# STATUS AND PERSPECTIVE OF TWO-PHASE FLOW MODELLING IN THE NEPTUNE MULTISCALE THERMAL-HYDRAULIC PLATFORM FOR NUCLEAR REACTOR SIMULATION

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Thermalhydraulic reactor simulation of tomorrow will require a new generation of codes combining at least three scales, the CFD scale in open medium, the component scale and the system scale. DNS will be used as a support for modelling more macroscopic models. NEPTUNE is such a new generation multi-scale platform developed jointly by CEA-DEN and EDF-R&D and also supported by IRSN and FRAMATOME-ANP. The major steps towards the next generation lie in new physical models and improved numerical methods. This paper presents the advances obtained so far in physical modelling for each scale. Macroscopic models of system and component scales include multi-field modelling, transport of interfacial area, and turbulence modelling. Two-phase CFD or CMFD was first applied to boiling bubbly flow for departure from nucleate boiling investigations and to stratified flow for pressurised thermal shock investigations. The main challenges of the project are presented, some selected results are shown for each scale, and the perspectives for future are also drawn. Direct Numerical Simulation tools with Interface Tracking Techniques are also developed for even smaller scale investigations leading to a better understanding of basic physical processes and allowing the development of closure relations for macroscopic and CFD models.

## 1. INTRODUCTION

At the end of the 90's, CEA made a comprehensive analysis of the industrial configurations involving two-phase flow and identified the limits of current simulation tools based on a State of the Art in physical modelling, numerical schemes, instrumentation and code architecture aspects (FASTNET, [1]). This work was extended to the European level within the frame of the EUROFASTNET [2,3] Concerted Action which was launched during the 5th European Framework Program (1998-2002). One of the main outcomes of the EUROFASTNET action was a State-of-the-Art analysis of the current thermal-hydraulics simulation tools. A priority list was also established ranking 44 industrial needs for which further scientific advances were expected both in physical modelling and numerical methods. For instance the improved prediction of Departure from Nucleate Boiling (DNB) ranked among the high priority needs since it is directly linked to fuel

performance. In the same way, the estimation of the fluid temperature on the Reactor Pressure Vessel (RPV) in case of a Pressurized Thermal Shock (PTS) is a major issue when controlling the lifespan of critical components. Another conclusion of EUROFASTNET was that to meet the challenges of tomorrow, the elaboration of a new generation of two-phase simulation tools was recommended. The analysis of the industrial needs pointed out that various interoperable simulation scales should be involved, including higher resolution 3-dimensional tools. Such a multi-scale approach has been developed (see Morel et al., [4]) for the next generation of codes and a strategy for improving two-phase 3-D modelling for nuclear safety applications was elaborated (Bestion et al., [5])

Following these reflections, the NEPTUNE Project [6] was launched at the end of 2001 by Electricité de France (EDF) and the Commissariat à l'Energie Atomique (CEA) as the thermal-hydraulic part of their long-term joint research and development program for the next generation of

nuclear reactor simulation tools. This program is also supported by the Institut de Radioprotection et Sûreté Nucléaire (IRSN) and Framatome-ANP. The project aims at building a new software platform for advanced two-phase flow thermal-hydraulics allowing easy multi-scale and multi-disciplinary calculations. In order to meet the industrial needs, new physical models and numerical methods are being developed for each simulation scale as well as for their coupling. The NEPTUNE activities include software development, research in physical modelling and numerical methods, the development of advanced instrumentation techniques and the performance of new experimental programs [7]. This paper focusses on the multi-scale approach and on the physical modelling.

The "System" scale is dedicated to the overall description of the circuits of the reactor with main application to accidental transient simulation for safety analysis, operation studies and real-time simulators. The CATHARE code developed by the same partners as NEPTUNE is the present generation of system code used in France. The primary and secondary circuits of a reactor are modelled by coupling 0D, 1D, and 3D modules, all based on the well known two-fluid 6-equation model. The "component" scale is dedicated to the design, safety and operation studies for reactor cores and tubular heat exchangers (steam generators, condensers, auxiliary exchangers). Rod or tube bundles are homogenized into the control volumes using the "porosity" concept. The minimum spatial resolution is fixed by the sub-channel size (about 1 centimeter). FLICA [8], THYC [9], and GENEPI [10] are the present generation of component codes used in France. Both the "system" and "component" scales are "macroscopic" scales and every 0D, 1D or 3D control volume (or mesh) contains walls and momentum and heat exchanges with these walls.

In order to allow a better description of the local flow processes in some components of a reactor, a finer resolution is necessary with the CFD (or CMFD) in open medium. It includes turbulence modelling using either RANS or LES. This "meso-scale" allows a local analysis in the critical parts of the cores, steam generators or other components including complex geometries. It is also the only scale able to predict the fluid temperature field for investigating thermal shocks or thermal fatigue of the reactor structures. A first experience in developing and applying the NEPTUNE two-phase CFD tool for Reactor Safety Analysis was presented by Bestion et al [11]. Advances in modelling two phase flow at the CFD scale were obtained in two Shared Cost Actions of the 5th European Framework Program: ASTAR project (Paillère et al, [12]) and ECORA project (Scheuerer et al, [13]). CEA and EDF contributed to these projects by using and developing modules of the NEPTUNE Platform.

A microscopic scale also exists with Interface Tracking Methods (ITM) and Direct Numerical Simulation (DNS) or pseudo-DNS. Such methods are being developed in the TRIO-U code in the frame of the NEPTUNE project.

They allow local simulations focusing on very small domains (e.g. containing a few bubbles or droplets). The use of such pseudo-DNS will help understanding the local flow phenomena and may be used for developing closure relations for meso-scale and macroscopic models.

The paper presents first the advances obtained so far in physical modelling for system and component codes including turbulence modelling, transport of interfacial area, and multi-field modelling. Future developments for macroscopic models are then identified. A methodology for using two-phase CFD or CMFD is presented with first applications to boiling bubbly flow for departure from nucleate boiling investigations and to stratified flows for pressurised thermal shock investigations. The perspectives for future developments of the CMFD are also drawn and the future role of Direct Numerical Simulation tools with Interface Tracking Techniques is defined.

## 2. ADVANCES IN TWO-PHASE FLOW MODELLING FOR MACROSCOPIC SCALE

### 2.1 Expected Improvements in System Codes and Component Codes

The current generation of "system" codes and "component" codes in France has reached a high level of maturity and they still will be used industrially for at least ten years. Further progress is now mainly expected from the following developments to be implemented in the NEPTUNE platform:

- system scale : multi-field modelling, interfacial area transport, modelling of turbulence effects (1D and 3D porous), with application to many accidental transients including the reflooding phase of LBLOCA, low pressure transients,...
- component scale: two-fluid and multi-field models for porous medium, modelling of turbulence, with application to PWR core in operation and in accidental transients (e.g. Steam Line Break), critical power in BWR, research reactors and propulsion reactors, SG tube vibrations, corrosion,...

### 2.2 Modelling Turbulence and Interfacial Area in Pipes and Rod Bundles

The prediction of turbulent scales in a pipe or in rod bundles (tube bundles) allows to predict many effects which were not modelled in previous codes:

- Coalescence and break-up of bubbles or droplets are mainly dependent on the turbulence. Then the prediction of the interfacial area requires a good prediction of turbulent scales and experimental data show that the turbulence in two-phase flow cannot be simply evaluated by single phase models and cannot be simplified using equilibrium between production and dissipation
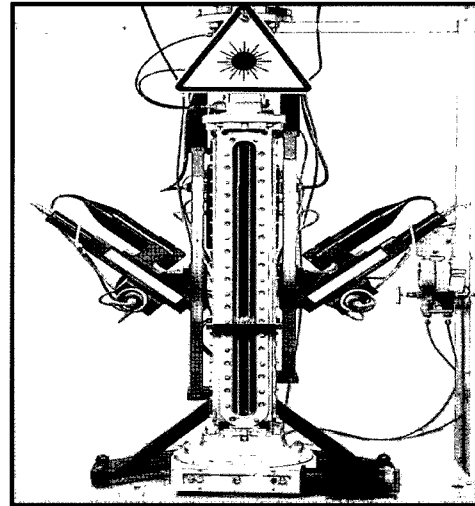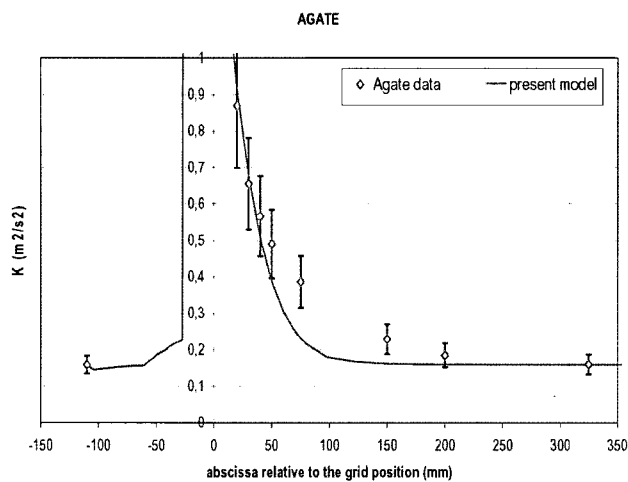
Fig. 1. Predicted and Experimental Axial Evolution of Turbulent Kinetik Energy k in a 5X5 Rod Bundle
with Spacer Grid in AGATE Experiment [16] Provided with Laser Anemometry. Calculations are Performed Using a k-$\varepsilon$ Model
(from Serre & Bestion [15])

· All interfacial transfers depend on turbulence through the interfacial area and transfer coefficients: Direct Contact Condensation due to ECC injection is very sensitive to liquid turbulence
· All wall heat transfers are also affected by the turbulence intensity
· In annular-mist flows, gas turbulence may control the droplet deposition
· In rod bundles and tube bundles turbulent mixing between subchannels depend on turbulent scales
· All singularities in the geometry of the duct will affect turbulent scales and all other flow parameters which depend on them. The effects of spacer grids in a core are of particular importance in both single phase and two phase flow conditions.

A first attempt to predict turbulent velocity and length scales was made using a transport equation for the turbulent kinetik energy k and an algebraic expression of the length scale (k-L model). It was found difficult to describe all flow situations with a simple algebraic model of the length scale. Then a k-$\varepsilon$ model was developed [14, 15] with a specific formulation of production terms due to wall shear and an additional term due to production in singularities. It was first validated for 1D single phase flows in pipes by comparison with 3D CFD predictions. Then it was validated against single-phase flows data in rod bundles with spacer grids. Figure 1 shows prediction of turbulence decay downstream of a spacer grid in the AGATE experiment [16]. The k-$\varepsilon$ model was found able to predict the strong increase of

turbulent kinetic energy due to the grid, and to predict also reasonably well the decay of turbulence downstream of the grid.

Then this k-$\varepsilon$ model was coupled with a transport equation for the Interfacial Area Concentration (IAC) and validated in two-phase bubbly flow in a pipe. In bubbly flows, velocity fluctuations in the liquid field result from coupled mechanisms such as the liquid turbulence generated by wall shear, the random stirring of the liquid phase due to the motion of the bubbles, the vortex shedding in the wakes of bubbles and the eventual deformation of the interfaces. The stirring of the flow induced by the bubbles random velocity field is irrotational and does not contribute to the turbulent cascade nor to the dissipation, and is called pseudo-turbulence. It is not separable from real diffusive and dissipative turbulence in measurements but it contributes to the random velocity field.

The complexity of coupling effects was simplified assuming that single phase and two-phase effects can be modeled separately and then linearly added. Pseudo-turbulence is also evaluated and added to the turbulent kinetic energy calculated by the (k-$\varepsilon$) model to allow comparison with measurements. The Dédale experiment run at EDF by Grossetête [17] is used for validation. In this low velocity flow, coalescence dominates break up and turbulence is mainly produced by bubble wakes. Coalescence and break up models of the literature were tested (Hibiki & Ishii [18], Wu et al. [19], Yao& Morel [20]) but a new efficiency of break-up is proposed. Figure 2 shows prediction of k and interfacial area Ai in the DEDALE experiment (from Serre
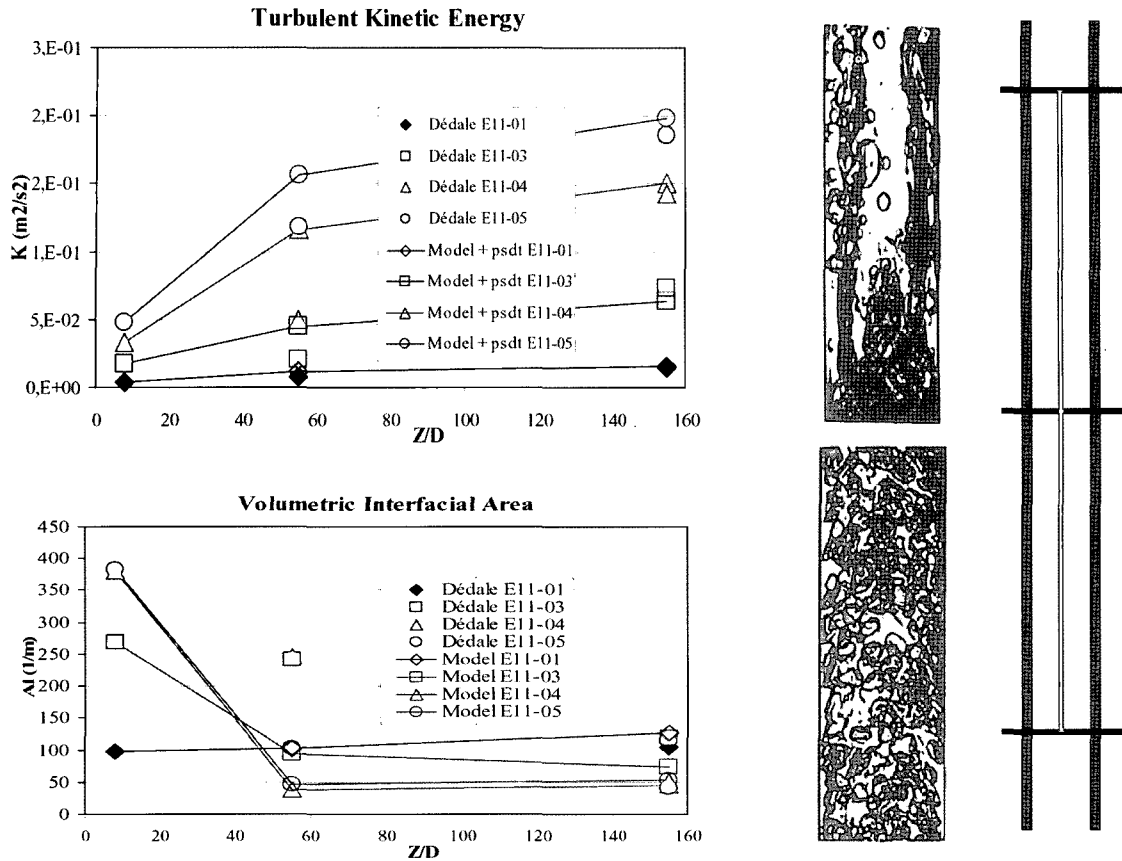
Fig. 2. Predicted and Experimental Axial Evolution of Turbulent Kinetik Energy k and Interfacial Area in the Vertical Pipe DEDALE Experiment [17]. Calculations are Performed with k-ε Model (from Serre & Bestion [15])

& Bestion [15]). Although interactions between interfacial area and turbulence models are very complex, a reasonable agreement could be obtained. In this range of void fraction, the two-group model of Ibiki & ishii [21] could probably better model bubbly-to-slug flow transition. However modelling with a better accuracy this bubble-to-slug transition in pipes was not identified as a major issue in nuclear reactor thermalhydraulics. Improvements are mainly expected in core geometry where specific geometrical effects affect the interfacial structure. When data in rod bundle will be available, the one-group model will be first tested since simplicity is preferred in codes when more complexity does not bring a high added value.

## 2.3 Modelling Annular-mist Flows with a 3-field Model

In the present generation of codes a major limitation of the two-fluid model was found when a phase is splitted into two separate fields. The annular-mist flow with co-
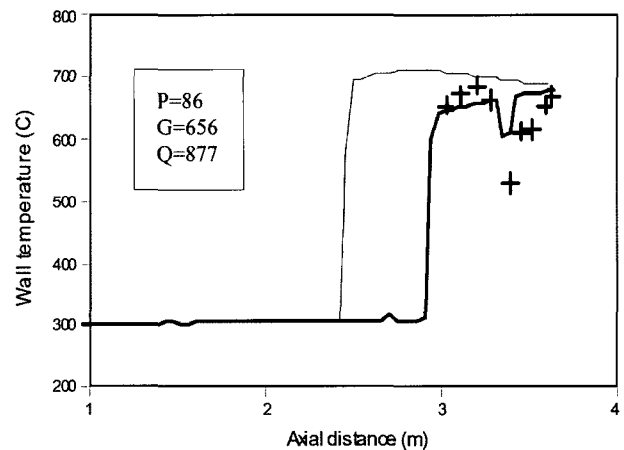


Fig. 3. Predicted and Experimental Axial Evolution of Wall Temperature in a Heated Vertical Rod Bundle. Calculations are Performed with (Solid Line with the Right Dry Out Location) and Without (Solid Line with Too Early Dry Out) Modelling the Geometry of the Spacer Grids (Reduction of Cross Section Area)

ntinuous liquid along walls and droplets in the gas flow is the first example where a 3-field model may improve the predicting capabilities. Valette & Jayanti [22] developed a 3-field model and validated against a large data base including pipe flows and flows in rod bundles corresponding to the geometry or a BWR core. The model is able to predict pressure drops, fraction of entrained liquid, dry-out quality, and Post-dry-out wall temperature for a heated flow.

A special attention was paid to the entrainment and deposition of droplets which controls the fraction of entrained liquid and the film dry-out. Figure 3 shows that by taking into account the geometry of spacer grids one can better predict the delayed dry-out occurrence and the clad cooling without quenching for grids in dry zone.

Application of the 3-field model is in progress for simulation of the Reflooding phase of a Large Break Loss of Coolant Accident.

## 3. FUTURE DEVELOPMENTS FOR NEPTUNE MACROSCOPIC MODELS

System code models and capabilities were described in successive State of the Art [1,2,24,25,26] analyses and perspectives for future were drawn. The intrinsic limitations of the two-fluid 6-equation model were reached in the current generation of system code. Further progress would require additional transport equations for interfacial area, for turbulent scales, and multi-field modelling. Then new options will be progressively developed and implemented in NEPTUNE-System scale with these new capabilities. The multi-field modelling will focus on annular-mist flow and stratified-mist flow regimes for which two liquid fields are necessary. Such flow regimes are encountered in nominal conditions in Boiling Water Reactors (BWR), and in many accident scenarios of PWRs such as low pressure transients, and late phase of LOCAs including Reflooding. Dynamic modelling of interfacial area and turbulence will focus on bubbly-slug-churn flows in reactor core and on the bubbly-to-stratified transition.

Stratified flow are often encountered in the Hot Legs of a Pressurised Water Reactor (PWR). Two flow regime transitions may also occur in Hot Legs which may play an important role in accident sequences:

· Transition from bubbly to stratified flow
· Transition from stratified to stratified-mist flow

Stratification of a bubbly flow in a horizontal channel also depends on a balance between turbulent dispersion force and the buoyancy forces acting on the bubbles. In Two-Fluid 6-equation models only a very simplified formulation of both effects was possible in the CATHARE code [23] and no relaxation time associated to the process could be properly described by an algebraic criterion. In this process, transport equations for turbulence and IAC are required to predict the evolution of the flow with bubble

sedimentation and progressive appearance of a continuous gas field at top of the pipe. A specific experimental programme [7] will be devoted to the investigation of such flow regime transition.

The transition from stratified to stratified-mist flow is often treated by system codes using extrapolations of models for onset of droplet entrainment in vertical annular flow. Moreover stratified mist flow also requires a two-liquid-field model to describe the separate behaviour of droplets and continuous liquid. A specific experimental programme [7] will be devoted to the investigation of stratified-mist flow in a horizontal pipe with measurements of entrainment and deposition rates, and of the droplet size and velocity.

The prediction of chocked flow by system codes still remains rather inaccurate. Flashing flows in a nozzle or at a break are non-established flows which require an accurate modeling of the flashing delay related to heterogeneous nucleation. It is expected that the activation of the nucleation sites depends on pressure turbulent fluctuations which might be estimated by a proper modeling of turbulent scales. After nucleation, myriads of small bubbles grow by flashing and may break up when reaching a limit size. The convective heat transfer controls the thermal non-equilibrium and the bubble size is the key parameter. Thus, using transport equations for turbulence intensity and IAC may allow a better prediction of flashing flows.

Component codes will also be further developed and on-going and future research and development will address the following issues :

· Mathematical derivation of two-fluid and multi-field system of equations in a porous medium using an homogenisation technique
· Development of wall friction and interfacial friction tensors taking into account the non-isotropy of the porous medium.
· Development and improvements of advanced numerical schemes including fully unstructured meshing and coupling with other scales.

## 4. ADVANCES IN TWO-PHASE FLOW MODELLING USING CMFD

### 4.1 Methodology for Developing and Using Two-phase CFD

Single-phase CFD codes are now increasingly applied to reactor investigations of some mixing problems, for both reactor circuit (boron mixing, thermal fatigue, thermal shocks), and containment thermalhydraulics (hydrogen mixing). Extension of CFD codes to two-phase flow is also in progress and offers an opportunity for design and safety investigations, by giving some access to smaller scale flow processes. Increasing computer performance will allow a more extensive use of 3D modelling with finer nodalization even in the field of two-phase thermalhydrau-

lics. However, models are not as mature as in single-phase flows and substantial work still has to be done regarding the physical modelling and numerical schemes to be implemented in such two-phase CFD.

The experience gained so far in using two-phase CFD for nuclear reactor thermalhydraulics was summarized [27]. Investigating a two-phase flow with CFD includes several successive steps:

- Identification of all important flow processes: this may require the analysis of some experiments.
- Selecting a Basic model: Single fluid, two-fluid or multi-field model may be used depending on the case
- Filtering turbulent scales and two-phase intermittency scales: following the RANS approach, all scales may be filtered. A two-phase LES (Large Eddy Simulation) may be adopted for filtering only the smaller scales. DNS or pseudo-DNS with ITM may also be used if all scales have to be simulated.
- Identification of Local Interface Structure: when a statistical approach is used, the interface structure must be identified based on calculated statistical parameters such as the void fraction, the interfacial area, ... Additional transport equations for IAC or bubble number density or other statistical parameter may be required for characterising the interfacial structure.
- Use of Interface Tracking Method: depending on the flow configuration and on the expected resolution scale, ITM may be used either for all interfaces or for some of them (free surface).
- Selecting a turbulence modelling: additional transport equations may be required for turbulent quantities: k-ε, Rij-ε,...
- Modelling Interfacial transfers and validation
- Modelling Turbulent transfers and validation
- Modelling Wall transfers and validation

This general methodology was already followed for two main applications :

- Boiling bubbly flow for DNB (Departure from Nucleate Boiling) investigations
- Free surface flows for PTS investigations

It is clear that present two-phase CFD simulation tools are not able to predict all flow regimes, all interface structure and that a rather long term research effort will be necessary to extend the modelling for all two-phase flow regimes.

## 4.2 Simulating Boiling Bubbly Flows with CMFD for DNB Investigations

The main objective of using CFD for boiling bubbly flows and DNB investigations is to provide a better understanding of local flow processes occurring at the scale of the two-phase boundary layers along heating walls. It should allow in the future to replace present industrial methods by a "Local Predictive Approach" where CHF

correlations will be based on local parameters instead of averaged parameters. Even if it is a rather long term objective, such investigations may bring a better understanding and may help in the modelling of non-uniform heat flux impact, grid impact, channel shape/size impact. It may help nuclear industry in the design/optimization of fuel assemblies and for optimizing CHF test procedures, reducing the number of tests. Finally a decrease of conservatisms through more general and accurate CHF correlations may result in additional operation margins.

As soon as nucleate boiling occurs, two-phase boundary layers appear along fuel rods in the subchannels. Many phenomena control the dynamics of these two-phase layers: bubble transport and dispersion, bubble growing and collapse due to vaporization and condensation, coalescence and break up, turbulents transfers of heat and momentum, local grid spacers effects.

Morel et al. [28] presented the status of modelling boiling flow with NEPTUNE CFD tool for open medium. The two-fluid model is used in a RANS approach where the equations are filtered with a time scale larger than all turbulent scales and large enough to allow the passage of several bubbles. A K-ε model for the turbulence in the liquid phase and a transport equation for the Interfacial Area Concentration (IAC) of the bubbles are also written. The balance equations of the two-fluid model include two mass balance equations, two momentum balance equations and two internal energy balance equations.

The closure of the Reynolds stress tensor for the liquid phase uses a turbulent diffusivity calculated by K-ε turbulence equations for the liquid, which include the effect of the bubble induced turbulence (Morel, [29]). Specific source terms model the turbulence production and dissipation in the wakes of bubbles .

The interfacial momentum transfer term is the sum of four different contributions corresponding to drag force, added mass force, lift force, and turbulent dispersion force. Interfacial heat transfer phenomena are modelled for both vaporization and condensation using the predicted interfacial area concentration.

The wall functions used in momentum equations are simply extrapolated from single phase models. The wall-to-liquid heat flux is classically divided into three parts:

- The wall to liquid heat transfer
- The heat flux due to the quenching effect
- The heat flux used for phase change : bubbles nucleated on the wall surface

In the closure relations, the bubble detachment diameter, the active nucleation site density, the fraction of the wall area occupied by the nucleated bubbles, the time delay between the detachment of one bubble and the apparition of the following one, the detachment frequency of the nucleated bubbles are all modelled. In the future, DNS simulations will allow to improve all these correlations.

The Interfacial Area Concentration (IAC) balance

equation for the particular case of boiling bubbly flow is written with source terms due to bubble nucleation at the wall, bubble size variation with pressure and temperature, bubble size variation associated to vaporization or condensation, and to coalescence and break-up. It should be noted that the contribution of the bubble to the IAC depends on its diameter. Generally speaking, the diameter probability density function is needed to determine the total changes in the IAC. Here, as a first approximation, a uniform bubble size for all the existing bubbles is assumed, given
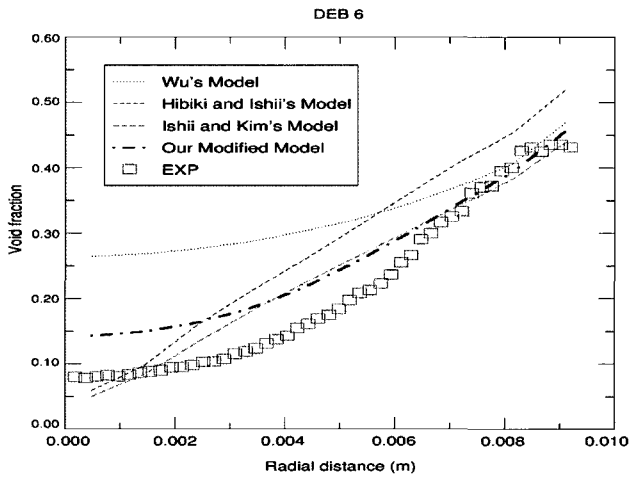


Fig. 4. Comparison of the Void Fraction at the End of the Heated Section Between the DEBORA Experimental Data and the Results of Four Different Models for Coalescence and Break-Up (from Morel et al. [27] )
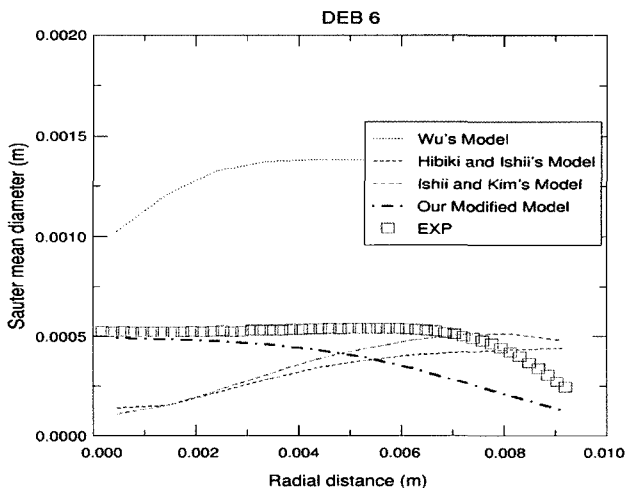


Fig. 5. Comparison of the Sauter Mean Diameter at the end of the Heated Section Between the DEBORA Experimental Data and the Results of Four Different Models for Coalescence and Break-Up (from Morel et al. [27])
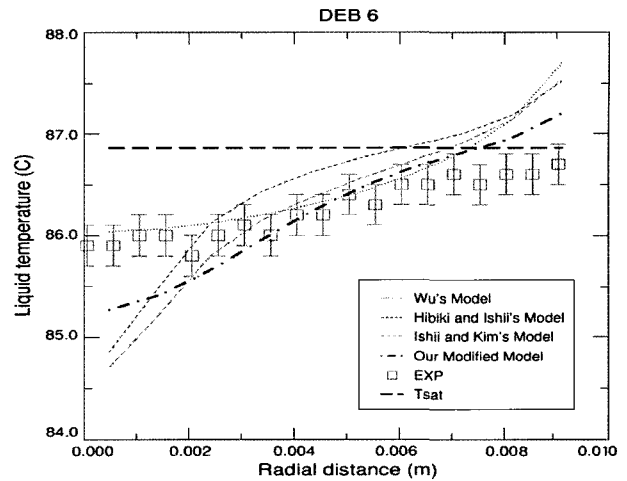


Fig. 6. Comparison of the Liquid Temperature Profile at the End of the Heated Section Between the DEBORA Experimental Data and the Results of Four Different Models for Coalescence and Break-Up (from Morel et al. [27])

by the Sauter mean diameter except for the newly nucleated bubbles which are characterized by the bubble departure diameter.

The model was compared to the DEBORA experimental data base [30]. The DEBORA experiment, which was carried out at the CEA-Grenoble, is a vertical heated pipe with freon R-12 flowing upwards. At the entrance of the tube, the R-12 is sub-cooled single phase liquid. Due to the wall heating, numerous bubbles are nucleated onto the wall surface. These bubbles grow, detach from the wall and are dispersed in the turbulent flow before partly condensing in the core region of the duct. The bubble size, void fraction, IAC, and also the liquid temperature radial profiles have been measured at the top end of the heated section. Calculated profiles with four different IAC models are compared to experimental profiles. An original IAC model proposed by Morel et al [27] was compared with three other bubble coalescence and break-up models of the literature.

Figures 4 to 6 compare the void fraction profile, Sauter Mean diameter profile and liquid temperature profile predicted with different coalescence and break-up models with the data.

Figure 5 shows that the best agreement on the bubble diameter profiles is generally obtained with the proposed model. Other existing models may be very far from the data qualitatively and quantitatively, which shows that coalescence and break-up play a dominant role in the boiling flows. Complex interactions exist between the bubble diameter (or IAC) and turbulence, void fraction and heat transfers. Larger bubbles create more turbulence, which improves bubble dispersion and turbulent heat diffusion to the center of the pipe where the water is subcooled and condenses bubbles. More turbulence also favours coalescence and

break-up. The model shows a reasonable agreement with all measured data. Further improvements would require more information on velocity and turbulence fields which affect bubble dispersion, liquid temperature profile, coalescence and break-up. Assuming a single bubble size is probably too limiting and the poly-dispersion should be taken into account. More recent simulations [31] of boiling flow in an annulus also showed that specific two-phase flow wall functions are required.

The complex effects of spacer grids in reactor fuel assemblies are rather challenging for the simulation tools. A turbulence promoter with mixing vanes was also implemented in the DEBORA tube test section and first validation calculations are reported by Guelfi et al. [6], which compare favourably with experiment.

Although many aspects of the model still require improvements, the application of CMFD to boiling bubbly flow already shows reasonable predictions and should be successful in a near future allowing first parametric studies on the fuel assembly design.

## 4.3 Simulating Free Surface Flows with Condensation by CMFD for PTS Investigations

Two-phase pressurized thermal shock (PTS) may occur when an Emergency Core Cooling (ECC) system is injecting cold water in a partially uncovered cold leg of a Pressurized Water Reactor (PWR). The knowledge of the liquid temperature field in the cold leg and in the downcomer is required to predict the thermal load on the pressure vessel wall. The interfacial heat and mass transfer related to direct contact condensation of steam on a subcooled liquid and the turbulence diffusion within the liquid control the liquid temperature field. Many research work support that turbulence behavior near the interface plays a dominant role for the interfacial transfers. For ECC injection cases, the turbulence mainly arises from the impact of the water jet and the shear (at the wall and at the gas-liquid interface). Thus, as a first step to simulate PTS, separate effects were investigated, i.e., interfacial friction and turbulence production, interfacial heat transfer, turbulence in a water pool induced by a water jet, in order to validate the developed models (see Yao et al. [32]).

A 3D two-fluid model for a turbulent stratified flow with/without condensation was used (see Yao et al, [32]). A modified turbulent K-$\varepsilon$ model for each phase is written with turbulence production induced by interfacial friction. A model of interfacial friction based on an interfacial sublayer concept was used, which is an extrapolation of the wall function approach to the interface. Three interfacial heat transfer models, namely, a model based on the small eddies using the surface renewal concept, a model based on the asymptotic behavior of the eddy viscosity and a model based on the interfacial sublayer concept (ISM) were implemented into the NEPTUNE code. Firstly, an experiment with adiabatic turbulent air-water stratified flow is calculated to evaluate the models which control
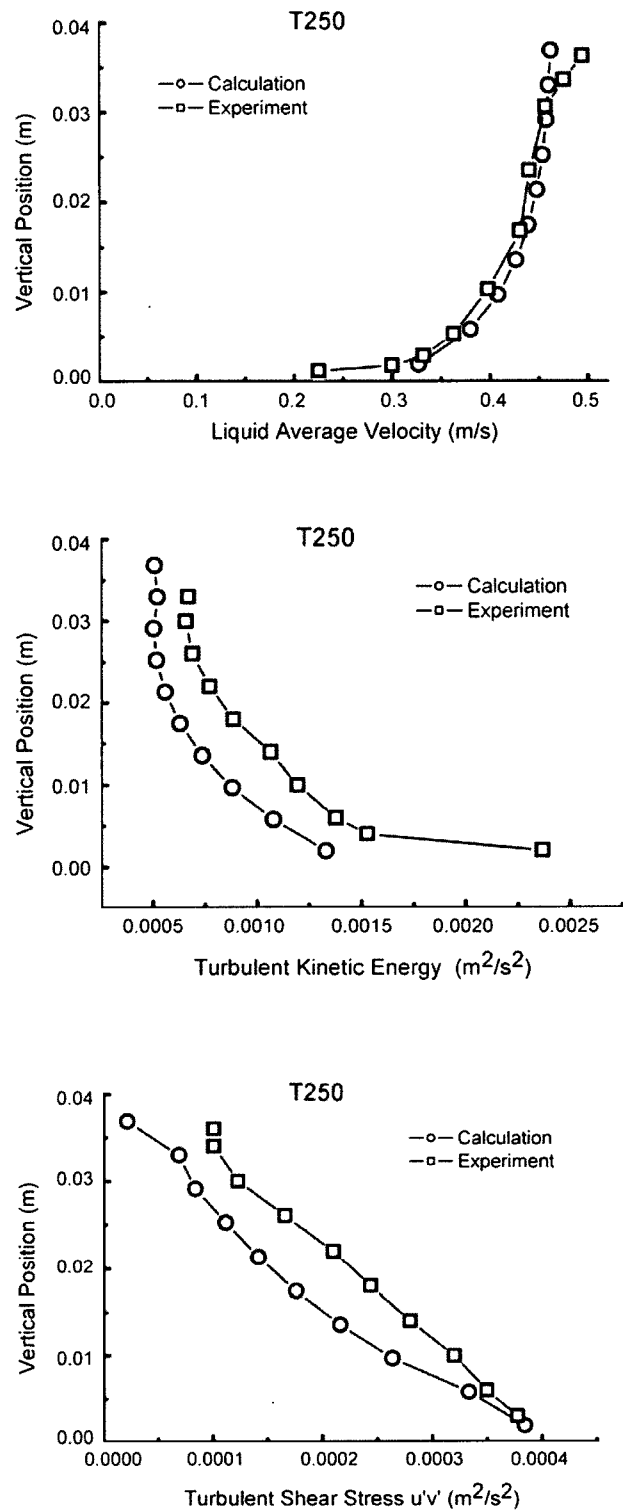


Fig. 7. Predicted and Experimental Profiles in an Air-Water Stratified Flow in a Rectangular Channel. Liquid Velocity Profile; Turbulent Kinetik Energy Profile in the Liquid; Turbulent Shear Stresses (from Yao et al., [32])

the velocity and turbulence profiles. Then an experiment of turbulent steam-water stratified flow with condensation is applied to compare the three interfacial heat transfer models mentioned above.

Models for turbulence diffusion and interfacial friction are evaluated by comparison with the experimental data (data of Fabre et al. reported by Yao et al. [32]) in a stratified air-water co-current flow in a horizontal channel of rectangular cross-section. In this experiment, systematic measurements of the components of the mean velocities and Reynolds stresses were performed under carefully controlled inlet conditions. Figure 7 presents the calculated profiles of mean longitudinal velocity, turbulent kinetic energy and turbulent shear stress. Calculations predicted well the liquid velocity, turbulent kinetic intensity and shear profiles in the liquid layer, compared to the experimental data, though with a little underestimation of turbulence and turbulent shear stress.

In a second step the interfacial heat transfer models are validated against data (data of Lim et al. reported in Yao et al., [32]) for a turbulent stratified condensing steam-water flow in a horizontal channel of rectangular cross-section. Pitot tubes are used to measure the steam velocity profiles at five test sections, giving the condensation rate. Several test cases were simulated with experimental conditions ranging from a glossy looking interface to a wavy interface. Experimental results showed a significant increment of condensation when the transition from glossy to wavy interface happened.

The comparison to the experimental data of the condensed stratified steam-water flow showed that ISM gave the best predicted results for the glossy interface conditions, but underestimated the condensation for the wavy interface possibly because the enhancement effects of interfacial waves on the interfacial friction and on turbulence were not taken into account. None of the models could well predict condensation with a wavy interface.

The two-fluid model with k-ε equations in each phase seems to be a reasonable first approach for this situation but a sufficiently fine meshing is required for the turbulence being correctly described. Interfacial transfers of heat and momentum (friction force) on the free surface require a specific modeling taking into account the space filter scale imposed by the meshing: the transfer coefficients depend on the distance to the interface in the same way as the distance to the wall is used in wall functions. However difficulties are encountered for modelling turbulence and heat transfers at the free surface in case of high interfacial shear and presence of waves and the capabilities of the two-fluid model with a RANS turbulence modelling may be questioned in this case.

Waves increase interfacial area and surface roughness. Friction coefficient and heat and mass transfer coefficients increase which may strongly affect the condensation rate. How to predict the local surface roughness associated to a wave structure which depends on what occurs on the

whole free surface? No correlation with local parameters is possible. Should we track the interface to predict the wave structure? The filtering of equations affects the capability to predict waves even when using ITM and using pure DNS without any filtering is not possible in a large scale industrial application.

Other difficulties were encountered when modelling PTS in two-phase situations. As an example, a possible entrainment by the ECCS jet of bubbles below the free surface may contribute to the condensation and it was found that this entrainment is controlled by a phenomenon having a very small scale, the entrainment and breakup into bubbles of a thin gas layer around the jet. It could be simulated by using DNS and ITM but is rather difficult to model within a CFD modeling (see [13]) having a larger filter scale than the scale of the phenomenon.

However considering the PTS scenarios of interest, interfacial shear should not be very high and the effect of bubble entrainment on the total condensation should remain relatively small. Therefore reasonable predictions may be expected in the near future but higher difficulties would be encountered in situations with higher mechanical interaction and/or condensation driven instabilities.

A validation matrix exists for PTS simulations (see [7]) including separate effect tests , more global tests (future TOPFLOW tests) and Integral Effect Tests (OECD-ROSA LSTF project).

# 5. FUTURE DEVELOPMENTS FOR NEPTUNE- CMFD MODELS

The two-phase CFD (CMFD) module of NEPTUNE will be applied in the future to many reactor issues with some priority to the improvements of DNB and PTS investigations, and with increasing effort for extending the application to more complex flows. Some of this activity will be performed in the frame of the NURESIM project of the 6th European Framework Program, where 14 partners join their efforts in two-phase CFD application to Direct Contact Condensation, PTS and Critical Heat Flux.

For DNB investigations the future modeling effort will address the following issues:

· The turbulence modeling in bubbly flow should better take into account the different nature of the turbulence produced in wall shear layers and the turbulence produced in bubble wakes. More advanced turbulence modelling such as Rij-ε could be necessary for rotating flow past a grid with mixing vanes.
· Modelling poly-dispersion effects either through multi-group or multi-field, or by transport of statistical moments of the bubble size distribution.
· More generic models for lift and turbulent diffusion forces are still necessary.
· Specific wall functions for momentum and energy equations are required for any two-phase flow conditions
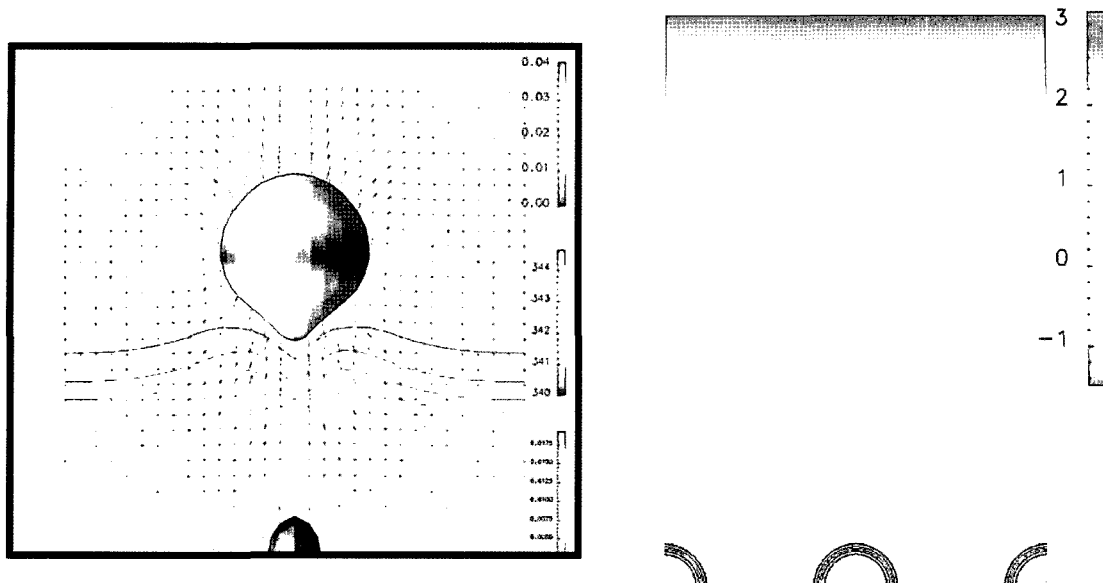
Fig. 8. DNS Simulation of Monosite Boiling on the Left by Matthieu et al [34] and Multi-Site Boiling
on the Right by C Fouillet [35]

- First attempts to develop a DNB criterion based on local parameters will be possible in the near future.

Further effort is required in the PTS investigations:

- Free surface: using an interface tracking technique to predict the exact position of the interface or adopting a simple interface sharpener technique remains an open question which requires further benchmarking.
- Turbulence modelling: beyond the K- ε model, other models may be evaluated to better deal with temperature stratification effects or for predicting large scale turbulence (LES).
- Interfacial transfers: the liquid to interface heat transfer should be validated in both separate effect tests and more integral tests and the formulation of the transfer should not be too sensitive to the mesh size or should allow a mesh convergence
- The effects of the ECCS jet on local turbulence and on bubble entrainment require further validation

More generally efforts will be made to try to define a Large Scale Simulation approach which could be in two-phase flow the equivalent of the Large Eddy Simulation in single phase flow. Such an approach seems to be necessary for two-phase flows with complex interfacial structure such as churn flow where small and very large and distorted bubbles co-exist or wavy stratified flow with possible entrainment of drop at wave crests and breaking of waves entraining bubbles in the liquid. In such complex flows, filtering all turbulent scales and two-phase intermittency

scales would not make sense since the main characteristics of the flow would be lost, and no filtering at all would be too expensive in required CPU time.

## 6. USING PSEUDO-DNS WITH ITM

### 6.1 DNS Simulations of Boiling Flows

DNS tools with ITM (Pseudo-DNS would be a more appropriate term since subgrid models exist in these tools) were implemented in the TRIO-U code [33,34] and have now reached some maturity to be used for helping the modelling of averaged models of NEPTUNE-CFD. These tools have already been able to simulate mono-site pool boiling and will be used to investigate multi-site boiling (Figure 8) up to DNB. Micro-visualisation experiments are also in progress to validate some aspects of the simulations.

DNB occurs at the very vicinity of the heating wall and all small scale phenomena occurring at the finest scale have to be taken into account: activation of nucleation sites, growing of attached bubbles, sliding of attached bubbles along the wall, coalescence of attached bubbles, bubble detachement, wall rewetting after detachement. Calculations with DNS including ITM are necessary to predict such small scale phenomena since detached bubbles have a diameter of a few tens of micrometers. However, today it may only be used for a very limited space domain.
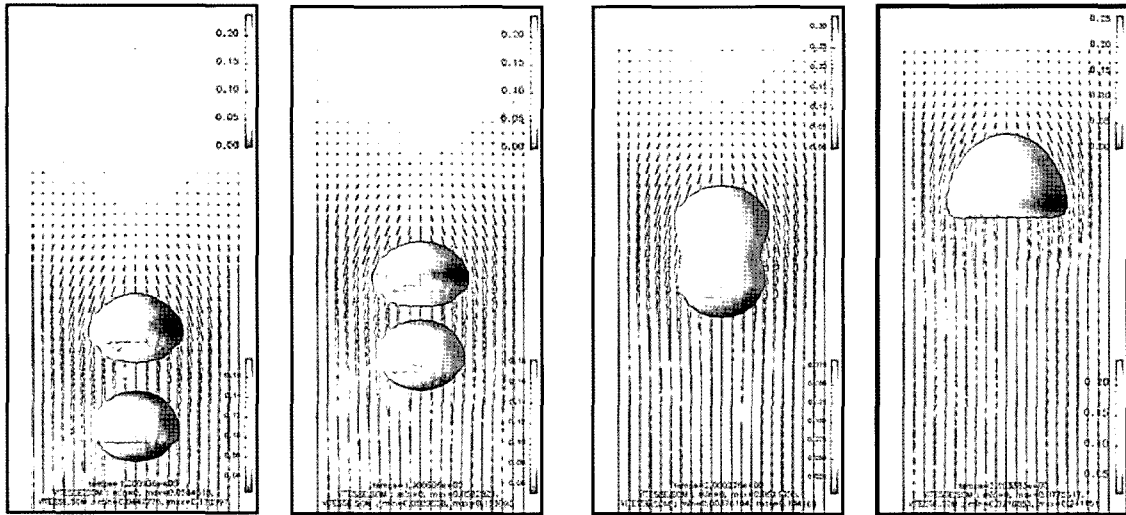
Such simulations may provide information on the

Fig. 9. DNS Simulation of a Coalescence of Two Bubbles        (B. Matthieu, [36] )
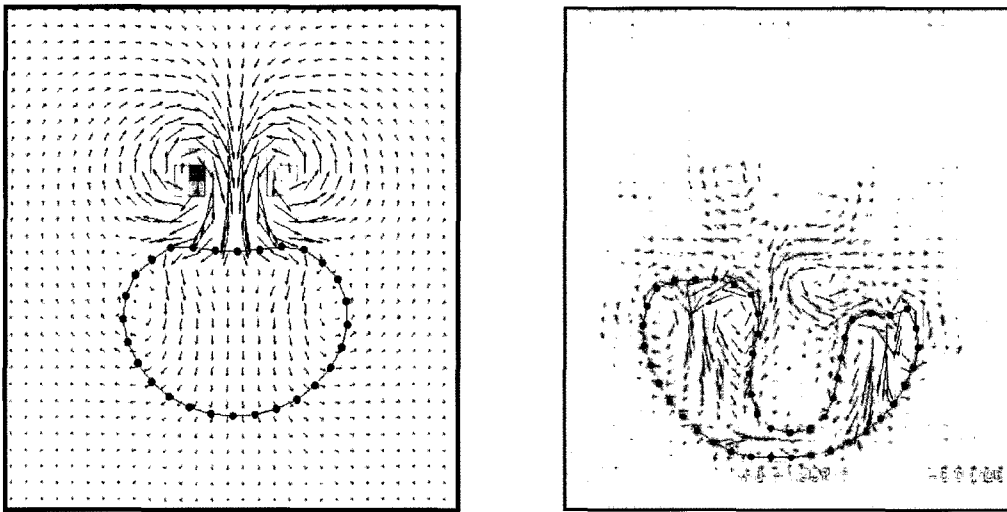


Fig. 10. Simulation with LES Coupled to and Interface Tracking Technique. Distortion of a Bubble Due to Large Scale Eddies
(Labourasse et al. [37])

bubble diameter when it leaves the wall, the frequency of bubble detachment, the heat transfer due to vaporization, liquid heating, wall quenching after a bubble departure. Many sensitivity tests are possible or will be possible in the future to learn about the influence of the nucleation site density, of the geometrical characteristics of the metallic surface, of the mechanisms leading to DNB. Is coalescence

likely to occur before detachment ? How a bubble detachment may affect the growing of neighbouring bubbles ? Such questions may be investigated through DNS and will help in developing adequate and physically based closure relations for the CMFD simulations.

After bubble departure, bubbles are entrained in the flow and they may grow or collapse by vaporization and

condensation. They may also either coalesce or break up. Figure 9 shows a simulation of a bubble coalescence due to entrainement in the wake (B. Matthieu, [36]). Figure 10 illustrates how a bubble can be distorted by turbulence up to break-up. Here the Large Eddy Simulation is used in the continuous phase together with a Front Tracking Method (Labourasse et al. [37]).

DNS methods for two-phase flow are still limited by the required computer power but progress is going on with improving efficiency of both numerical schemes and computer power. The methods used in the examples above are implemented with a parallel solver and future applications on massive parallel computers will allow much more complex simulations.

## 6.2 DNS and LES Simulations of Stratified Flow

Lakehal et al [38,39] have used LES and an ITM to investigate stratified counter-current air-water flow with high interfacial shear and developed a specific subgrid scale modelling. Such finer scale simulations may be of great interest for understanding the complex interactions at the free surface between friction forces, surface tension, wave propagation, condensation or vaporization, turbulence of both the gas flow and the liquid flow for evaluating more macroscopic modelling such as RANS approaches and can be used as complementary to experiments to develop closure relations. These results of LES with ITM will be used for developing closure relations for CMFD in the frame of PTS modelling in the NURESIM project.

## 7. CONCLUSIONS

Reactor simulations of tomorrow will require a combined use of at least three scales, the CFD scale in open medium, the component scale and the system scale. DNS will be used as a support for modelling more macroscopic models. The major steps towards the next generation of thermalhydraulic codes lie in new physical models and improved numerical methods.

Two-phase CFD in open medium is much more recent than other scales but it opens promising perspectives for industrial simulations, allowing to zoom on some component in some specific situations. It was a priority of NEPTUNE phase 1 (2002-2003) to produce the first principal release of the NEPTUNE CFD application.

New coupling methods between the scales or with other disciplines such as neutronics or fuel thermo-mechanics are in progress.

## 8 ACKNOWLEDGEMENTS

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