

VALIDATION METHODOLOGY FOR THE EVALUATION OF THERMAL-HYDRAULIC SUB-CHANNEL CODES DEVOTED TO LOCA SIMULATIONS

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Abstract

This study focuses on thermal-hydraulic simulations, at sub-channel scale, of a damaged PWR reactor core during a Loss Of Coolant Accident (LOCA). The aim of this study is to accurately simulate the thermal-hydraulics to provide the thermal-mechanical code DRACCAR with an accurate wall heat transfer law. This latter code is developed by the French Safety Institute “Institut de Radioprotection et de Sûreté Nucléaire” (IRSN) to evaluate the thermics and deformations of fuel assemblies within the core. The present paper first describes the methodology considered to evaluate the capabilities of existing codes CATHARE-3 and CESAR to simulate dispersed droplet flows at a sub-channel scale and then provides some first evaluations of them.

1. Introduction

This study focuses on the cooling capacity of a damaged PWR reactor core (Pressure Water Reactor) during a Loss Of Coolant Accident (LOCA). During such an accident, as the temperature of the fuel assemblies are very high (600-1200°C) and the clad external pressure well below this internal pressure, some clad ballooning could occur jeopardizing the cooling capability of the core during the following reflooding phase. During this accident phase, core cooling is first provided by a hot vapour flow. Then, as the quench front rises and gets closer to the balloon regions, water droplets appear within the vapour. They experience evaporation, deviation, break-up and coalescence and may impact the ballooned fuel cladding. Numerous dynamical and thermal phenomena should be taken into account to well describe the thermal hydraulics of this dispersed droplet two-phase flow and thus the heat removed from the rods (figure 1). As the quench front hits the ballooned regions, the heat flux removed from the walls reaches its maximum.

The French Institut de Radioprotection et de Sûreté Nucléaire (IRSN) is currently developing the DRACCAR code to simulate the thermal-mechanical behaviour of a rod assembly during LOCA reflood phase with a 3D multi-rod description [1].

This code is a simulation tool for cooling assessment of a geometry having experienced a LOCA. This geometry could be either a complete assembly (including control rods, guide tubes, instrumental tubes, spacer grids) or be reduced to a part of it or a test bundle surrounding by a shroud. The application field of this tool gathers any LOCA transients, different kinds of fuels (UO₂, MOX...) even simulated rods (using electrical devices) and cladding material (Zircaloy-4, M5 and Zirlo) as well as various burn-up. The main goal is to estimate the structures

deformation, coolability and embrittlement before and after the reflooding. The results would be transposed onto a reactor scale to carry out safety studies involving best-estimate computations and uncertainties.

The thermal-mechanical approach is based on a 3D creep model at each axial level, with boundary conditions (constraints) only due to pressure (without retroaction of the neighbour level constraints). Four different modes of ruptures are considered : total elongation, strain, stress and temperature. In this way, thermal-mechanical behaviour of fuel cladding such as deformation, bowing phenomenon and failure are simulated. The Zircaloy oxidation is also taken into account. Models for fuel fragmentation and relocalisation, release of fission gases and hydriding process, which can change mechanical properties, are under-development.

In the first version (DRACCAR V1), delivered in 2008 [1], the thermal-hydraulics was a stand-alone three-dimensional single-phase gas model with a multi-channel water level model. This version was suitable to perform the interpretation of most of the strain and burst experiments, which are generally carried out under vapour flow and of experiment with a reflooding phase.

DRACCAR V1 has been validated on the basis of available experimental data (EDGAR, PHEBUS LOCA, PERICLES, REBEKA, HALDEN, etc.)

However, fluid phenomena occurring during a typical LOCA, as shown in figure 1, are complex and require an advanced 3D sub-channel two-phase flow thermal-hydraulic code [2]. Moreover, a multi-field approach could be required to deal with thermal and dynamical out of equilibrium. Possible coexistence and separated and dispersed flow makes attractive the distinction between two liquid fields (continuous and droplet fields). Finally, closure models need to be suitable for reflooding calculations. Two options are envisaged for the sub-channel code coupled to the next version DRACCAR V2 based on code capabilities and availabilities: the CATHARE-3 and the CESAR code. Both codes are able to handle reflooding at sub-channel scale in intact assemblies and the main features of these two codes will be quickly recalled in this paper.

Beside the development of such a thermal-hydraulic code, a reflection has been conducted to establish the specificities of the coupling of the thermal-dynamical part of the DRACCAR code to any suitable thermal-hydraulic code. The resulting Application Programming Interface has been achieved and released within the framework of the European Project NURISP.

This paper focuses on the validation methodology of these sub-channel thermal-hydraulic code, that should handle at the same time vapour convective heat transfer, phenomena upstream the quench front and the quench front itself. As no local experimental results are available until now, this validation methodology is based on the assessment of sub-channel code results on spatially averaged CFD results. The proposed validation methodology is described in the first section pointing out the chosen parameters for comparison purpose. Then, some exploratory and preliminary results of this validation will be presented; the features of the two module candidates to be coupled to DRACCAR code (CESAR and CATHARE-3) are described, as well as the input deck, and first result comparison for, on one hand, an isothermal two-phase flow and, on the other hand, super-heated vapour flow carrying saturated droplets.

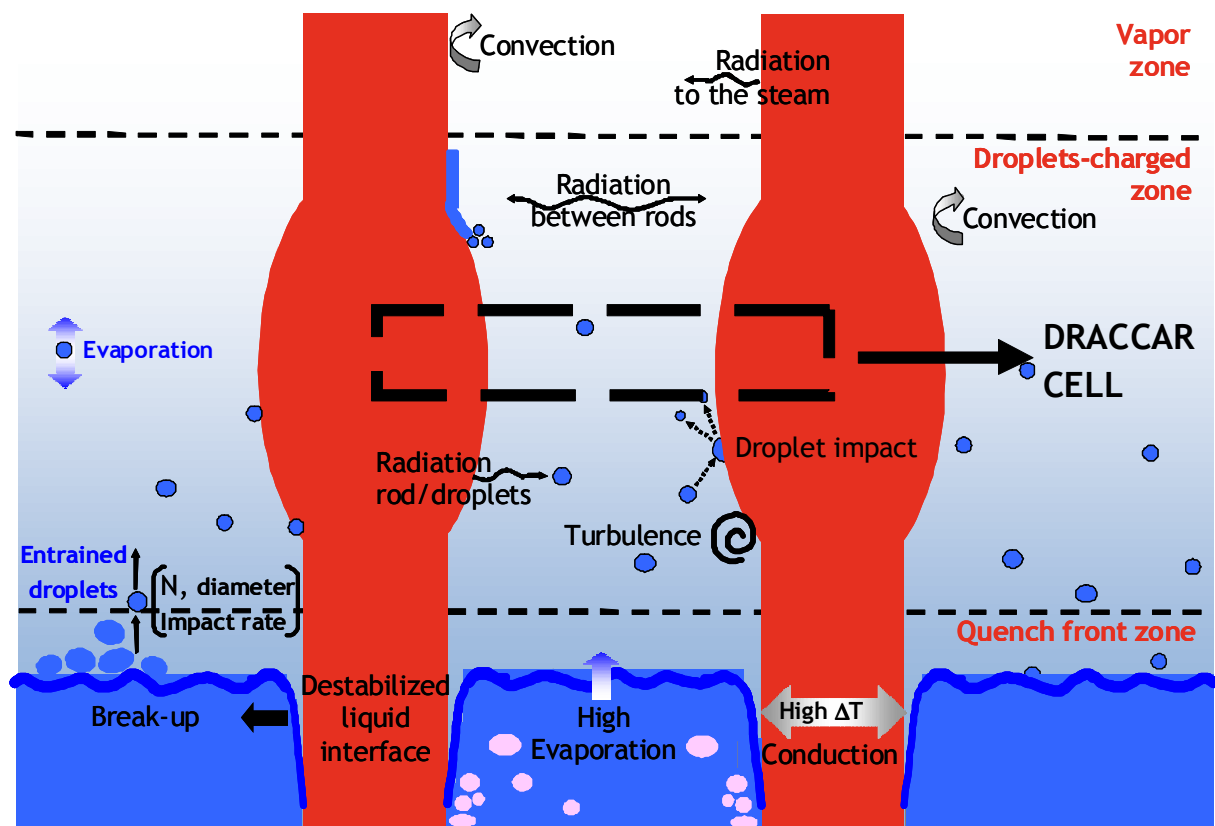


Figure 1 : Thermal-hydraulic phenomena occurring during the reflood phase of a LOCA which need to be modelled at the sub-channel scale of the DARCCAR cell.

2. Validation methodology for advanced sub-channel TH software

Currently only global tests of intact assembly reflooding have been considered for the validation matrix of the CATHARE3 and CESAR codes. The validation is achieved by comparisons between measured and simulated clad temperatures and quench front motions. This analysis validates to a certain extent the global wall heat transfer in the dispersed flow region and does not allow to identify the relative contribution of heat transfer modes and to extrapolate to ballooned configurations.

Unfortunately no local measurements downstream the quench front in balloon regions (i.e. two-phase flow temperature, droplet diameter and spatial distribution ...) are actually available for validation purpose. At present time only global data are available (pressure at the exit, average flow rate, collapse liquid level, cooling rate etc) and do not allow to accurately validate the effects of droplet diameters and difference of velocities between the two phases on the cooling capability of such dispersed droplet flow in ballooned regions.

Thus, a validation methodology was proposed by IRSN in the framework of a wide Research and Development Program on LOCA, launched in 2006. The methodology is based on the adaptation of the CFD code Neptune_CFD (mainly devoted to bubbly and separated-phase flows) to the simulations of dispersed droplet two-phase flows involving steep thermal gradients and thus heat

transfers. Neptune_CFD code is a three dimensional two-fluid code based on the classical two-fluid one pressure approach, including mass, momentum and energy balances for each phase [7], [8]. The final goal of this task [6] is to develop an operational tool in order to, on one hand, study the cooling capability at CFD scale of various two-phase flow features and, on the other hand, provide adequate closure laws for the study of reflooding phase in such LOCA conditions at a component scale. To achieved this adaptation of the code Neptune_CFD, each main heat transfer process, influencing the global heat transfer balance, has been independently studied, modelled and validated on IRSN's separated experiments (such as tests of droplets impacting on very hot plates or radiation attenuation through a spray ramp) [6]. Furthermore, at the end of this development task, the Neptune_CFD results will be validated against a global experiment providing local two-phase flow measurements. This global experiment, called COAL, is foreseen to be performed within the framework of the IRSN's CYCLADES program.

The validation methodology of the thermal-hydraulic sub-channel codes is then planned to be achieved against the CFD simulations of Neptune_CFD in ballooned configurations and under LOCA conditions. Results of candidates sub-channel codes, CATHARE-3 and CESAR, are compared to these CFD results which are spatially averaged over a sub-channel horizontal flow section. The comparisons are performed between two-phase flow features obtained with Neptune_CFD and the sub channels codes. Along the simulated domain elevation (fig.2), the spatially averaged adopted parameters for comparison purpose are vapour and liquid axial velocities, void fraction, phase temperature and interfacial heat fluxes, evaporation rate and wall to phase heat transfers. The radial velocity (cross-flows) would be also investigated downstream and upstream the ballooned regions.

The assessment methodology considers increasing physical complexity of the flow in a realistic LOCA geometry (four ballooned rods as presented in figure 2):

- first isothermal dispersed droplet two-phase flows,
- then dispersed two-phase flows including saturated droplets and superheated vapour with adiabatic wall.

The preliminary results of these two former steps will be presented in this paper.

- In a latter stage, not yet achieved, wall heat transfer will be considered.

At the same time, reflooding of two-phase flow global tests including ballooned regions will be carried out (CEGB [9], CODEX[10]). But this will not be presented in this paper.

3. Reference results

3.1 Studied geometry

The geometry consists of three sub-channels, defined as the fluid space between eight adjacent fuel rods (fig. 2). To simulate flow across partially deformed assemblies, the first and second sub-channels are constricted due to the ballooning of four adjacent fuel rods, while the third sub-channel has a constant cross-sectional area along its whole length. The considered ratio of

ballooning¹ is 61% in the first sub-channel. For this ratio, the rods touch each others and there are no cross-flows between adjacent sub-channels within the balloon region. The total length of a sub-channel is about the typical distance between two horizontal grids (350 mm), and the length of the balloons is 196 mm (figure 2). The CFD meshing of this geometry consists of 78732 cells.

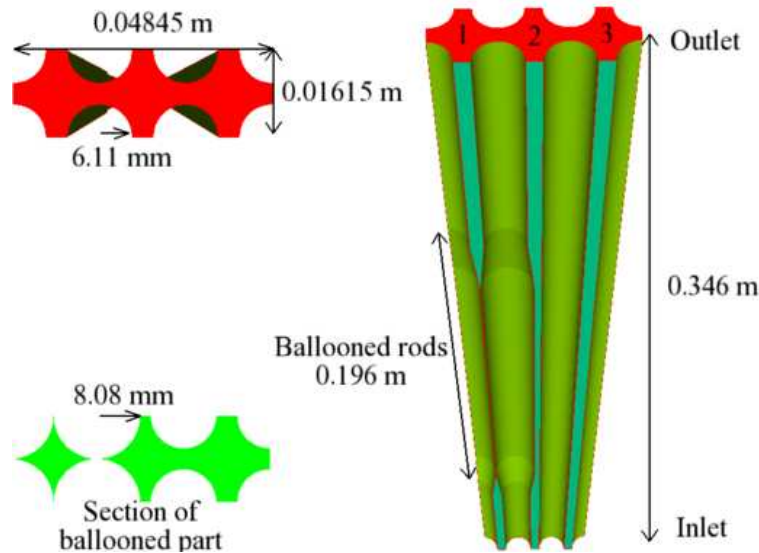


Figure 2: Studied geometry: the four ballooned rods surround the sub-channel denoted 1.

Two-phase flow inlet conditions are imposed at the bottom of the calculation domain. Range of values for droplets and vapour velocities (v_l , v_g), temperatures (T_l , T_v) and liquid volumetric fractions (α_l), are representative of a flow downstream a quench front during LOCA reflooding phase (v_l : 1-5 m/s, v_g : 1-10 m/s, α_l : 10^{-4} - 10^{-2} , T_l around saturation, T_v from saturation to 1000 °C) [9]. Symmetry boundary conditions are considered on the sub-channels vertical boundaries. The rods wall could be adiabatic, as for the test case presented in this article, or heated. Outlet boundary condition is an imposed level of pressure. The mesh convergence of the different simulations has been checked.

3.2 Spatial average

CATHARE-3 and CESAR involve a porous approach to simulate the rods. When using them at sub-channel scale, there is one cell per sub-channel (figure 4).

To compare CFD results from Neptune_CFD with both sub-channel results (CATHARE3 and CESAR), CFD variables are averaged on sub-channel horizontal surfaces located at corresponding cell elevations of the CATHARE-3 and CESAR meshes. As these two codes deal with staggered meshes, the elevations considered for scalar or vectorial variables are different.

¹ This ratio is defined as $(1 - S_{bal}/S_{nbal}) S_{bal}$, resp. S_{nbal} , being the cross section in the ballooned, resp. intact, region.

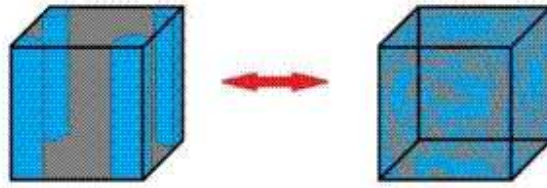


Figure 4 : Illustrations of CATHARE-3 and CESAR cells and the porous approach.

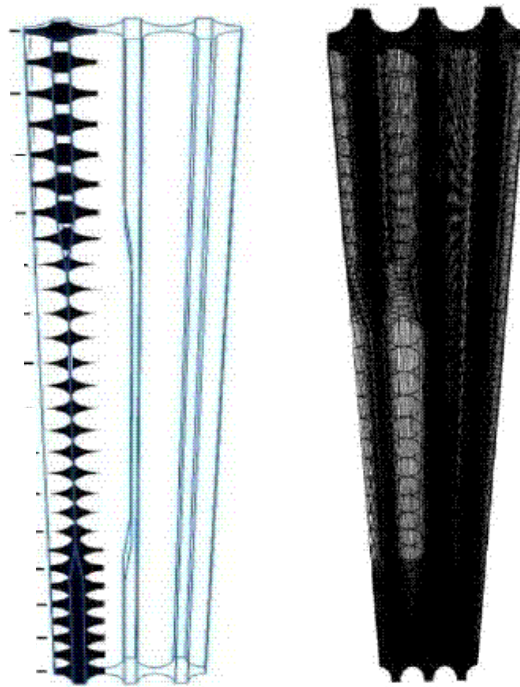


Figure 5 : Illustrations of surfaces used for averaging the vectorial variables within the first sub-channel and overview of the CFD mesh.

4. CATHARE-3

4.1 Current status of CATHARE-3 code

CATHARE-3 [11] is a system code developed by CEA within the NEPTUNE multi-scale thermal-hydraulic platform [12]. In addition to the two-fluid 6-equation model already used in CATHARE-2, an “advanced” three-field model has been implemented in CATHARE-3 [11], featuring a set of balance equations for mass, momentum and energy for the liquid droplets, the continuous liquid and the vapour fields. This model has been developed in order to improve the flow simulation when liquid droplets and continuous liquid flow at significantly different velocities as during the reflooding phase of a LB LOCA. It has already been assessed in 1D and

3D modules of CATHARE-3 against global reflooding experiments [14]. Some other evolutions of CATHARE-3 concern additional equations for interfacial area transport or two-phase turbulence models [13], the improvement of the 3D module of CATHARE-2 whose physical assessment will be extended, and finally the revision of the numerical methods to deal with non-conforming meshing of the vessel. A complete redefinition of the junction data structure and a new solver to optimize computing efficiency are foreseen. Therefore, CATHARE-3 with its sub-channel approach, is a good candidate for the DRACCAR thermal-hydraulics.

4.2 CATHARE-3 input deck

The CATHARE-3 input deck, mainly consisting of a 3D module, has been built to enable result comparisons with Neptune_CFD simulations. Ballooning ratio, height, rod diameter of the geometry define the CATHARE-3 meshing and corresponding cell and faces properties (surfacic and volumetric porosities and hydraulic diameters). As the version V1.250 of CATHARE-3 used in this study is a prototype, the symmetry boundary condition is not available yet. The CATHARE-3 calculation domain is thus enlarged around the 3 sub-channels of the initial geometry with symmetrical neighbouring sub-channels, see figure 6.

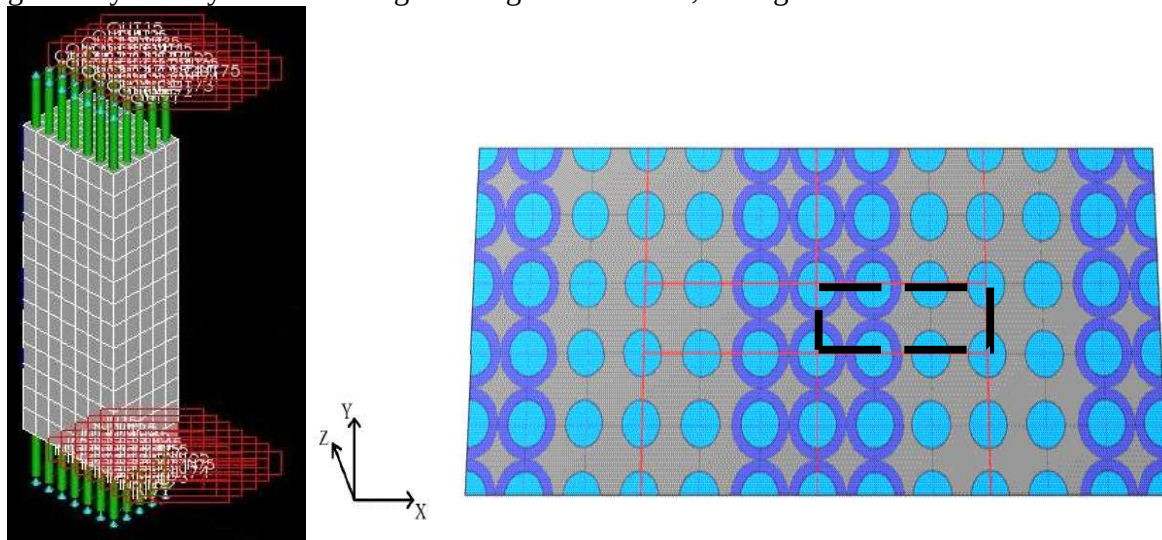


Figure 6: Full view (left) and Horizontal cut (right) of the CATHARE-3 geometry, the three sub-channels studied are in the dashed box .

5. CESAR

5.1 Current status of CESAR code

The CESAR thermal-hydraulics modelling is based on a 1-D 2-fluid 5-equation approach. Up to $N=5$ non-condensable gases are available. As a result $5+N$ differential equations and 1 algebraic equation are solved:

- $2+N$ mass balance equations (for the vapour phase, the liquid phase, and the N non-condensable gases),
- 2 energy balance equations (one for the gas mixture and one for the liquid phase),

- 1 mixture (liquid and gas phases) momentum balance equation,
- 1 algebraic equation, which models the interfacial drag between the liquid phase and the gas phase. It must be underlined here that the interfacial drag is a complex model, which has been assessed on a large number of experimental data [3].

Thermal non-equilibrium is considered between phases, with the possibility of sub-cooled liquid and superheated steam, and mechanical non-equilibrium between phases is considered too, with the possibility of counter-current flows and stratified flows. Most of the CESAR physical constitutive laws are issued from the correlations, which are included in the French best-estimate thermal-hydraulics CATHARE2 code. The different heat transfer processes all along the boiling curve are modelled. Moreover a droplet projection model is implemented which enables CESAR to simulate the quasi-intact core reflooding.

The numerical method follows the finite volume technique. The space is discretized using a staggered grid with the use of the donor cell principle. The time integration is performed using a Newton's method and a fully implicit scheme is used. The Jacobian matrix inversion is based on a highly optimized Lower Upper (LU) algorithm that makes CESAR a fast running and at the same time stable module. Moreover, a special coupling, based on a prediction-correction method, is applied between the CESAR and DRACCAR modules.

5.2 CESAR input deck

The CESAR input deck consists of cells connected through vertical and horizontal junctions. Each of the three sub-channels is modeled by a column of 14 cells. Ballooning ratio, height, and rod diameter define the horizontal and vertical junctions and modules. Furthermore, singular head losses model the flow cross-section variations in the first and second sub-channels. The geometry is displayed in figure 7 where the sub-channel of the left hand side presents 61% of ballooning ratio. The cross-flows around the balloons are illustrated by arrows.

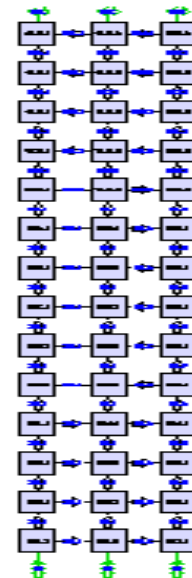


Figure 7: CESAR mesh of 3 sub-channels

6. Comparison of Results

6.1 Single –phase flow

Isothermal single-phase vapour flow simulations with different ballooning ratios (61% and 90 %) and lengths (148 and 58 mm) have first been simulated with CATHARE-3 and CESAR code. The simulated vertical vapour velocities in each sub-channel have been compared to analytical evaluations from a head losses model inspired by Fairbain et al. [15] but also to surface averaged results obtained with CFD softwares; the Neptune_CFD and CFX codes. Table 1 gives the

results obtained for a ballooning ratio of 61% and a length of 148 mm, at atmospheric pressure and an inlet vapour velocity of 10 m/s.

	analytical	Neptune_CFD	CFX	CATHARE-3	CESAR
balloon	11.6	13.8	12.6	11.8	9.5
bypass	14	14.3	13.9	16.2	16.6

Table 1 : Vertical velocity in the ballooned sub-channel (first sub-channel) and the bypass (third sub-channel) [m/s] .

The different codes at the various scales (CFD and sub-channel) reproduce the vapour flow deviation. The surface averaged velocities given by CFD codes in the bypass are very close to the analytical value, whereas the velocities in the balloon are a little bit over-estimated. On the contrary, the sub-channel codes largely over-estimate the velocities in the bypass. CATHARE-3 well predicts the velocity in the balloon and CESAR under-estimates it.

6.2 Two-phase flow with adiabatic wall

Two-phase flow simulations have also been performed. The presented results are obtained at atmospheric pressure, for the following inlet conditions: $v_l=1\text{m/s}$, $v_g=10\text{ m/s}$, $T_l=372.15\text{ K}$, $T_v=573.15\text{ K}$, $\alpha_l=0.01$. The droplet diameter is $d=500\mu\text{m}$.

The vertical pressure profiles along the three sub-channels obtained with CATHARE-3 and Neptune_CFD are very similar: the pressure within the ballooned sub-channel remains a little bit higher than in the other sub-channels. On the contrary, the pressure calculated by CESAR in the ballooned sub-channel drops rapidly at the inlet of the restricted section ($\Delta P \sim 75\text{ Pa}$) well below the pressure evaluated inside the other sub-channels. However, the overall pressure loss obtained along the geometry is of the same order of magnitude; 120 Pa with Neptune_CFD, 200 Pa with CATHARE-3 and 170 Pa with CESAR.

The vertical vapour velocity evolutions along the height of the simulation domain are displayed in figure 8. Results are given for each sub-channel: ballooned (bal in fig. 8 or 1 in fig. 2), intermediary (inter in fig. 8 or 2 in fig. 2), and bypass (bypass in fig. 8 or 3 in fig. 2). Global evolutions are consistent for the 3 approaches: in the ballooned sub-channel, the velocity decreases upstream the ballooned region, remains uniform along the balloon, and decreases as cross-section enlarges downstream. CATHARE-3 results are the closest to the CFD in the balloon region prediction whereas CESAR results are the closest in sub-channel 2 (inter). And the velocity in the bypass is largely under-estimated by CATHARE-3 and overestimated by CESAR.

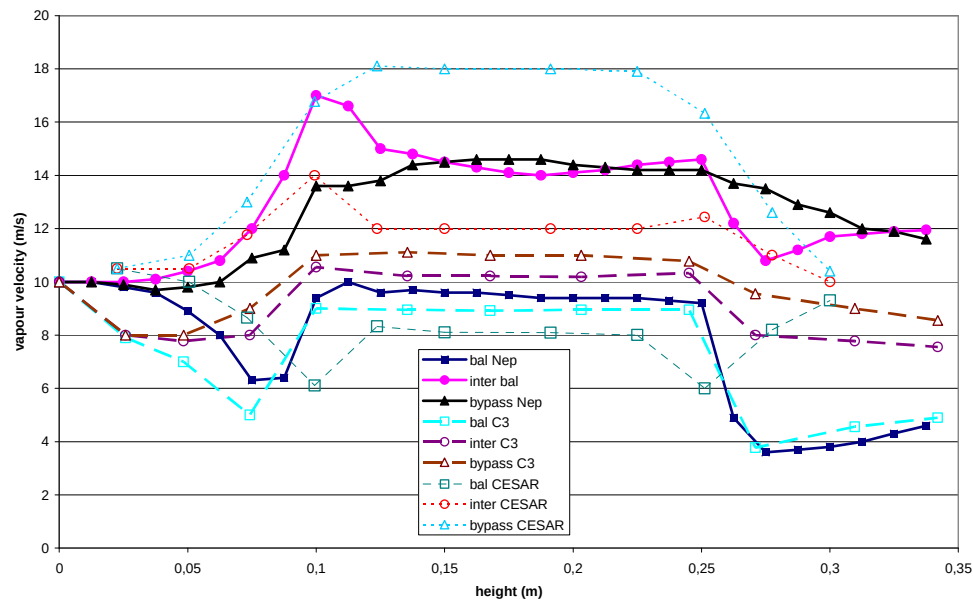


Figure 8 : Vertical vapour velocity evolution along the height of the domain in the three sub-channels (Neptune_CFD, C3 and CESAR results)

The CESAR model for the interfacial drag between the liquid phase and the gas phase is not adapted to configurations involving inclusions with inertia. From CESAR results, the droplet vertical velocity (injected at 1m/s) quickly reaches the vapour velocity and then evolves in accordance with it keeping a very low difference of about 0.05 m/s, whereas the droplet field simulated with CATHARE-3 experiences an inertia as illustrated in figure 9.

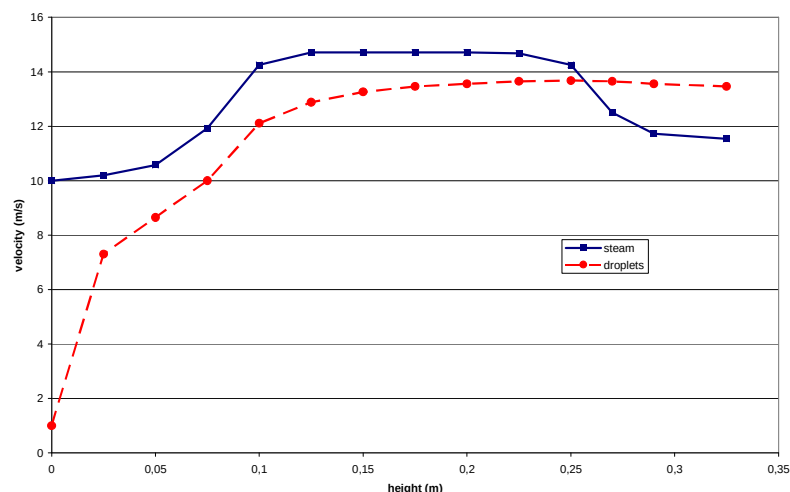


Figure 9: Liquid and vapour vertical velocity evolutions in the bypass along the height of the domain, CATHARE-3 results.

The void fraction profiles in the three sub-channels obtained with Neptune_CFD and CATHARE-3 are displayed in figure 10. Although, the void fraction at the bottom of the

geometry is a little bit different (0,992 with Neptune_CFD and 0,988 in CATHARE-3), its evolution along the different three sub-channels are the same with Neptune_CFD and with CATHARE-3. The void fraction decreases in the balloon and increases downstream.

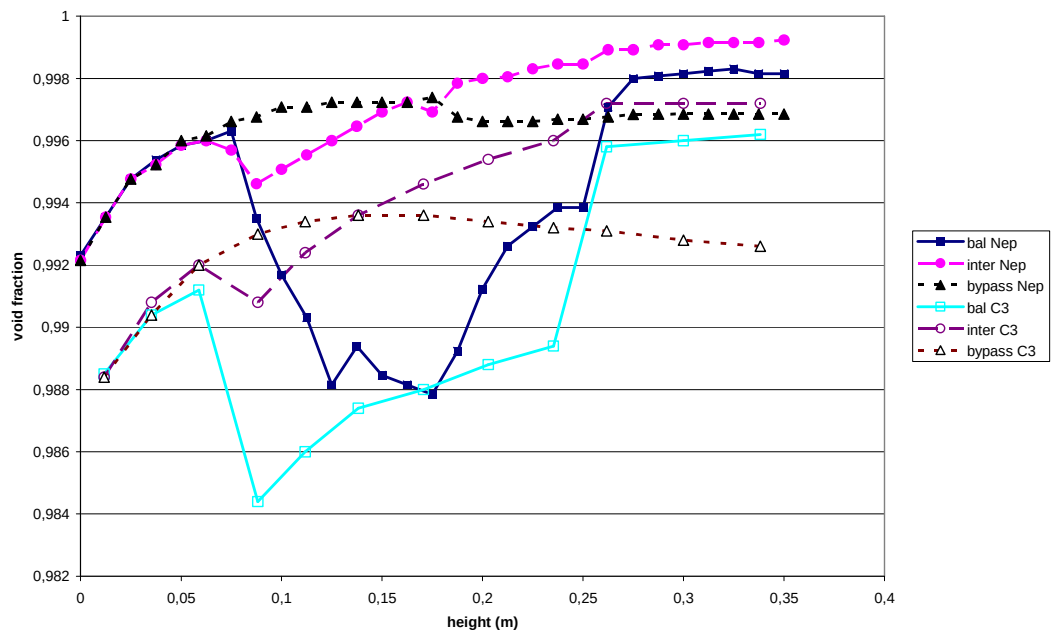


Figure 10 : Void fraction evolution in the three sub-channels along the height of the domain (Neptune_CFD and C3 results)

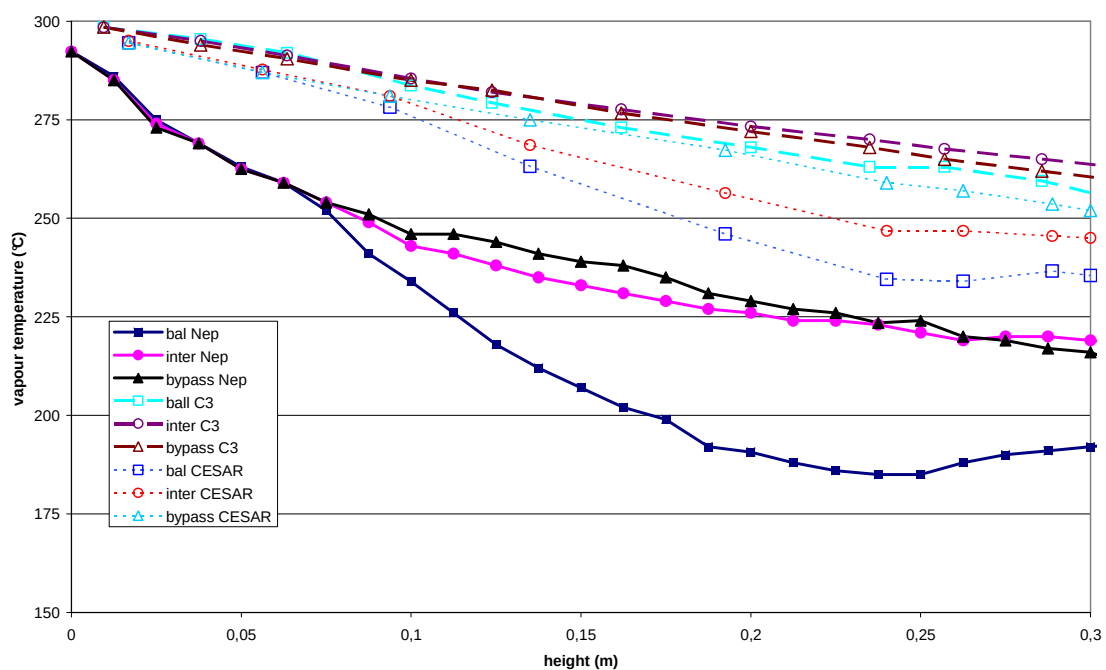


Figure 11 : Vapour temperature evolution along the geometry height in the three sub-channels (Neptune_CFD, C3 and CESAR results)

The second sub-channel is only a little bit affected by this void reduction. Finally in the upper part of the geometry the void fraction increases owing to saturated droplets evaporation in the surrounding overheated vapour. The void fraction obtained with the CESAR code is quite constant to 0,999 (although 0.99 is injected) along the geometry height and is slightly lower in the ballooned sub-channel. This gap is consistent with the 5 equation approach of the code. Indeed, the inlet information of vapour and liquid velocities as well of the inlet liquid fraction are lost in the mixture velocity and interfacial drag. A new dynamical equilibrium is found which does not correspond to the non-equilibrium inlet condition.

Finally the vapour temperature vertical profiles are compared in figure 11. The overall vapour cooling-down is simulated by CATHARE-3 and CESAR but they are very less than CFD predictions. The ballooned sub-channel is the most cooled down. A finer investigation should be carried out to understand this vapour temperature decrease as the amount of liquid remains constant to about 0.001. Also a further work will be to accurately evaluate the heat fluxes between phases (through droplet interface) in CATHARE-3 to understand the lower cooling down with a higher amount of liquid than in Neptune_CFD.

7. Conclusion and Perspectives

This paper summarizes the preliminary assessment of the CATHARE-3 and the CESAR codes for sub-channel thermal-hydraulics treating dispersed droplet flow in ballooned region of a Nuclear Water Reactor core during the reflood phase of a LOCA. This thermal-hydraulics is required for the DRACCAR code, devoted to the simulation of thermal-mechanical behaviour of a rod bundle under LOCA with a 3D multi-rod description. With respect to fluid phenomena occurring in this region, the need is a 3D two phase flow sub-channel thermal-hydraulics with two liquid fields (continuous and droplet fields) and models suitable for reflooding calculations. CATHARE-3 gathers all these characteristics and could be a good candidate. CESAR is a 5 equations code with an algebraic equation modelling the interfacial drag between phases which is not adapted to heavy particles in gaseous flow. However, the CESAR code is a sub-channel code including a reflooding model and already coupled to DRACCAR. Furthermore no local measurement is available on dispersed flow features during a reflood phase. The validation of the thermal-hydraulic sub-channel code for LOCA simulation purpose is based on a methodology involving, on the one hand, comparison results to local surface averaged results obtained with the adapted Neptune_CFD code [6] and, on the other hand, global comparisons to experimental tests with ballooned regions.

In this paper, the preliminary results of the local part of this methodology has been presented. CATHARE-3 and CESAR input decks have been build for this purpose. Preliminary results underline that CATHARE-3 well fits to the requirements for the DRACCAR thermal-hydraulics. Its prediction of the void fraction evolution is very accurate and of velocity in the good order of magnitude. The interfacial heat transfers would be more further investigated before treating cases with hot cladding. On the other side, this preliminary study has underlined the limitations of the CESAR code, in particular in term of velocity and void predictions and an important work of improvement of code capabilities (at least the accounting of a second momentum balance equation) should be considered.

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