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Project Report

An Overview of the Pressurized Thermal Shock Issue in the Context of the NURESIM Project

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Within the European Integrated Project NURESIM, the simulation of PTS is investigated. Some accident scenarios for Pressurized Water Reactors may cause Emergency Core Coolant injection into the cold leg leading to PTS situations. They imply the formation of temperature gradients in the thick vessel walls with consequent localized stresses and the potential for propagation of possible flaws present in the material. This paper focuses on two-phase conditions that are potentially at the origin of PTS. It summarizes recent advances in the understanding of the two-phase phenomena occurring within the geometric region of the nuclear reactor,that is, the cold leg and the downcomer, where the "PTS fluid-dynamics" is relevant. Available experimental data for validation of two-phase CFD simulation tools are reviewed and the capabilities of such tools to capture each basic phenomenon are discussed. Key conclusions show that several two-phase flow subphenomena are involved and can individually be simulated at least at a qualitative level, but the capability to simulate their interaction and the overall system performance is still limited. In the near term, one may envisage a simplified treatment of two-phase PTS transients by neglecting some effects which are not yet well controlled, leading to slightly conservative predictions.

1. Introduction

Pressurized thermal shock (PTS) in general denotes the occurrence of thermal loads on the reactor pressure vessel (RPV) under pressurized conditions. PTS was identified by the European project EUROFASTNET as one of the most important industrial needs related to nuclear reactor safety since the integrity of the RPV has to be assured throughout the reactor lifetime; it is one of the barriers against fission product release, and its replacement is not feasible. A very severe PTS scenario is cold water emergency core cooling (ECC) injection into the cold leg during a hypothetical small-break loss of coolant accident (SB-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 (see Figure 1). High thermal gradients may occur in the structural components while the primary circuit pressurisation is partially preserved. Therefore, the transient fluid temperature must be reliably assessed to predict the loads upon the RPV and the pressure wall toughness. The cooling fluid can either be in single-phase or in two-phase condition, depending on the leak size, its location, and on the operating conditions of the nuclear power plant considered. The PTS has been the objective of a number of international cooperative programmes in the past, for example, the OECD-ICAS as given by [1].

PTS-scenarios were considered in the NURESIM project for the French 900 MW CPY PWR, the German 1300 MW Konvoi reactor, the Loviisa 500 MW VVER, and the Russian VVER-1000. Typical diameters of the cold leg are between 700 mm and 850 mm while the sizes of the ECC injection nozzle vary between 170 mm and 225 mm. Loss of coolant accident (LOCA) scenarios, with different leak sizes and leak locations, are considered as initial events leading to ECC injection, which can create PTS situations. For all the scenarios, there is a high-pressure injection (HPI) into the cold leg. For some of the scenarios, the pressure can be stabilized to remain within single-phase flow conditions in the cold leg. However, for all reactor concepts, there are also scenarios that lead to two-phase flow situations in the cold leg. Injection from the hydroaccumulators needs to be considered in addition to the HPI. While the accumulators are connected to the cold leg for some PWR, the accumulators inject the cooling water into the downcomer and into the upper plenum in case of the VVER reactors. In the two-phase flow scenario, the cold leg is either partially uncovered or totally uncovered. Both situations have to be covered by two-phase flow simulations; in particular, stratified flow with a void fraction range from 0 to 100% needs to be considered for a partially filled cold leg.

In all the two-phase flow scenarios, the pressure is below 7.5 MPa. The liquid flow rates in the cold leg at the exit of the pumps are close to zero but may have fluctuations in the range from -100 kg/s to $+100$ kg/s. Maximum steam flow rates in the considered scenarios are up to 50 kg/s in case of a steam flow from the downcomer towards the steam generator and up to 15 kg/s for a flow from the steam generator towards the downcomer. Mass flow rates from the HPI are limited to a maximum value of 80 kg/s, while the temperatures are in the range between 283°C and 298°C. The maximum accumulator flow rates for the reactor designs with an injection into the cold leg are up to 30 kg/s. The temperature of the injected water is between 25°C and 60°C.

The PTS work package within the frame of the NURESIM Integrated project of the 6th Framework Programme focuses on a two-phase flow configuration resulting from a partially or fully uncovered cold leg. In the case of a partially uncovered cold leg, a stratification of cold water on the bottom of the cold leg with counter-current flow of hot water and steam on top of this cold-water layer may occur (see Figure 1). There is a mixing between hot and cold water. Condensation takes place at the free surfaces of the cooling water jet and of the stratified flow. The process is strongly dependent on the turbulence in the fluids. If the water level in the downcomer has dropped below the cold leg nozzle, cold water is injected into vapor with direct contact condensation on the steam-water interface and heating along walls of both the cold leg and the downcomer. Stripe cooling will occur in the downcomer. Direct contact condensation (DCC) is of prime importance in this situation since it is the main heat source for the cold water. Interfacial transfers (momentum—including turbulence—mass and energy) have then to be considered in the jet area as well as in the stratified flow.

As shown in Figure 1, different flow phenomena occur. There are flows with separated surfaces (jet interface, horizontal interface), but also dispersed flows occur due to bubble entrainment (at jet impingement and possibly also in the horizontal flow region by entrainment caused by waves). Since there is a strong thermal nonequilibrium at these interfaces, momentum transfer as well as heat and mass transfer have to be considered. The various two-phase phenomena taking place are strongly coupled, both within the fluids and in regard to the heat transfer to walls. The different phenomena depend on very different characteristic length-scales, from the size of the smallest eddy up to the system scale. Some of the involved phenomena are not yet well understood regarding their physics. The simulations of the whole system during the ECC injection process and then accurate reproduction of the thermal loads on the RPV are thus a considerable challenge.

In detail, the following “geometrical” flow regions or flow patterns connected with the listed single phenomena can be distinguished for the two-phase PTS situation (e.g., [2], see also Figure 1).

(i) Free liquid jet:
   (a) momentum transfer at the jet interface, including instabilities,
   (b) splitting of the jet,
   (c) condensation on the jet surface.

(ii) Zone of the impinging jet:
   (a) surface deformation by the jet including generation of waves,
   (b) steam bubble entrainment,
   (c) bubble migration and de-entrainment,
   (d) turbulence production below the jet.

(iii) Zone of horizontal flow:
   (a) momentum exchange at the gas-liquid interface, including generation of waves and growth or damping of these waves,
   (b) heat and mass transfer (condensation) at the gas-liquid interface including its influence on the momentum transfer,
   (c) heat transfer to the walls,
   (d) turbulence production at the interface,
   (e) turbulence production at the walls,
   (f) influence of the phase change on turbulence and on wave pattern,
   (g) mixing/stratification of hot and cold water streams.

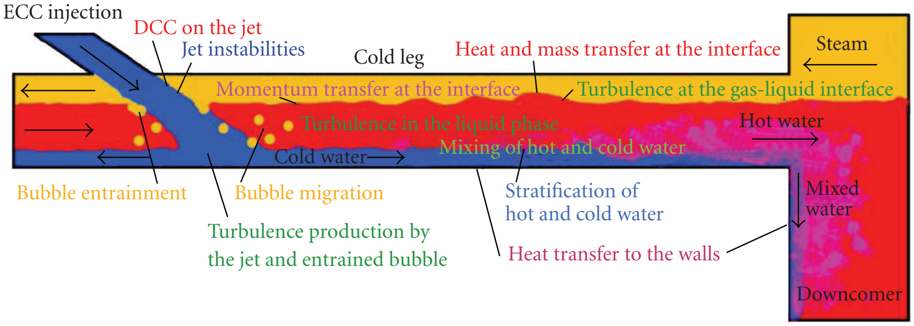

Figure 1: Most important flow phenomena during a PTS situation with partially filled cold leg.

(iv) Flow in the downcomer in the case of a partially filled cold leg:
  (a) turbulence production at the walls,
  (b) mixing/stratification of hot and cold water,
  (c) heat transfer to the walls.

(v) Flow in the downcomer in the case of the water level being below the cold leg nozzle:
  (a) separation of the incoming water jet from the downcomer wall or not,
  (b) momentum transfer at the jet interface, including instabilities,
  (c) splitting of the jet,
  (d) phase change at the jet surface,
  (e) heat transfer to the walls.

There are strong interactions between the listed flow regions and related flow patterns. The effect of noncondensable gases has to be considered due to nitrogen degassing from ECCS water.

It is not possible to reproduce experimentally in full scale, the whole ECC injection process, starting from the injection location to the inner downcomer, considering the various two-phase flow regimes. Reliable numerical simulations are required, and two-phase PTS constitutes one of the most challenging exercises for a computational fluid dynamics (CFD) simulation. Improvements of the two-phase modelling capabilities have to be undertaken to qualify the codes for the simulation of such flows. A really accurate simulation of all the phenomena that occur in the scenario will only be possible in the far future. To reach this aim, it is necessary to go step-by-step and to improve the quality of the forecasts. However, the use of CFD in industrial studies related to PTS is already possible, but with some limitations.

The main goal of the NURESIM project is the development of a common European multiscale and multidisciplinary platform for NUclear REactor SIMulation (NURESIM). During the current NURESIM project, the simulation of PTS, including DCC scenarios, should be enhanced beyond the current state of the art by improving substantially the two-phase flow modelling capabilities of current CFD-codes. The Neptune_CFD (see [3, 4]) code is used as the initial framework for the common platform, and both the CFX and FLUENT CFD tools are also used for PTS investigations.

Within the above framework, the objective of the paper is on the one hand to provide a critical evaluation on the present status in the simulation of thermal-hydraulic aspects of PTS and on the other hand to show how the NURESIM project uses available experimental data for improving and validating the models. A detailed presentation of scenarios leading to two-phase PTS situations as well as a discussion on the status of CFD capabilities for PTS at the beginning of the NURESIM was given by Lucas [5].

2. Experimental Data Basis

CFD methods use many turbulence and two-phase flow models which have a certain degree of empiricism. The accuracy and universal validity of these models have to be assessed by comparison of the numerical results with experimental data. Depending on the suitability of the data, test cases are used for validation and calibration of statistical models and for demonstration of model capabilities.

2.1. Validation Experiments. Validation cases focus on separate effects as they test different aspects of a CFD code and its physical models. The successful simulation of the single separated effects is a prerequisite for a complex industrial PTS flow simulation. In a validation test, the quality of the statistical model is checked for a given flow situation. Validation tests are the only method to minimize and quantify modelling errors and to ensure that new models are applicable with confidence to certain types of flows. In an ideal case, a validation test case gives sufficient details to allow for an improvement of the physical models. In NURESIM, validation data are also obtained from direct numerical simulation (DNS) studies.

In the NURESIM database [6], test cases were selected which clearly identify the main features of the CFD models that are to be tested and which are dominant in the validation case. In order to ensure completeness of information, all experiments are described according to the following template:

(i) general description and flow features,

(ii) description of measurements and geometry,

(iii) detailed information on boundary and initial conditions,

(iv) availability of experimental data,

(v) information on previous work and related experiments.

Next to the completeness of the data, their quality is of primary importance for a successful validation exercise. The quality of the data is mainly evaluated by error bounds provided by the experimentalists. Unfortunately, most experiments still do not provide this information. Moreover, even if error estimates are available, they cannot exclude systematic errors by the experimentalist. In addition to error bounds, it is therefore desirable to have an overlap of experimental data, which allow for testing of the consistency of the measurements. To this end, experiments have been gathered investigating the same or similar PTS phenomena but performed by different experimental groups in different facilities using different experimental techniques.

Experiments investigating jet impingement on a free surface and bubble entrainment were performed by Bonetto and Lahey [7] and Iguchi [8] as follows.

(i) The Bonetto and Lahey experiment investigates jet impingement on a free surface using an axisymmetric, turbulent jet impinging orthogonally on a free surface. The flow was statistically steady-state; the fluid was water in an air environment. A laser Doppler anemometer (LDA) system was used to measure the liquid gas velocities (both mean and fluctuations), and both a fiber phase-Doppler anemometer (FPDA) and an impedance probe were used to measure the void fraction, depending on the bubble size created by the impinging jet. The void fraction was measured at varying depths below the undisturbed surface.

(ii) A turbulent nonfragmented water jet impinging on a free surface in air environment was investigated by Iguchi et al. [8] at the University of Hokkaido. LDA was used to measure mean velocities and RMS values of the vertical and radial velocity below the free surface. However, no measurements of bubble entrainment were made.

Air water flows in horizontal channels were investigated at Forschungszentrum Dresden-Rossendorf (FZD) by Vallée et al. [9] and at INP Toulouse by Fabre et al. [10]:

(i) A horizontal channel with rectangular cross section was built at FZD for the investigation of co- and counter-current air water flow at atmospheric pressure. The measurements were focused on the behaviour of slug flow. Optical techniques, like video observation, were used to record the flow pattern and to determine the water level. Velocity-fields are measured using particle image velocimetry (PIV). Data is available for all NURESIM partners on the basis of bilateral agreements.

(ii) In the Fabre experiment, air-water turbulent stratified flow was investigated in a quasi horizontal (descending) rectangular channel. Systematic measurements of the components of the mean velocities and Reynolds stresses were performed with LDA and hot wire anemometry under carefully controlled inlet conditions. The data was used by [11] for validating the turbulence modelling near a free surface and below the free surface in the liquid including the interfacial production terms in adiabatic conditions. Selected data is made available to NURESIM partners by CEA.

Stratified steam water flows with condensation were investigated by Lim et al. [12] and Ruile [13] as follows.

(i) Lim investigated steam-water turbulent stratified flow with condensation in a horizontal channel with a rectangular cross-section. In the experiment, Pitot tubes were used to measure the local mean steam velocity, and conductivity probes to measure the water height at five locations. The data was used to validate interfacial condensation models by Yao et al. [14].

(ii) Ruile [13], Hein et al. [15], and Goldbrunner [16] investigated contact condensation in horizontal stratified flows of subcooled water and saturated steam in the LAOKOON test facility at the University of Munich. The experimental equipment was designed to set up co-current and counter-current flow conditions in a straight channel with adiabatic walls. Available measured data include the water and steam flow rates at the water feed cross section, the inlet water temperature, and the temperature distribution across the water layer at one location, where a vertical array of thermocouples was installed. The pressure level inside the channel and the water layer height were also measured. Data for selected test cases is available for NURESIM partners.

Water hammer in a horizontal section of a steam-line, induced by the injection of the cold water, was experimentally analysed at PMK-2 test facility of the Hungarian Atomic Energy Research Institute KFKI [17]. For the NURESIM project, mesh sensor data can be useful for the development and verification of the heat and mass transfer models in a horizontally stratified flow. However, it is well known that due to the Helmholtz instability measurement error can be as large as 50%.

Condensation pool studies were performed in the Nuclear Safety Research Unit at Lappeenranta University of Technology, LUT [18]. They were designed to correspond to the conditions of a postulated accident in BWRs in Finland. In the first tests, the formation, size, and distribution of noncondensable gas bubbles were studied in the condensation pool facility POOLEX. In the frame of the national SAFIR programme, steam instead of noncondensable gas was injected into the condensation pool test rig in order to study bubble dynamics issues such as bubble growth, upward acceleration, detachment, and breakup. The experiments usually consisted of several individual steam blows, where the key parameters of the experiments (pool subcooling, steam mass flux) were varied. High-frequency instrumentation and a high-speed camera were used in the experiments. Structural loads were evaluated with the help of strain gauge measurements.

2.2. Demonstration Experiments. The purpose of a demonstration exercise is to build confidence in the ability of a CFD method to simulate complex flows. While validation studies show for a number of building block experiments that the physical models can cover the basic aspects of the PTS application, demonstration cases test the ability of the CFD methods to predict combined effects, including geometrical complexity. Typically, the level of completeness of the data for demonstration cases is much lower than for validation cases. Even though the density of data is usually lower, the NURESIM selection required that the quality satisfies the same criteria as for validation cases. Error estimates are desirable and so are independent measurements.

Suitable demonstration experiments were selected with complex flow phenomena for PTS-scenarios as follows.

(i) The 1 : 2 scaled HYBISCUS experiments where local temperature measurements were taken in the cold leg and in the downcomer of a PWR simulating ECC-injection. However, data is property of EDF and only available on special bilateral agreement.

(ii) The COSI experiments (see [19]) which provide temperature measurements for ECC injection scenarios in a cold leg with focus on direct contact condensation in the injection zone. The analysis of COSI tests data concluded that the jet-induced local turbulence in the water was the main phenomenon controlling the global condensation rate since most of the total condensation occurs close to the jet where this jet-induced turbulence enhances heat mixing below the free surface. Data is property of CEA and EDF, and there is no published data available.

(iii) Selected 1 : 1 scaled UPTF experiments where condensation and mixing phenomena during ECC injection were studied in the test series TRAM C1 and TRAM C2. Temperature measurements were taken in the cold legs, downcomer, lower, and upper plenum and in the core region. A detailed description of the geometry, the instrumentation, and selected data is made available in the frame of the NURESIM project.

(iv) The 1 : 48 volumetrically scaled ROSA test facility which was originally designed for the investigation of system behaviour. However, several spinoff experiments in the ROSA-IV and ROSA-V test programmes are focused on stratified flows. Data for temperature and concentration measurements are restricted to the ROSA group. Future experiments are planned with focus on the simulation of ECC injection and temperature stratification.

(v) Structural mechanics data resulting from thermal stresses assuming PTS conditions are also made available in the NURESIM database. They relate to thermal shock cryogenic experiments on steel plates which were performed at the University of Pisa, DIMNP.

Although there are a number of experiments available where flow phenomena are investigated as separate effects and as integral effects, there is still a need for well-instrumented validation data and demonstration experiments where experimental parameters are varied in order to investigate PTS phenomena. The data are required in a high resolution in space and time for the whole domain of interest and should include local and time-dependent information on interface between the phases, mean, and fluctuations (turbulence parameter) values for temperature and velocity.

For this purpose, the *TOPFLOW PTS experimental programme* has been conceived. Its objective is to provide a well-informed experimental database for both validation of CFD modelling of the two-phase flow in the cold leg and the downcomer including flow-wall heat transfer, and the improvement of the understanding of key thermal hydraulic (TH) phenomena involved. Besides the operational standard instrumentation (pressure, differential pressure, temperature, flow rates), the instrumentation will comprise thermocouples, heat-flux probes, wire-mesh sensors, local void probes equipped with a microthermocouple, high-speed camera observation, infrared camera observations and a local conductivity probe. It is planned to operate the test mockup in steady-state conditions with and without mass transfer due to condensation as well as in transient operation.

3. CFD Capabilities for the Simulation of Two-Phase PTS

3.1. Free Liquid Jet. The cold liquid jet injected into the horizontal cold leg pipe interacts first with the surrounding hot steam environment. These interactions are strongly dependent on the position and shape of the interface between the cold water and the hot gaseous environment. Interface tracking methods (ITM) are needed for a detailed description of these interactions. Depending on various characteristics of both the liquid and the gas, such as the relative velocity between the two phases or turbulence properties, instabilities at the surface of the jet can occur. Instabilities can also be directly generated by the condensation process [20]. They affect the heat and mass transfer. Models for DCC at the jet surface have to be applied. The instabilities also influence the gas entrainment at the jet impingement point on the liquid surface by capturing gas. Adequate modelling of the interface, in connection with a suitable coupling of the turbulence fields of the single phases and local mass and heat transfer, is needed.

Numerous theories relating to mechanisms on generation and growth of jet instabilities exist. Several numerical approaches have been used, such as DNS or large-eddy simulation (LES) for the prediction of their behaviour using various conditions [21, 22]. Even if the individual effects of some parameters, such as gravity or nozzle internal flow, have been separately studied, no computations exist taking into account all these effects simultaneously. Actually, some models for the treatment of these instabilities are based on restrictive assumptions, which limit strongly their applicability. The LES approach seems the most suitable for the modelling of this specific flow situation, not presuming what would be the best choice for the simulation of the whole PTS.

DCC at the jet surface resulting from the temperature difference between the two phases is responsible for a non-negligible part of the total condensation in the considered flow domain of the cold leg [19]. For the condensation rate at the jet surface, correlations exist [19], but no representative experimental data are available to confirm this model. No special models were developed for DCC at the jet surface. The variations of the condensation rate along the jet and the effects of the noncondensable gases have been qualitatively reproduced [23], but the quantitative prediction was not fully mature.

3.2. Zone of the Impinging Jet.

Appropriate modelling of the turbulence production below the jet is highly important, since turbulence is responsible for the mixing of the fluid. Gas entrainment caused by the jet impingement influences the characteristics of the turbulence below the free surface. The properties of the entrained gas (e.g., bubble size, penetration depth, horizontal migration, and total amount of entrained gas) are dependent on various properties of both phases and jet. The jet velocity is one of the most critical parameters. Depending on it, several scenarios for the gas entrainment below the free surface have already been experimentally identified [24, 25]. Most of the attempts for the development of theories able to reproduce the properties of the entrained gas below the free liquid surface have resulted in global correlations, which are limited to the corresponding operating conditions and geometric configuration. Several studies have highlighted the absence of theoretical approach and of valid correlations for the prediction of the minimal jet velocity at which the gas entrainment occurs. The modelling of the impinging jet zone requires simultaneous consideration of separated (surface) and dispersed (bubbles) flow within one flow domain.

Two issues have to be considered regarding turbulence production: the turbulence generated by the impingement of the jet itself and the influence of the bubbles on the turbulence. In the NURESIM project, investigations are done on the turbulence production below the jet by CEA and University of Pisa which simulated [8] tests of a plunging jet [26]. Together with Neptune_CFD standard models, a CEA/Grenoble modified k-ε model was tested. Quite good agreement with experimental data was achieved with best performing models: numerical predictions of the mean velocity field were always good, and turbulence was generally not bad but with significant underestimation far from the jet axis region.

In most simulations, the effect of the liquid turbulence on the bubbles is modelled, but the opposite effect (corresponding to the influence of the bubbles on the liquid turbulence field) is only considered in regards to the turbulent viscosity, for example, using the Sato model [27], despite this effect being important in the dense bubble region (near the impingement point). Some studies have thus to be conducted to improve understanding and modelling of the coupling between these various processes.Both LES and RANS models can be used for the simulation of the zone of the impinging jet. A more general investigation on the applicability of RANS and LES models for bubbly flow, including bubble plumes, was undertaken in the frame of the NURESIM project by PSI.

In the impinging jet zone, four different interface structures have to be considered: (1) the surface of the jet, (2) the free surface of the pool (i.e., liquid level in the cold leg), (3) the entrained bubbles, and (4) the complicated surface structure in the region where the jet impacts the surface. Separated (jet surface and pool surface) as well as dispersed (bubbles) flow regions exist simultaneously in one flow domain. The most difficult thing is to model the transitions between the two types of interfaces (i.e., bubble entrainment and de-entrainment). For the different interfacial structures, different closure models are needed, for example, for drag. The identification of the interfaces for separated flows is thus of crucial importance.

Some computations of the whole plunging jet process (starting from the jet, to the bubble de-entrainment, considering the impingement zone, the bubble migration below the free liquid surface and the free surface) have been performed with some success in the past [28]. These were able to reproduce the global behaviour for the free liquid surface (small waves at the free surface and shape at the impingement point), the gas entrainment, the bubble migration below the free surface, and the bubble de-entrainment at the free surface. Even if the entrainment process has been more or less well reproduced numerically (generation of entrained bubbles at the impingement point), the total volume flow rate of entrained gas has been largely overestimated. One of the most critical problems pointed out during these computations is the treatment of the liquid/gas interfaces. To overcome the discrepancies, the two kinds of interface mentioned above have to be modelled using two different models (or at least the same model with different values for the parameters). In the frame of the NURESIM project, investigations are done by FZD regarding these problems. This resulted in the suggestion to use so-called algebraic interfacial area density (AIAD) models which allow to apply two different drag coefficients for free surface and for bubbly flow. A blending function based on the gas void fraction is used to apply the adequate drag coefficient depending on the flow regime.

The behaviour of the entrained gas bubbles below the free liquid surface is determined by several forces acting on individual bubbles. The most important of these forces are buoyancy, drag, virtual mass force, lift force, and turbulent dispersion force. All these forces are strongly dependent on the bubble size (see, e.g., [29]). For bubbly flow in vertical pipes, a combination of Tomiyama lift- and wall force together with the Favre-averaged drag force [30] was found to reflect the experimental findings in poly-dispersed flows [31]. In the case of developing flows, some differences have been pointed out between calculations and experimental data [32]. In the frame of the NURESIM project, the influence of the bubble forces on bubble migration is investigated by FZD for an impinging jet configuration.

In most computations, the bubble diameters are assumed to be constant. In principle, CFD models which allow consideration of a number of bubbles classes already exist [33], but calculations are then very time consuming. The bubbles size distribution is strongly influenced by bubble coalescence and breakup, for which various models exist in the literature (e.g., [34–36]). The models for bubble forces, as well as the models for bubble coalescence and breakup, have consequently to be validated for the plunging jet configuration.

There are also some attempts on a direct tracking of interfaces at zone of the jet impingement. Interface tracking techniques have indeed been applied, in combination with LES of the fields in each phase, to interfacial, sheared, two-phase flow [37, 38]. These authors incorporated the VOF approach to an LES simulation and applied it to the case of air/steam injection into a water pool, as investigated previously by Meier [39]. It is obvious that the available computational resources will not allow this approach to be used to capture the details of a dispersed bubbly flow; the routinely used two-fluid formulation remains much less demanding. Nevertheless, the LES/VOF combination may be a candidate future technique for tackling flows involving large interfacial inclusions. Novel analytical developments to the method have now been made by Liovic and Lakehal [38], namely, in the treatment of turbulence near sheared deformable interfaces.

3.3. Zone of Stratified Flow in the Cold Leg. In the horizontal cold leg pipe, a stratified flow has to be considered. In the context of PTS, the interface is characterised by intense heat, mass, momentum, and turbulence transfer. Heat transfer between the fluids and the wall of the cold leg pipe has also to be considered.

3.3.1. Momentum and Turbulence Transfer. Depending on the relative velocities of the gas and the liquid phases, the liquid/gas interface is strongly or mildly perturbed. For low relative velocities, the interface is quasistatic. For higher relative velocities, the interface is perturbed, and small waves are generated. Depending on the actual conditions, these waves can be amplified during their propagation in the horizontal pipe. The so-called *Kelvin-Helmholtz instability* can occur when a velocity shear is present within a continuous fluid or when there is sufficient velocity difference across the interface between two fluids. The CFD modelling of this instability was investigated in the frame of the NURESIM project by UCL. The classical theory can be used to predict the onset of instability in fluids of slightly different densities moving at various speeds. In the absence of surface tension, all wavelengths are unstable. The existence of surface tension stabilises the short wavelength condition; the theory then predicts stability until a velocity threshold is reached. For this reason, interface tracking methods or any method which includes surface tension effects have to be used [40, 41]. For cases with high-density differences, such as steam and water in the case of PTS, the situation is much more complicated (see [42]). It was found that either a single-fluid approach with VOF (FLUENT) or a two-fluid model with a large interface recognition (Neptune) could predict reasonably wave generation and growing and that condensation-induced instability could also be qualitatively predicted by Neptune and CFX.

In cases with high relative velocities in horizontal pipes, the waves are strongly amplified, and a *slug flow* with a complex system of interactions (presence of gas bubbles and liquid droplets) between the two phases can occur. The generated waves can, in certain cases of high relative velocity, entirely block the cold leg pipe. The slug flow regime is usually characterised by an acceleration of the gaseous phase and by the transition of fast liquid slugs carrying a significant amount of liquid with high-kinetic energy. The two-phase flow regimes in horizontal pipes are not only dependent on the local conditions but depend also on the characteristics of the free falling jet which may itself generate waves.

A systematic study of numerical simulation of slug flow in horizontal pipes using ANSYS CFX was carried out by Frank [9] and Vallée et al. [43]. It was shown that the formation of the slug flow regime strongly depends on the wall friction of the liquid phase. In simulations using inlet/outlet boundary conditions, it was found that the formation of slug flow regimes strongly depends on the agitation or perturbation of the inlet boundary conditions. Furthermore, Frank showed that the length of the computational domain also plays an important role in slug formation. Similar experimental data are being used in NURESIM for benchmarking the Neptune_CFD code by UCL, while University of Pisa and CEA do simulations of Fabre et al. [10]. A new modelling approach of large interfaces is developed considering an interfacial layer of 3 cells [44].

Momentum transfer is closely connected with turbulent transfer. In the case of the turbulence predicted by the k-ε model, the interfacial momentum can be modelled using several closure laws. The interfacial sublayer model (ISM, [14]) in the gas phase supposes, due to the significant difference between the gas and liquid densities, that the interface can be treated as a "moving solid wall" with a velocity equal to the liquid velocity. The gas region close to the interface is modelled with the two sublayer models, which is similar to the wall function concept. It is also possible to use the average viscosity assumption (AVM, [14]). This model is based on the simplified momentum equation in the case of a thin layer near a smooth interface without phase change, which permits the interfacial friction and velocity to be evaluated. Morel [45] has proposed a modification of the Taitel and Dukler model (TDM, [46]) for multidimensional calculations.

3.3.2. Turbulence Modelling. The mixing of hot and cold water is mainly determined by turbulence. The turbulence fields for both the liquid and the gas phases and the coupling between them play also important roles on the interfacial transfer and on the two-phase flow regime in the cold leg, and for the transition between different regimes (i.e., smooth surface, wavy flow, slug flow). Close to the interface, three turbulence sources have been identified: turbulence diffused from wall boundaries, turbulence production by the interfacial friction, and turbulence induced by interfacial waves. Close to the interface, the anisotropy of the turbulence has to be considered. It is not reproduced by any classic model. In most of the cases, the turbulence is modelled using the k-ω or the k-ε (classic or modified) models, together with a specific hypothesis at the interface [47, 48]. Without any special treatment of the free surface, the high-velocity gradients at the free surface generate too high turbulence when using eddy viscosity models like the k-ε or the k-ω model. Therefore, a symmetric damping procedure for the solid wall-like damping of turbulence in both gas and liquid phases has been proposed by Egorov [28]. A numerical database obtained by DNS simulation of the interface was generated in the frame of NURESIM by ASCOMP [49, 50].

Vallée et al. [51] employed the shear stress transport (SST) turbulence model for each phase. The k-ω based SST model [52] accounts for the transport of the turbulent shear stress and gives good predictions of the onset and the amount of flow separation under adverse pressure gradients. The qualitative slug formation in the simulations (ANSYS-CFX) was in good agreement with the experiment.

3.3.3. Modelling of the Free Surface. According to Zwart [53], numerical models for free surface flow may be divided into three categories: surface adaptive methods, interface-capturing methods, and interface-tracking methods.

Surface-adaptive methods are typically single-phase approaches in which the kinematic condition is used to update the location of the free surface interface, and the mesh boundary conforms to this interface at all times. These methods inherently involve mesh motion. While these methods are successful for certain classes of flows, they are typically restricted to modest degrees of interface deformation. Methods of working around these limitations have been devised, including periodic remeshing and interpolation, characteristic streamline diffusion finite element methods [54], and the integrated space-time finite volume method [55]. Despite these advances in tracking significant interface deformation, it remains the case that surface adaptive methods are useful primarily when the interface topology is straightforward. Effects such as splashing, breaking, and colliding of waves remain difficult challenges. Moreover, the geometries themselves must be simple in order to calculate how to move the mesh at interface-wall intersections.

These limitations may be overcome by having a fixed mesh, which spans the interface location. The *interface is captured* within the mesh by specific algorithms. Most commonly, the algorithm makes use of the continuity equation for one of the phases, in which the dependent variable is the volume fraction of that phase; these methods are called volume-of-fluid (VOF) methods. They differ widely in their detailed implementation. Many of them are interface-capturing and solve the VOF equation using a continuum advection scheme. If standard techniques are used for the advection operator, numerical diffusion will lead to significant smearing of the interface. A variety of compressive advection schemes have been devised to minimize this diffusion. The compressivness is often obtained by using a controlled downwinding of the fluxes, as with the donor-acceptor [56] and CICSAM [57] schemes. Controlled downwinding schemes have compressive characteristics which depend upon the time-step and therefore require small time steps to retain sharp interfaces, even for steady-state free surface flows. More recently, a new scheme having compressive characteristics independent of the time step size has been developed [58].

Other VOF methods are *interface-tracking* and explicitly track the free surface interface. For a particular volume fraction field, the interface is reconstructed using a piecewise representation (constant, linear, or parabolic) in each cell. The volume fluxes may be calculated either geometrically or using an advection operator as described above. Further details of these algorithms can be found in [59, 60]. Another fixed grid strategy for free surface flow problems involves the use of level set method [61]. The level set strategy formulates and solves an equation representing the signed distance to the free surface interface; the interface itself is extracted as the zero-distance isosurface. This method has the advantage that the level set variable is smooth, rather than discontinuous across the interface, and is therefore easier to solve. Its disadvantage is that the level set needs to be reset periodically, and this process is not strictly mass-conservative.

Surface tension effects are important in many free surface flows as well, as mentioned above. The continuum surface force method [62] formulates the surface tension force as a volumetric force. A key ingredient of this method is evaluating the interface curvature; it is challenging because it in effect requires second derivatives of the discontinuous volume fraction field. Care must be used in order to avoid errors in this calculation. Further details are discussed by Kothe et al. [60].

In addition to the surface adaptive, interface-capturing, and interface-tracking methods, Coste has developed a method of large interface recognition in a two-fluid model [44]. This method allows to define the position of large interfaces (the characteristic length scale being larger than the mesh size) like a free surface or a surface of the jet in order to being able to model interfacial transfers by an extension of the wall function approach. The objective is to combine the merits of the two-fluid model which models statistically "small interfaces" (e.g., for bubbles and droplets) with the specific treatment of large interfaces required for PTS simulations.

3.3.4. Direct Contact Condensation. In the context of PTS, the gas-liquid interface is characterised by intense heat and mass transfer in addition to the effects discussed in the previous section. Some simulations exist on the safety analysis of a nuclear reactor in which rapid contact condensation of vapour occurs during the emergency injection of cold water [63–67]. The following condensation models were tested by

Yao et al. [14] in a turbulent stratified steam-water flow of Lim's experiment [12].

(i) Interfacial sublayer concept (ISM), using "wall function" approach to model the sublayer that exists at a gas-liquid interface. The modelling of the interfacial heat transfer is based on approaches similar to the interfacial friction transfer. Schiestel [68] and Jayatilleke [69] have proposed relations for the temperature profile and the Prandtl number, using a formulation similar to the interfacial sublayer model.

(ii) A model based on asymptotic behaviour of the eddy viscosity model (EVM) [70–72] describes the turbulent viscosity in the boundary layer with a Gaussian function.

(iii) A model based on surface renewal concept [63, 64, 73, 74] with small eddies (HDM) was proposed by Banerjee [75]. He has proposed a relation for the heat transfer, that was modified by Hughes and Duffey [64] by introducing the Kolmogorov time scale for the small eddies. The use of these models with the steam-water flow is theoretically questionable as discussed by Yao et al. [14].

An alternative model was then proposed [23] in order to avoid this question. The time scale in this model is built with the Kolmogorov length scale and the turbulent velocity (velocity fluctuations due to turbulence) which gives in the theoretical framework of surface renewal an acceptable domain of validity compatible with steam water flows. This model has been validated with SIMMER and Neptune_CFD codes calculations of eighteen COSI tests and a LAOKOON test [76]. It is being tested and used within the 3D two-fluid models for the stratified flow condensation during the PTS related transients.

Various experiments are being used to test these condensation models in the stratified flow with two-fluid models of various 3D CFD codes.

(i) Condensation of hot steam in the stratified flow of the LAOKOON test facility [77] at Technical University of Munich is being modelled in the frame of the NURESIM project by GRS, CEA, and University of Pisa with two-fluid models of the computer codes Neptune_CFD and CFX.

(ii) Condensation-induced water hammer experiment, where a cold liquid is slowly flooding a horizontal pipe filled with hot steam, has been performed at KFKI, Budapest [78, 79]. The first phase of the transient is another example of condensation of hot steam on a stratified cold liquid, that can lead to the slug formation and severe pressure peaks due to the condensation-induced slug acceleration. CFD simulations of this experiment for benchmarking Neptune_CFD and CFX are done in NURESIM project by JSI. The development and implementation of new models are planned.

(iii) Test STB-31 at the POOLEX experimental facility is the test case for the condensation modes in a different geometry of a stratified flow: steam is being introduced into the cold water pool through a vertical pipe, and the selected test case exhibits a condensation over a flat and stable gas-liquid interface in the vertical pipe. The experiment was done by LUT in the frame of the national SAFIR programme for the NURESIM project. Simulations of the experiment are done by LUT and VTT using Neptune_CFD.

The KFKI water hammer experiment and the POOLEX experiment of LUT might require conjugate heat transfer calculations that take into account heat transfer in the structure walls and thus present a test case also for that physical phenomenon relevant for the integral PTS simulations.

In the frame of the NURESIM project, a database generated by DNS simulations of a stratified air/steam water flow is used by ASCOMP to obtain new scaling laws for the normalized heat transfer coefficient for both the steam and liquid phases. The database has been initially developed to infer modelling approaches to turbulence transport at interfacial two-phase flows without phase change. In a second step, a thermal DNS database for the steam-water stratified flow has been exploited in order to understand the importance of the relative driving mechanisms for the condensation heat transfer in both phases [50]. New scaling laws for the normalized heat transfer coefficient have been derived for both the steam and liquid phases. On the gas side of the interface, condensation heat transfer was found to scale with the interfacial friction velocity and Prandtl number like in the passive heat transfer case studied by Lakehal et al. [49]. In the liquid phase, the DNS results produced a condensation heat transfer coefficient that remains roughly constant at a given total shear velocity. However, an augmentation of heat transfer due to the combined effects of mass exchange and interfacial waviness has been observed. The surface divergence model of Banerjee et al. [80] is found to apply in the liquid phase, with an excellent agreement in the low-to-mild interfacial shear regime in particular. Regarding the interfacial friction, the DNS data confirm that in the presence of condensation, the interfacial shear stress is influenced by the mass exchange, and a correction factor based on the rate of condensation is needed to correctly predict the variation of the friction coefficient.

3.4. Flow in the Downcomer and Wall Heat Transfer.

In the case of a partially filled cold leg, the flow in the downcomer can be assumed to be single phase, and the temperature distribution of the fluid cooling the pressure vessel wall is mainly influenced by ECC injections, local mixing phenomena, and geometrical constraints. On the other hand, if the water level in the downcomer is below the nozzle of the cold leg, a complex two-phase flow regime occurs. Because of the low liquid level in the downcomer, another impingement region has to be considered. The same modelling approaches have to be applied as discussed for the impinging jet. Depending on the water velocity when entering the downcomer, a detachment of the flow from the walls is possible. If this detachment occurs, the heat transfer between the water and the walls is decreased. Because of the variations in the flow regime and the presence of waves in the cold leg pipe, the velocity is not constant when the liquid enters the downcomer. The presence of the walls modifies the liquid flow behaviour by changing the turbulence properties, the liquid temperature, and the velocity field. Some calculations of the flow in the downcomer have been performed [81] and have been able to reproduce the water temperature oscillations in the downcomer.

The prediction of the transient and local heat transfer to the RPV wall is the final aim of the thermal fluid dynamic simulation of the PTS situation. However, the heat transfer to the cold leg wall has also to be considered, since there is a feedback from the wall temperatures on the flow. The various flow regimes taking place in the different regions influence the heat transfer at the walls. The numerical prediction of the transfer with the walls is strongly dependent on the accuracy with which the other phenomena are represented. The variations of the temperature fields for both the liquid and the gas phases are strongly dependent on the mixing between the phases, which results in the local phenomena. Conversely, the heat transfer at the walls influences the behaviour of the other phenomena by changing the temperature fields of the fluids.

As far as the simulation of the wall heat transfer is concerned, models valid for single phase should be sufficient. Various models exist and have been extensively studied. In most of the CFD codes, some heat transfer models with a solid wall are available. These models require the definition of the wall properties, depending on their composition. These models have already been used successfully in various configurations but not for the jet impingement where the local Nusselt number is not properly predicted [82].

3.5. Integral Simulation. The thermal-hydraulic phenomena at the origin of the two-phase PTS event have been split into several parts or subphenomena in the sections above. Each of those subphenomena, that is, Sections 3.1 to 3.4, actually implies the presence of inherent: (a) transient conditions, (b) thermo-dynamic non equilibrium, (c) mechanical nonequilibrium, (d) three-dimensional situation, and (e) nonfully-developed flow condition. Starting from this premise, any attempt to perform an integral simulation (i.e., considering all together the listed phenomena and the related interactions) of the PTS thermal-hydraulics phenomena are at worst meaningless, or more positively tainted by unreliable results, as also pointed out in the text before (e.g., attempts to consider together some of the identified subphenomena).

Three calculation types can be identified:

(A) licensing analysis accepted or acceptable by regulatory authorities;

(B) support (i.e., to licensing) calculations performed by “advanced” methods;

(C) scoping calculations by “advanced” methods to understand the phenomena or the use of the computational tools.

Advanced methods mean two-phase CFD in this case. Analyses of type (A) are performed by system thermal-hydraulic codes and typically based on conservative assumptions and do not fit with the content of the present paper (however, see below): there is no or limited consideration for phenomena, and the calculations are addressed to the estimate of the safety margins rather than to the prediction of the physical system transient evolution. At the basis of those analyses, there is the experience of safety technologists, including the consideration of experimental data and of deficiencies of the available computational tools. At the bottom end, comparison of expected conservative results from analyses of type (A), and results from methods discussed in this paper, when these will be available, will definitely prove the quality of the adequacy of the adopted conservatism. Analyses of type (B) are not accepted by licensing authorities nowadays. Therefore, only analyses of type (C) can be carried out. The analyses of type (C) suffer from all the limitations and the problems discussed in Sections 3.1 to 3.4.

In the frame of the NURESIM project, simulations are done by CEA for the COSI experiments (see Section 2) using the Neptune_CFD code. They found that some results are generally within a reasonable range, namely the water level, the liquid heat up in the cold water injection region, and the global condensation rate. Some other results are not satisfactory, for example, water temperature profiles upstream of the injection, and even in the downstream region in some cases. Simulations of UPTF TRAM experiments were done by EDF and GRS.

Further code improvements are required to allow reliable simulations of the two-phase PTS situation considering all the involved phenomena.In the near term, one may envisage a simplified treatment of two-phase PTS transients by neglecting some effects which are not yet controlled like the bubble entrainment and the possible effects of waves on the free surface. A better modelling of interfacial transfers of heat and mass at the free surface allowing convergence with a reasonable coarse mesh is still required to be able to predict the minimum liquid temperature entering the downcomer. It is very likely that neglecting entrained bubbles and interfacial waves leads to conservative predictions since both phenomena may increase condensation and mixing.

4. Conclusions

A comprehensive overview of the thermal-hydraulic phenomena (and subphenomena) connected with PTS in pressurized water reactors has been provided, with emphasis given to two-phase conditions.

The outline given in relation to single-phase phenomena shows that coupling techniques involving system thermal-hydraulics and CFD codes are mature enough to be used for technological purposes, with main reference to the evaluation of safety margins, though improvements are still needed (as expected when nuclear safety is part of the game) in the area of convection heat transfer.

The detailed analysis performed in relation to the two-phase flow phenomena shows the complexity of those phenomena. Computation techniques are capable to reproduce qualitatively the individual aspects (also called subphenomena) but fail, so far, in the prediction of the interaction among the subphenomena and of the overall system behaviour.

The NURESIM EC project, that constitutes the key source of information for this paper, gave a unique possibility to a dozen EU institutions to cooperate and create a synergy for better understanding and modelling the overall thermal-hydraulic phenomena at the basis of PTS, and a continuation of the project is envisaged to address the open issues listed in Sections 3.1 to 3.5. Best practice guidelines [52] have to be applied for the integral simulations.

List of Abbreviations

AIAD:	Algebraic interfacial area density.
AVM:	Average viscosity model.
CFD:	Computational fluid dynamics.
DCC:	Direct contact condensation.
DNS:	Direct numerical simulation.
ECC:	Emergency core cooling.
EVM:	Eddy viscosity model.
FPDA:	Fiber-phase doppler anemometry.
HPI:	High pressure injection.
HDM:	Hughes &Duffey model.
ISM:	Interfacial sublayer model.
ITM:	Interface tracking methods.
LES:	Large eddy simulation.
LDA:	Laser Doppler anemometry.
LOCA:	Loss of coolant accident.
PIV:	Particle image velocimetry.
PTS:	Pressurized thermal shock.
PWR:	Pressurized water reactor.
RANS:	Reynolds-averaged Navier-stokes.
RMS:	Root mean square.
SB-LOCA:	Small break loss of coolant accident.
TDM:	Taitel and Dukler model.
VOF:	Volume of fluid.

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