

Numerical study on the influence of simplified spray boundary conditions for the characterization of large industrial safety spray systems used in nuclear reactors

J. Malet¹, A. Foissac^{1,2}, C. Vayaboury¹, T. Gélain¹, S. Mimouni²

¹ Institut de Radioprotection et de Sûreté Nucléaire, BP 68 Gif-sur-Yvette, France

² EDF, MF2E, Chatou, France

jeanne.malet@irsn.fr; thomas.gelain@irsn.fr; stephane.mimouni@edf.fr

Introduction

During the course of a severe accident in a Pressurized Water Reactor (PWR), hydrogen can be produced due to reactor core oxidation, leading to potential combustion and deflagration, as observed in Three Mile Island and Fukushima accidents. In some reactors, spray systems are placed at the top of the containment to prevent overpressure. Spray modelling is thus part of thermal-hydraulic containment codes. The two major phenomena involved in spray behaviour under such accidental conditions are the thermodynamical effect of a spray (steam condensation on droplets, leading to a local increase of hydrogen concentration) and the dynamical effect (mixing of gases, leading to a decrease of hydrogen concentration). The competition of these two coupled phenomena is an important issue for nuclear safety and can be assessed using CFD codes.

For nuclear reactor (containment vessel of around 60 000 m³), simplifications have to be done to simulate a nuclear accident in the containment where gas mixture (steam, hydrogen and air) is mixed by the spray systems. Up to now, no CFD calculations are available in the open literature on spray systems in a real-scale nuclear containment, using detailed spray initial conditions, accurate droplet modelling and droplet-gas momentum interaction. Many simplifications can be performed in the computer simulation to reduce the computational time of such sprays induced flow in a very large containment: atomization zone is neglected, considerations of only one droplet size and velocity at one single injection point, consideration of so-called ‘dynamical equilibrium’ between gas and droplet, etc. [1]. The objective of this paper is to evaluate the influence of several simplifications performed on spray boundary conditions, on some selected ‘output’ parameters that can influence the overall gas mixing in nuclear reactors.

This evaluation is performed on a real-scale PWR spray nozzle (hollow cone) having an outlet diameter of 9.5 mm and a maximum diameter of the induced spray envelope of about 2 m. CFD calculations are performed using the ANSYS code (lagrangian approach) and the EDF NEPTUNE_CFD code (eulerian approach).

1. Description of PWR spray systems

Spray systems are emergency devices designed for preserving the containment integrity in case of a severe accident in a PWR. They are used to prevent overpressure, to cool the containment atmosphere, to remove fission products from the atmosphere and to enhance the gas mixing in case of hydrogen presence in the containment. The efficiency of these sprays can depend partially on the evolution of the droplet size distribution in the containment, due to gravity and drag forces, heat and mass transfers with the surrounding gas, and droplet collisions. Spray systems in PWR are composed of over 500 interacting water droplet sprays, placed in circular rows, which are activated under gaseous mixture composed of steam, hydrogen and air at a total pressure of around 2-3 bars and under gas temperature around 100-120°C. A schematic view of the spray rings, the associated theoretical spray envelopes, as well as the spray nozzle (Lechler, 373.084.17.BN) are presented in Figure 1.

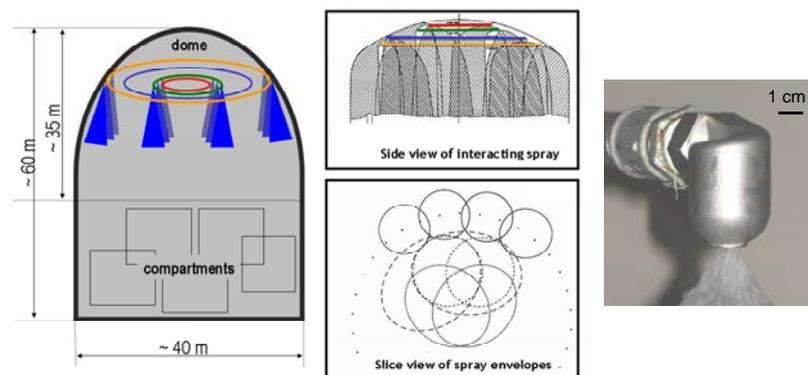


Figure 1: Spray rings and envelopes in a French PWR (not at scale) and PWR spray nozzle

2. Description of the experimental facility

The experiments have been carried out at the Institut de Radioprotection et de Sûreté Nucléaire (IRSN), in the CALIST facility (Characterization and Application of Large and Industrial Spray Transfer, 160 m³) sketched in Figure 2. The set-up is composed of a hydraulic circuit supplying, for those experiments, a single spray nozzle with a flow-rate of 1 l/s at a relative pressure of 3.5 bar. The pulverized water is collected in a 5 m³ pool. The axial position of the spray nozzle can be changed using a monitored carriage.

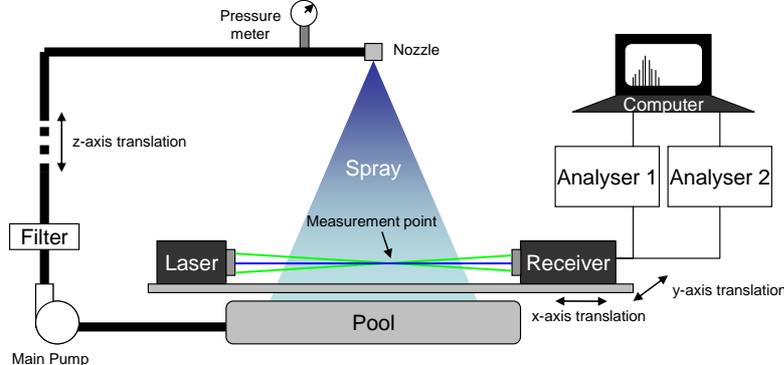


Figure 2: CALIST water-spray experimental facility

Spray characteristics are measured by Phase-Doppler Interferometry (PDI, distributed by LAVISION/ARTIUM, Bachalo and Houser, 1984 [2]). In order to determine where atomization ends, i.e. where droplets are spherical, visualization has been performed with a Phantom high-speed camera. More information on these PWR spray measurements can be found in [3] and [4] where droplet sizes, droplet velocities and droplet size-velocities correlations are given. All measurements are performed in air under atmospheric conditions (1 bar, 20 °C).

3. Description of the numerical calculations

3.1 NEPTUNE-CFD code

Numerical simulations have been performed using the NEPTUNE_CFD code (Mimouni et al. [5]). The solver belongs to pressure based methods and is based on a finite volume discretization. It is able to simulate multi-component multiphase flows by solving a set of three balance equations for each field. The data structure is totally face-based which allows the use of arbitrary shaped cells including non conforming meshes. The main interest of the numerical method is the so-called “volume fraction – pressure – energy cycle” [6] that ensures mass and energy conservation and allows strong interface source term coupling. In the simulations, gas turbulence is associated to the k-ε model, whereas dispersed phases turbulence is modelled with the Q2-Q12 model (Simonin [7]). The dispersed phase is considered as a set of continuous ‘fluid’ media: each ‘fluid’ corresponding to a statistical average between two fixed droplet size (Greenberg et al. [8]).

3.2 ANSYS/FLUENT-CFX code

The CFD code ANSYS 13, based on the conservative finite-volume method, is also used to calculate the gas flow induced by this PWR spray. Calculations are performed under incompressible, isothermal, steady-state and turbulent flow. The Lagrangian-droplet-Eulerian-fluid (LDEF) approach tracks the particle’s accelerations with Newton’s second law (gravity and drag forces) and imposes the particle-fluid (gas) interaction through a source term (drag force) in the Navier-Stokes momentum equations. The standard k-ε turbulence model is used here. CFX and FLUENT solvers are used for these calculations but mainly CFX results are presented here, since CFX has a so-called ‘hollow-cone’ spray injection option. The obtained results lead us to test other spray injection options.

3.3 Computational domain and boundary conditions

The CALIST facility room is 7 m x 6 m large and 3.5 m height and the spray nozzle is placed at the center of a horizontal slice of the room. Using symmetries, the computational domain is reduced to 1/4th of the CALIST facility, so that it is 3 m x 3.5 m large and 3.5 m height. The mesh is obtained using GAMBIT (structured-grid) for the NEPTUNE-CFD calculations, and using ANSYS-Meshing for the ANSYS/CFX calculations (unstructured grid). Examples of the meshes are given on Figure 3. The way of mesh refinement used with both codes is different: in the NEPTUNE-CFD calculations, the whole ‘spray zone’ is refined and in the ANSYS calculations, the expected spray envelope, assuming an angle of 60 degrees, is refined.

The atomisation process of the spray nozzle is not modeled, since the objective is to perform a calculation using droplet characteristics (size and velocities) as boundary conditions: it is not planned to use an atomisation model in a whole scale nuclear reactor containment vessel, considering already the huge computational time requested by such a calculation. Nevertheless, as it will be briefly discussed at the end of the paper, this could be an option for future studies.

Since atomisation process is not modelled, boundary conditions have to be given for the spray: droplet size and velocities have been measured 20 cm below the nozzle outlet and can be used as boundary conditions. In this paper, this height 20 cm below the nozzle will be called the ‘droplet injection zone’. It is situated at 1 m from the ceiling of the CALIST facility.

The gas (air) is initially at rest. Depending on the kind of ‘droplet injection zone’, a boundary condition on the gas velocity will be applied or not (this will be specified in the paper sections).

Two ‘lateral faces’ of the computational domain are two symmetry planes and the two other lateral faces are treated as walls. The bottom face is treated as a wall. Conditions on wall are the non-slip condition for the gas and extraction of the domain for the droplet.

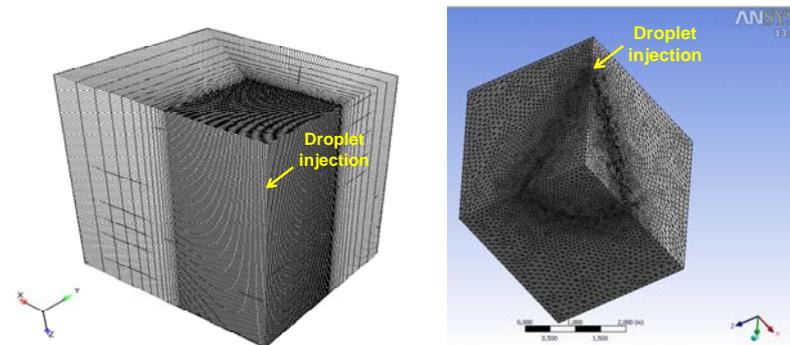


Figure 3: Meshes (left: for NEPTUNE-CFD calculations, right: for ANSYS calculations)

3.4 Preliminary verifications

Mesh dependency has been checked for calculations performed with both codes. The tested meshes characteristics are given in Table 1. Examples of the results on the mesh sensitivity obtained with both codes are given in Figure 4 (radial profiles over the horizontal axis X). The selected data on this figure are especially taken as the one where the mesh sensitivity is the highest. For both codes, similar results are obtained with the standard and finer mesh, whereas the coarser mesh lead to significant differences. Major differences are obtained with the ANSYS calculations probably because the coarser mesh used with ANSYS is coarser than the coarse one used with NEPTUNE-CFD. It is thus concluded that mesh convergence is reached with both “standard” meshes.

Table 1: Meshes characteristics of all calculations

	Coarse mesh		Standard mesh		Refined mesh	
	NEPTUNE	ANSYS	NEPTUNE	ANSYS	NEPTUNE	ANSYS
Typical dimension of the cell (spray refined zone)	3 to 5 cm	7 cm	2 to 3.5 cm	5 cm	1 to 1.5 cm	2.5 cm
Total number of cells	262 500	116 500	787 500	451 500	4 750 000	1 650 00

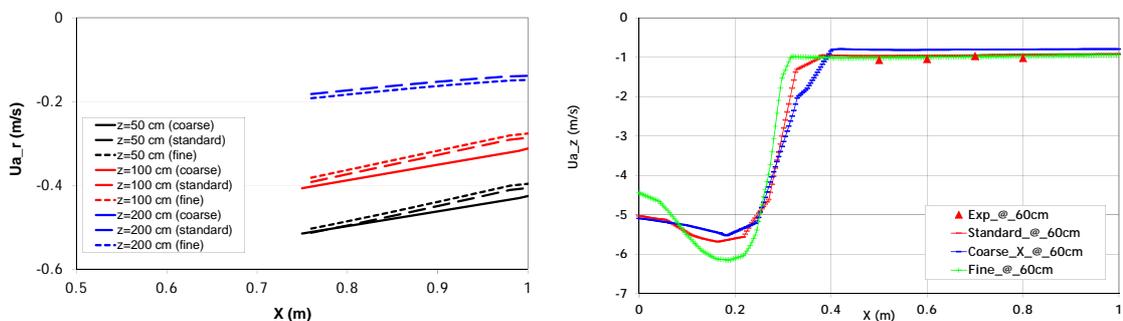


Figure 4: Examples of gas (air, U_a) velocities radial profiles (radial $U_{a,r}$ and axial $U_{a,z}$ gas velocities) for different meshes (left, NEPTUNE-CFD, right, ANSYS/CFX)

Concerning ANSYS/CFX lagrangian calculations, the convergence to the injected droplet number is also achieved. Examples of results are presented in Figure 5. From all results obtained, the convergence is achieved with 10^5 particles.

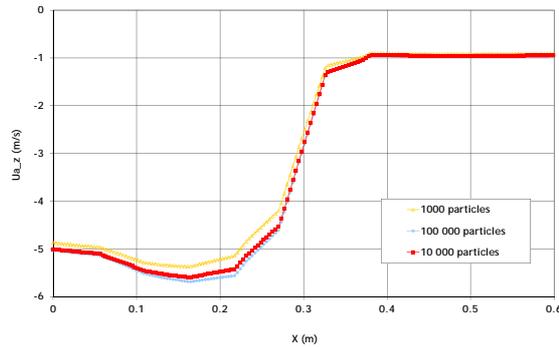


Figure 5: Convergence to injected particle number in the lagrangian tracking approach, shown for one gas vertical component of the velocity radial profile

More sensitivity calculations have been done with the ANSYS/CFX code that offers a wide range of possible investigation. Two other turbulence models (SST and BSL) have been tested, as well as the influence of the numerical scheme. Small influences are observed but are not relevant for the present study so that it is chosen not to present them in this paper.

4. Results

4.1 Main results

Main results presented on Figure 6 are as expected for hollow-cone spray calculations: the main gas entrainment occurs inside the spray (Figure 6), so that the smallest droplets ($150\text{-}200\ \mu\text{m}$), with less inertia, are easily entrained in this region, and can thus be mainly found in the spray center. It can be observed that the biggest droplets ($400\text{-}500\ \mu\text{m}$) are concentrated on the spray envelop, since they are less influenced by the induced air flow field, whereas small drops respond to the air flow.

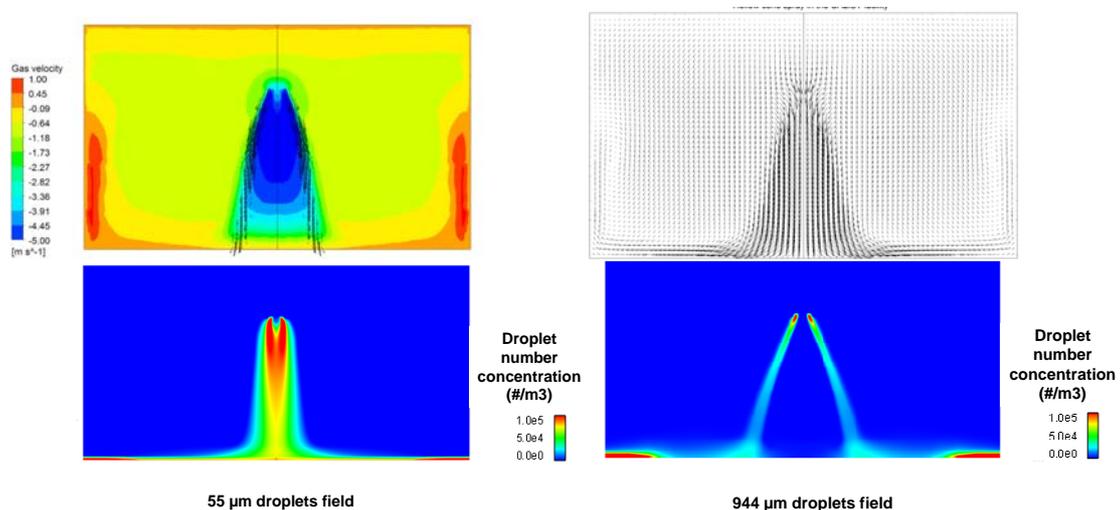


Figure 6: Up: Vertical component of the gas velocity and droplet velocities vectors (left), gas velocities vectors (right), ANSYS/CFX calculations, Down: Droplet volume fractions field for the smallest size droplets (left) and largest size droplets (right), NEPTUNE-CFD calculations

The code-experiment comparison is given in Figure 7 for both codes. It can be seen that results on the droplets velocities (radial and axial) are rather in good agreement with the experiments. The spray is dispersed on approximately the same widths on the different heights: from a 10 cm width injection zone at 20 cm below the spray nozzle (boundary conditions of the calculations) up to almost 30 cm width at 95 cm from the nozzle outlet. The levels of the velocities, as well as the shape of the velocity profiles are rather coherent with the experimental data even if some discrepancies remain for both codes, especially far away from the spray nozzle. Further analysis could be performed to enhance the reliability of the calculations.

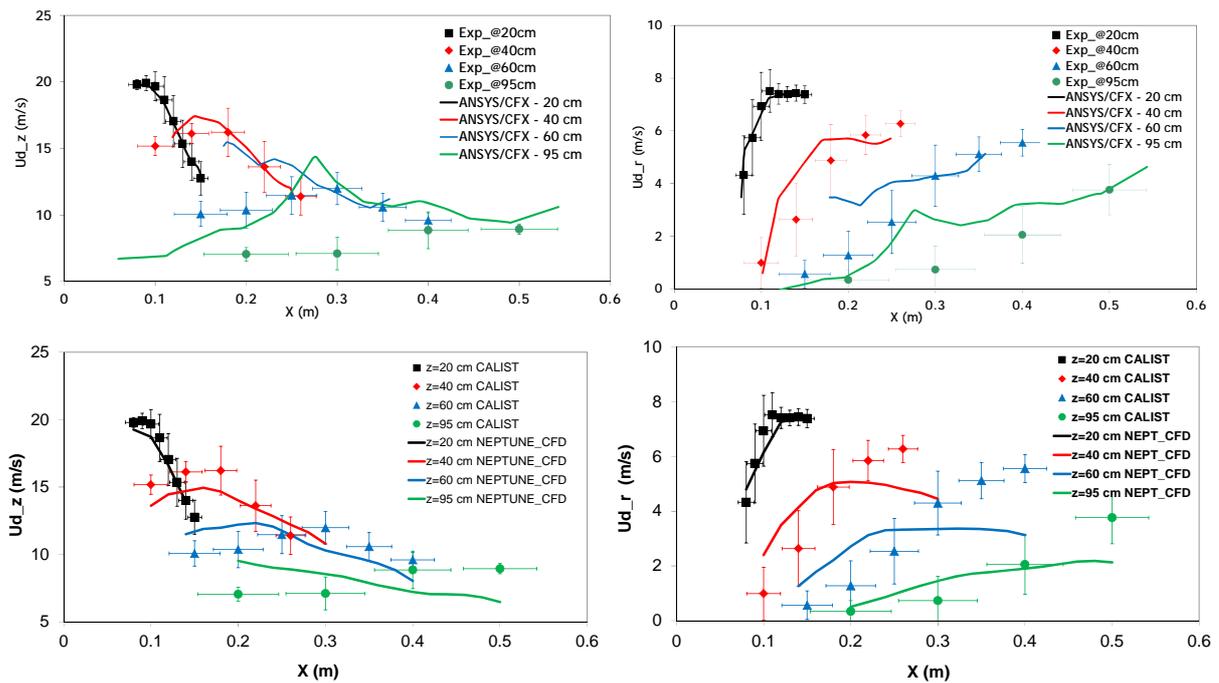


Figure 7: Droplet axial (left) and radial (right) velocity profiles at different distances from the spray nozzle, ANSYS-CFX (up) and NEPTUNE-CFD (down) versus CALIST experiments

4.2 Studies on the effect of simplified spray boundary conditions

In nuclear reactor applications, considering the large volume (60000 m^3) and the important number of various phenomena to be simulated to represent accidental conditions, some simplifications have to be made. Here, so-called ‘simplifications studies’ in which simplified conditions are used for the calculations, are performed in order to see their impact on the results. Most of the simplifications studies have been performed using the ANSYS/CFX code, even if NEPTUNE-CFD results lead, as we will see on section 4.2.4, to similar conclusions.

4.2.1 Impact of the use of a constant velocity profile at the injection

In the results presented above, the exact experimental droplet size distribution and velocity profiles have been used as boundary conditions for the droplets, imposing the creation of a mesh object that define droplet ‘inlet’ conditions (see curves at 20 cm in Figure 7). However, for lagrangian tracking of commercial codes, several different ‘particle injections’ are proposed for the user: these ‘particle injections’ give the interesting possibility not to model this ‘inlet’ zone. This can be very useful for CFD calculations of spray systems in a nuclear reactor containment, since the mesh of such a small region regarding to the size of the containment would be a great constraint. For example, plain-orifice atomizer, pressure-swirl-atomizer, flat-fan atomizer, full-cone, ring cone and hollow-cone are ‘particle injections’ available in ANSYS.

The ‘ring’ cone ‘particle injection’ of CFX has been tested here, since the PWR spray characteristics obtained experimentally at 20 cm are found to be over an annulus ring. In such ‘ring cone’ calculation, the input data that lead to the closest droplet initial velocities profiles (at 20 cm) is the one considering a ring from 10 to 13 cm (instead of 8.5 cm to 14.5 cm), having an angle of 25 degrees (30 degrees is the angle at the middle position in the ring), and using an amplitude for the droplet velocity of 18 m/s. The droplet sizes are modelled with the experimental size distribution presented in Foissac et al. [3] (data called CVP_DSD for Constant Velocity Profile and Droplet Size distribution). They are compared with the data presented in Figure 7 having the exact experimental injection velocity profile (data called EVP_DSD, EVP stands for Experimental Velocity Profile). It can be seen on Figure 8 that at boundary conditions (20 cm), the droplet velocities (curves CVP) are not exactly fitting the measured experimental data using such ‘ring cone particle injection’ due to the interpolation of the imposed data with the mesh (whereas with an inlet model, the experimental conditions can be applied perfectly to the boundary zone). The consequences of these different boundary conditions are shown on Figure 9 at 40 and 95 cm from the nozzle outlet: the droplet dispersion, the droplet gas velocities, and the entrained gas velocities are not the same. For example, the maximum value of the axial velocity is changed of 50 %.

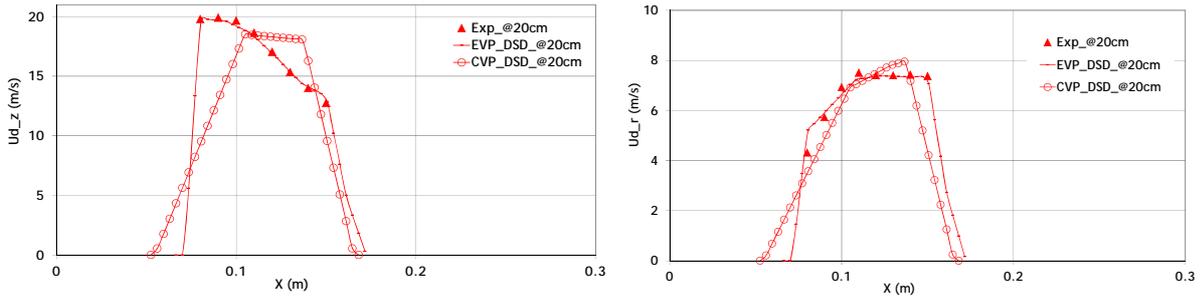


Figure 8: Droplet injection velocity (U_d) radial profiles with ANSYS/CFX using an exact mesh object as boundary (EVP_DSD) and a ‘particle injection’ without injection mesh object, with a constant velocity profiles (CVP_DSD)

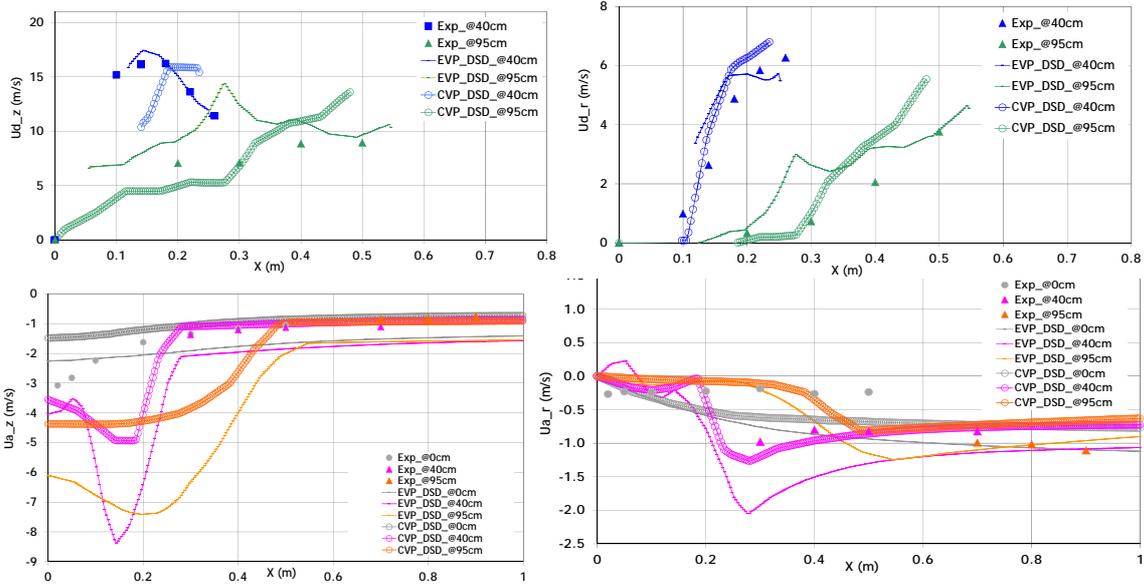


Figure 9: Droplet (U_d) and gas velocity (U_a) radial profiles using an exact mesh object as boundary (EVP_DSD) and a ‘particle injection’, with a constant velocity profiles (CVP_DSD), ANSYS/CFX

4.2.2 Impact of the use of a single diameter instead of a mean droplet size distribution at the injection

Because of the large size of the reactor containment, studies using spray systems at the real scale are generally performed using a spray characterized by one mean droplet size instead of a droplet size distribution. Figure 10 shows the impact of such assumption on droplet velocities. It can be seen that under conditions with a single droplet size (data called ‘MONO’), all droplets have almost the same trajectories, leading to a different spray envelope than in a case considering an initial size distribution (‘POLY’). In the case presented here, the spray envelope is reduced (the largest droplets of a size distribution define the spray envelope) and there is no droplet at all in the center of the spray (no small droplets to be entrained). This has an effect on the entrained gas velocity, since the maximal axial velocity is changed of around 25 %. The radial velocity is also impacted.

4.2.3 Impact of the choice of the gas boundary conditions at the spray injection zone

One other feature is the boundary conditions applied for the gas at the location of droplet injection. At this location, where the atomization process is assumed to be completed, the gas is already entrained. Here, we examine one case where the gas is considered at rest in the droplet injection zone (so called REST), one case where the gas velocity is equal to the droplet velocities in the droplet injection zone (AS_DROP), and one case similar to the ‘AS_DROP case’, but considering also a 10 m/s constant gas velocity profile inside the spray, assuming entrainment is already established inside the spray (AS_DROP_IN_ENTR). The value of 10 m/s comes from 50 μm droplet velocity measurements on the spray axis. These boundary conditions are summarized in Table 2. Results are presented in Figure 11. It can be seen that initialization of the gas velocity leads to different results in the entrained gas velocity. Experimental data are needed to validate the most appropriate boundary conditions.

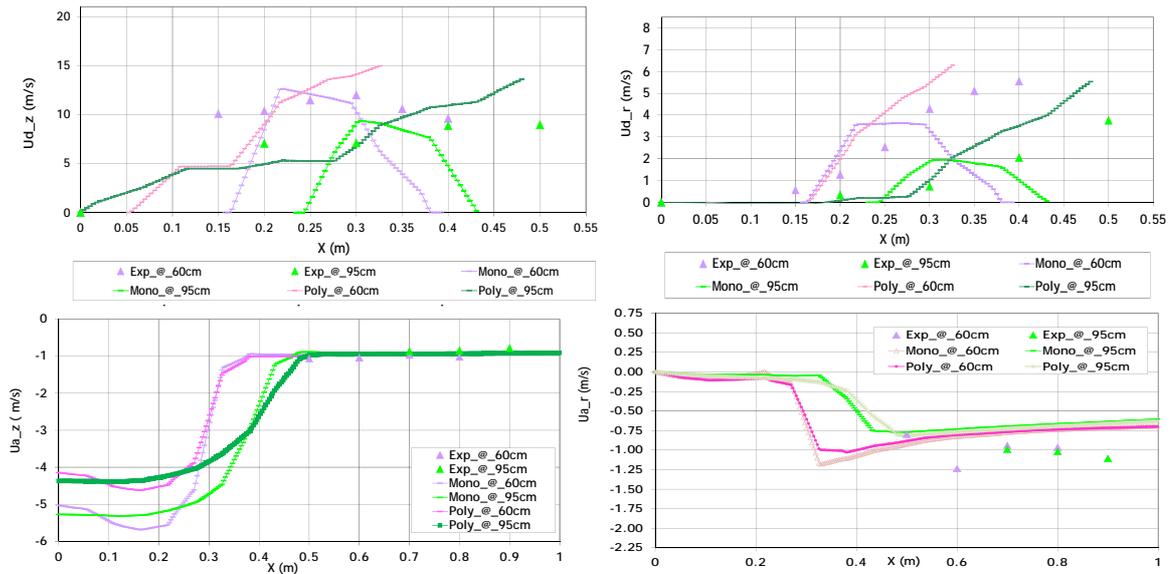


Figure 10: Comparison on droplet and gas velocities between ANSYS/CFX results obtained with single mean diameter (MONO) and size distribution (POLY) at the inlet spray boundary conditions

Table 2: Different boundary conditions applied for the gas velocity

Velocities (m/s)	REST		AS DROP		AS DROP IN ENTR	
	Ua _z	Ua _r	Ua _z	Ua _r	Ua _z	Ua _r
Inside the cone (almost no droplets)	free	free	free	free	10	0
On the spray envelope (droplets are present)	0	0	17.7	7.6	17.7	7.6
Outside the spray	free	free	free	free	free	free

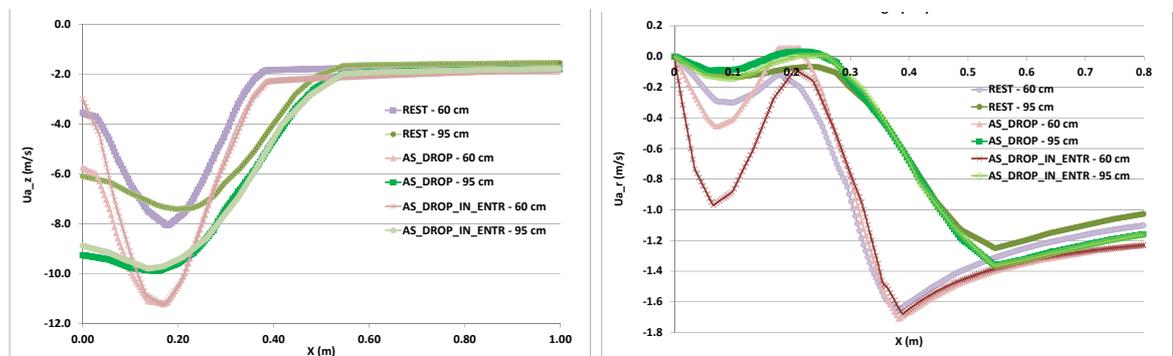


Figure 11: Comparison on gas velocities between results obtained with different gas inlet boundary conditions (with same droplet inlet boundary conditions)

4.2.4 Impact of the choice of combined simplifications on droplet size and velocities

Combining the two sensitivity studies described above, i.e. imposing a monodispersed size instead of a size distribution, as well as a constant mean velocity instead of a velocity profile, has also been investigated. Results are presented for the NEPTUNE-CFD code on Figure 11. The droplet velocities profiles for the ‘MONO_CVP case’ show values generally higher in the spray center and lower on the spray envelope, which can be explained easily since no droplet ‘separation’ by inertia occurs. ANSYS results lead to the same conclusions.

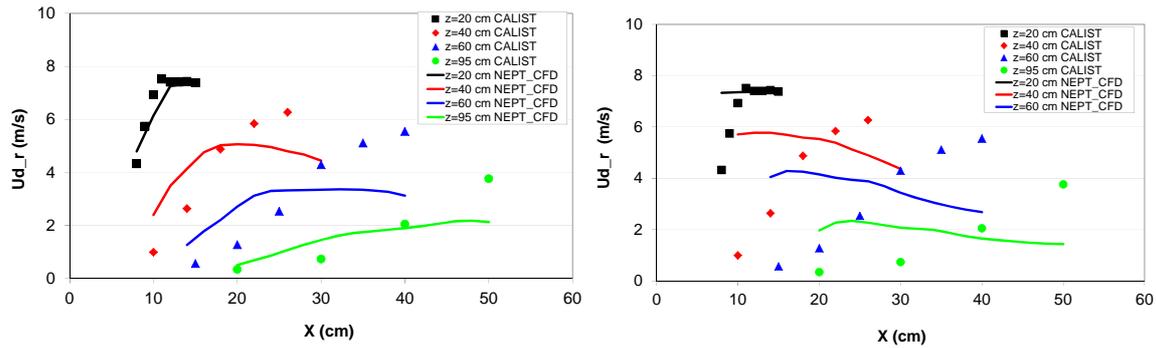


Figure 12: Droplet velocities obtained with mean diameter and a constant velocity profile (right) and a size distribution and a real velocity profile (left) applied at the inlet spray boundary conditions

5. Conclusion and perspectives

CFD calculations on a real PWR spray nozzle have been investigated here with two different CFD codes, both using different approaches for the droplet transport: Eulerian model for the NEPTUNE-CFD code, and Lagrangian tracking for the ANSYS/CFX code. Several simplifications have been made in the calculations, especially based on the boundary conditions applied at the location where droplets and gas are injected. It is found that the use of a constant droplet velocity instead of the velocity profile at the injection mainly influences the entrained gas axial velocity. The use of a mean droplet size plays mainly a role on the spread of the spray, i.e. on the thickness of the annulus where droplets are found. The influence of the gas conditions applied at the droplet injection location plays mainly a role on the axial entrained gas velocity. Such simplifications are realistic for nuclear containment calculations that do not allow, for the today computer power, to use exact boundary conditions.

We have shown here that such simplifications influence droplet and entrained gas characteristics. The next step will be to study their impact on the droplet sizes profiles inside the spray and to translate these conclusions in terms of interesting parameters for nuclear safety. One important concern is the competition between depressurization of the containment by the cold spray and gas (hydrogen) mixing induced by the spray entrainment.

It is known that droplet condensation will mainly occur in a reduced region compared to the size of the reactor containment, since droplet will rapidly reach the thermodynamical equilibrium (in less than 1 or 2 meters below spray nozzle). As a result, this competition between depressurization and mixing should be addressed very locally in the vicinity of the spray nozzle. This competition is also probably different 'inside' the spray, where droplets are tiny and entrained gas velocities higher, and on the spray envelope, where droplets are bigger and entrained gas velocities lower. To investigate analytically the competition of these phenomena is rather difficult since the evolution of the droplet characteristics depends on phenomena that are strongly coupled. As a conclusion, CFD calculations, focused on the zone where most of the heat, mass and momentum transfers occur, are recommended in order to bring some insights for different configurations typical for safety concerns.

6. References

- [1] J. Kim, L. Unjang, S.-W. Hong., Kim S.-B., Kim H.-D., Spray effect on the behaviour of hydrogen during severe accidents by a loss-of-coolant in the APR1400 containment, *Int. Comm. in Heat and Mass Transfer*, 33, pp. 1207-1216, 2006.
- [2] W.D. Bachalo and M.J. Houser, Phase Doppler spray analyzer for simultaneous measurements of drop size and velocity distributions, *Opt. Eng.*, Vol. 23, pp 583-590, 1984.
- [3] Foissac, J. Malet, M.R. Vetrano, J.M. Buchlin, S. Mimouni, F. Feuillebois and O. Simonin, Droplet size and velocity measurements at the outlet of a hollow-cone spray nozzle, *Atomisation and Sprays*, Vol. 21, pp. 893-905, 2011.
- [4] Foissac A. Modélisation des interactions entre gouttes en environnement hostile, PhD Thesis, Univ. Paris VI, France, 2011.
- [5] S. Mimouni, J.-S. Lamy, J. Lavieville, S. Guieu and M. Martin, Modelling of sprays in containment applications with a CMFD code, *Nuclear Engineering and Design*, Vol. 240 (9), pp 2260–2270, 2010.
- [6] N. Mechtoua, J. Lavieville et al., An unstructured finite volume, solver for 2-phase water/vapor flows modelling based on an elliptic oriented fractional step method, in *Proceedings of the 10th International Topical Meeting on Nuclear Reactor Thermal-Hydraulics (NURETH '03)*, Seoul, South Korea, October, 2003.
- [7] O. Simonin, Combustion and turbulence in two-phase flows, *von Karman Institute for Fluid Dynamics, Lecture Series*, 1996-02, 1996.
- [8] J.B. Greenberg, I. Silverman and Y. Tambour, On the origin of spray sectional conservation equations, *Combustion and Flame*, Vol. 93, pp 90–96, 1993.