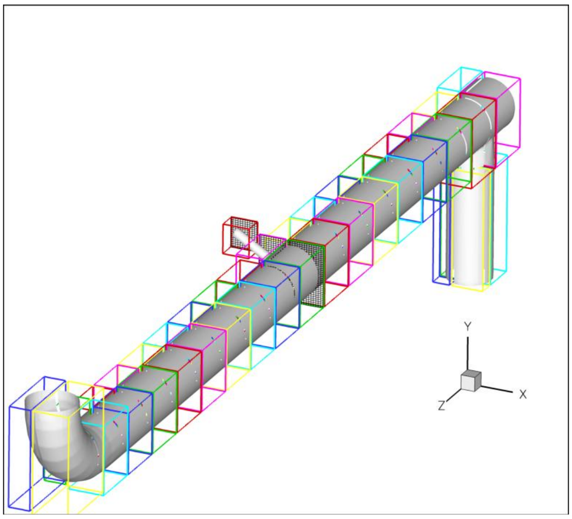

Figure 1: Computational multi-block domain and grid using IST/BMR.

Here we have employed LEIS combining V-LES and level set (Eq. 2) modified to account for phase change heat transfer using (Eqs. 3-5). The grid was generated using the IST method for meshing, 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 results of the coarse grid simulation are available in our former contributions [2]. The final grid consists of one 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 both time and space discretization. The overall simulation time was 135 H on a 4 processors PC under LINUX. Parallel scaling under these conditions is actually not meaningful, but it was still around 100% using OpenMP parallel protocol (no MPI). The same problem was tested – not run till convergence though - on leading MPI supercomputer (256 Proc.); it showed a speedup factor of 25 using MPI protocol. The convergence criteria set for pressure was (maximum) 0.5e-3 for each time step. Mesh sensitivity study has revealed that a 1 million cell provides virtually the same results as a 2 million cell mesh. To reduce any numerical errors, the aspect ratio of the grid was limited to 1.2. No error analysis was conducted in the sense of VUQ.

3.2 VLES transient results

In this section, only V-LES simulation results are discussed. Qualitative flow features are depicted in Fig. 2, 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), and turbulent kinetic energy fields as the flow mixes downstream towards the downcomer. Note that these are taken from a late instant where the flow stabilizes reaching almost steady state condition (not to confuse with ergodic time averaged results). The deformations of the sheared surface are most intense in the region below water 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 first panel of Fig. 3. TKE contours depicted in the lowest panel of Fig. 2 suggest that turbulence is essentially generated at the gas-side of the surface due to interfacial friction, but more intensively around the jet and immediately downstream. This suggests that most of the condensation occurs indeed in these zones, which is well confirmed when looking at the 2D snapshot shown in the second panel of Fig. 3.

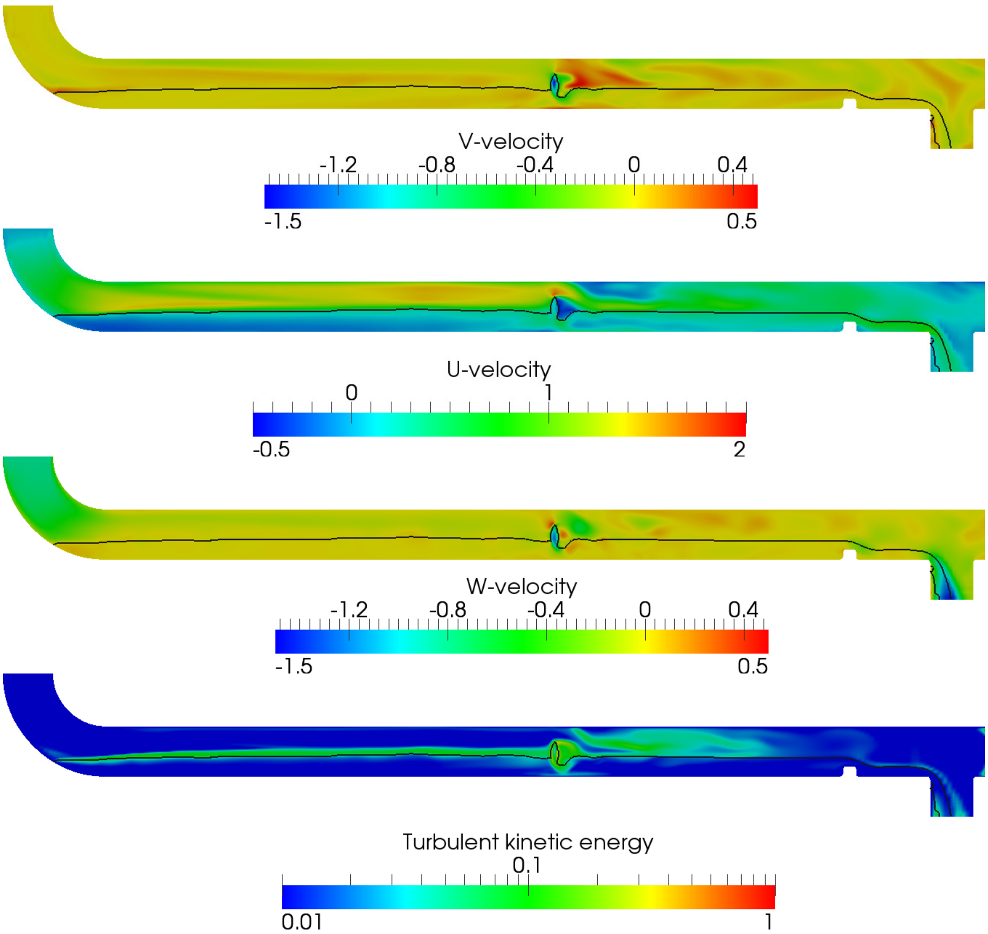

Figure 2: surface deformations at the injection and velocity and TKE contours

Figure 4 depicts several cross-flow planes inside the cold leg, showing time-averaged secondary velocity vectors and magnitude, interface level, condensation rate and temperature contours. Only selected results are shown here; more details can be found in [3]. The figure depicts the time-average (the instantaneous pictures show more vigorous deformations) water level in the leg subsequent to coolant injection at injection level only. 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 at other cross-flow locations (results not shown here) show that the cooling along the leg occurs on the side, not at the centre, even when analysed under time-averaged conditions. The heat diffuses from the steam to the water in the leg rather gradually prior to injection, and more sharply downstream. 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.

The results of steam condensation rate (normalised by the experimental value) are discussed in the context of Fig. 5. 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.

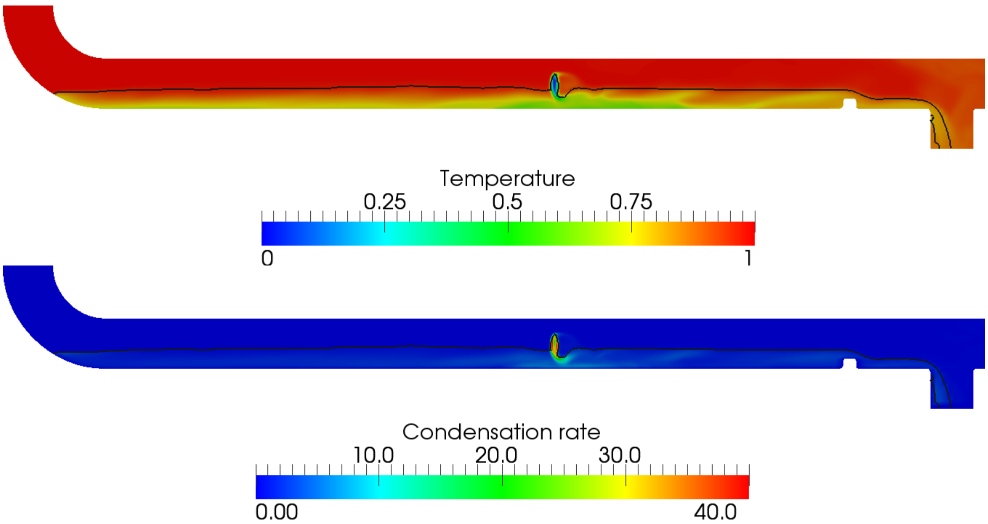

Figure 3: Late instantaneous snapshots of temperature and steam condensation rate contours

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 to achieve ergodic steady state conditions and storage resources, as discussed next. Note that the COSI problem has been simulated using the two-fluid-based code NEPTUNE_CFD, using URANS for turbulence and other interfacial phase change models [16-18].

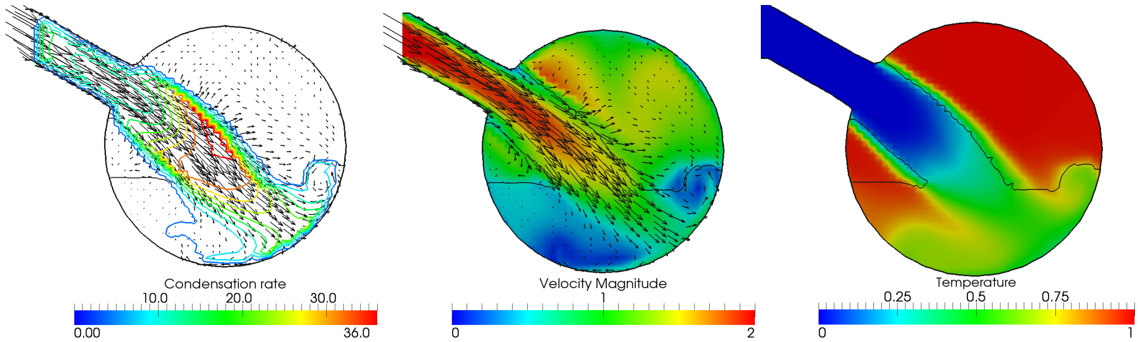

Figure 4: Cross-sectional contours of condensation rate, velocity and temperature

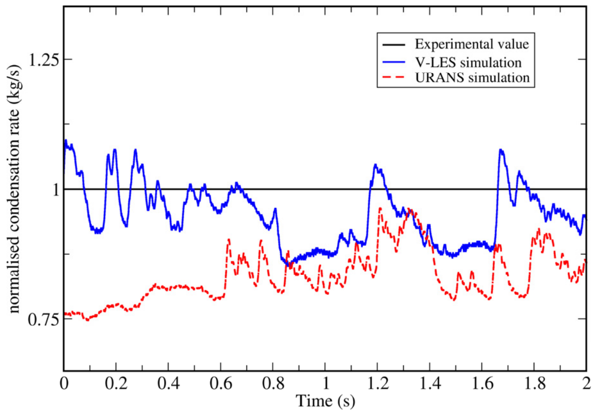

Figure 5: Time evolution of condensing steam rate: URANS and VLES vs. experiment

3.3 New LES results

The flow has been calculated now using LES, where the transport equations (1) were filtered, and subgrid scale quantities were modelled using the Smagorinsky model, modified to account for near interface decay of turbulence [14]. The grid was finer than the one employed in VLES, consisting of two million cells (87x65x387) with 50x50 nodes for the pipe. Second order central scheme was employed for space discretization, and 3rd order RK scheme for time marching. The overall simulation time was 440 H on a 8 processors PC, using OpenMP parallel protocol. For LES TransAT uses explicit time stepping rather than implicit. Werner and Wengle's [19] Wall Functions were employed. An initial turbulent field was generated based on the wall shear. Time stepping was reduced by one order compared to implicit VLES (CFL~0.1-0.3 against ~0.5-0.8).

The energy spectra of the fluctuating velocity components taken before and after injection at x/D=7.5 and 10 (injection is at x/D=9.2) are shown in the upper panel of Fig. 6; those of the interface deformations taken at same locations in the lower panel. The spectra depict a strong turbulence activity in the near injection zone, with decay slopes oscillating between -5/3 and -2/3. The streamwise velocity fluctuations carry more energy than the other components before injection, while a sort of isotropy in energy distribution takes place in the post injection area. The decay behaviour is totally different from pre- to post-injection. The oscillation of the water holdup beyond injection reveals how surface fluctuations correlate with turbulence intensity.

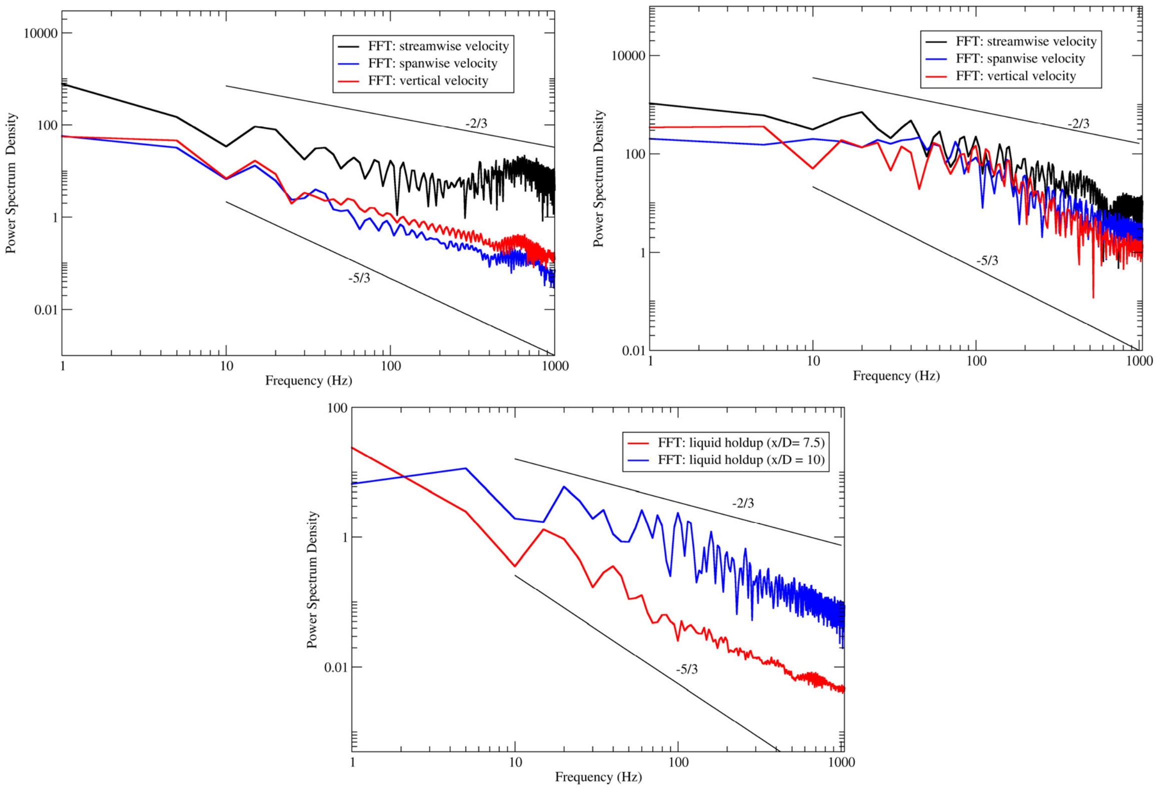

Figure 6: Energy spectra of the velocity fluctuations (upper) and interface deformations (lower)

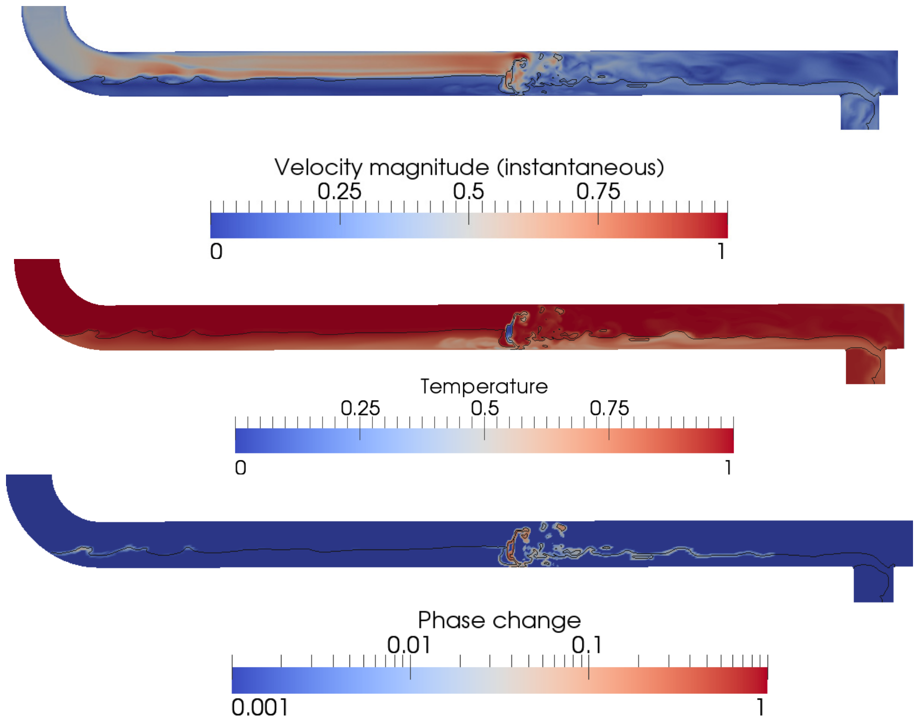

Figure 7: Snapshots of temperature and steam condensation rate contours

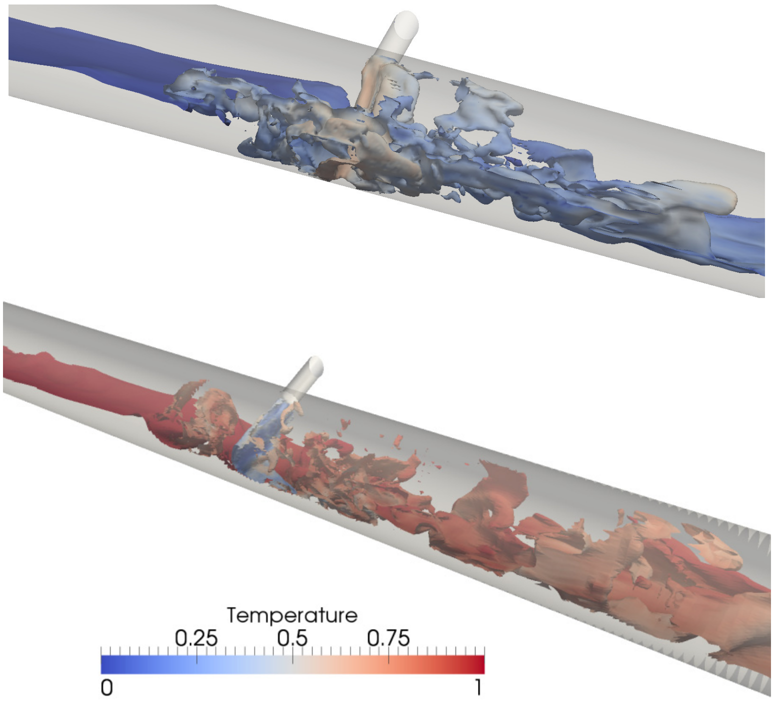

Figure 8: 3D snapshots of steam condensation rate and heat contours with surface deformations

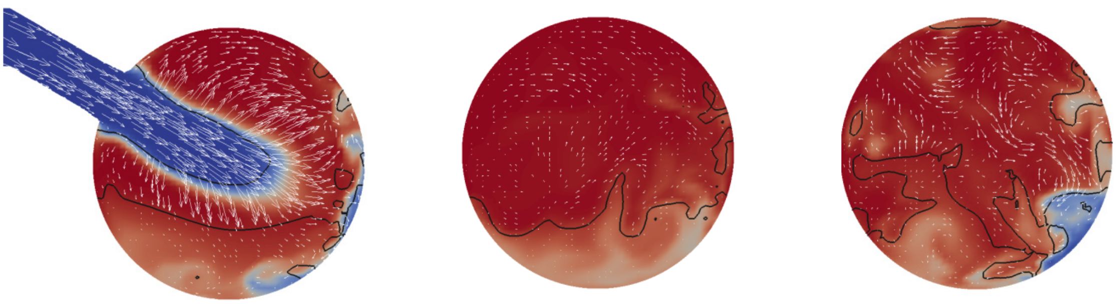

Figure 9: Cross-sectional surface deformations, velocity vectors and contours of temperature

The results depicted in Figs. 7-9 reveal that the LES is amenable to reproduce more transient and small scale motions as compared to RANS and VLES. Fig. 7 reveals in particular the prediction of Kelvin-Helmholtz type of interface instability, prior to injection, which were not observed in VLES and URANS simulations. Figs. 8 and 9 show the interaction between turbulent flow and topology changes in the vicinity of coolant injection. The rate of heat mixing is significantly affected by these interactions, a feature that is out of reach of URANS for instance, and is very critical for predicting thermal stripping. The other side of this superiority of LES is that the simulations require longer reaching statistical convergence than VLES and obviously URANS. Regardless of that aspect, LES could actually provide a faithful instantaneous picture of might be expected to happen in ECC injection problems in localised regions of the leg.

4. Conclusions

The paper describes the way computational thermal-hydraulics is migrating to more sophisticated modelling techniques. The novel modelling technique transcends phase-averaged models for two-phase topology description combined with RANS for turbulence by integrating interface tracking methods within the LES and V-LES framework, referred to as LEIS. The scale-adaptive SD model is integrated to account for condensation. For mesh generation, use is made of the Immersed Surfaces approach. The combined approach can be successfully employed to generate realistic transient simulations in reasonable computing times. The perspectives for its generalization to a variety of thermal-hydraulics problems are real and should be further explored.

The present extensive simulation campaign reveals though that the key success of the model is the way interfacial shear under turbulent conditions is determined. The extension of the mass transfer models by blending the exponent based on turbulence strength was meant to clearly distinguish the low-to-medium from the strong turbulence case, which will obviously remain a problem-dependent issue. Similarly, predicting correctly the water depth in this class of flows is another key issue, which the modelling strategy should overall be capable to maintain to the right level, otherwise the results will be biased. Overall VLES is superior to URANS and returns excellent mass transfer results. While LES seems to remain quite expensive to reach statistically converged results, it can deliver instantaneous local flow-events with valuable flow details.

Acknowledgements

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