

**BENCHMARKING OF CFD AND LP CODES  
FOR SPRAY SYSTEMS IN CONTAINMENT APPLICATIONS:  
SPRAY TESTS AT TWO DIFFERENT SCALES IN THE  
TOSQAN AND MISTRA FACILITIES**

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**Abstract**

The TOSQAN (IRSN) and MISTRA (CEA) projects have been created to perform separate- and coupled-effect tests representative of typical post-accident thermal-hydraulic flow conditions in the reactor containment, such as those created by the operation of spray spray systems, with detailed instrumentation suitable for code validation. Gas entrainment and heat and mass transfers between gas, droplets and walls are the main phenomena involved under spray conditions. In order to improve the modelling of the latter phenomena, a global benchmark exercise is organized in the frame of the European SARNET Network. The paper will focus on the results of the TOSQAN benchmark exercise on test 101, where a cold water spray is injected into a steam/air mixture, resulting in partial depressurization. The TOSQAN test 113 (cold spray injected into a helium-air stratified mixture), the MISTRA MASP and MARC2b tests (similar respectively to TOSQAN 101 and 113, but at larger scale) are then briefly presented.

**Introduction**

During the course of a hypothetical severe accident in a Pressurized Water Reactor (PWR), spray systems are used in the containment in order to prevent overpressure in case of a steam break, and to enhance the gas mixing in case of the presence of hydrogen. Spray models are thus part of thermal-hydraulic containment codes. The two major phenomena involved in spray behaviour in such applications are the thermodynamical effect of a spray (steam condensation on droplets, evaporation, ...) and the dynamical effect (entrainment and mixing of gases).

The objective of the SARNET benchmark is to evaluate the spray models of containment codes.

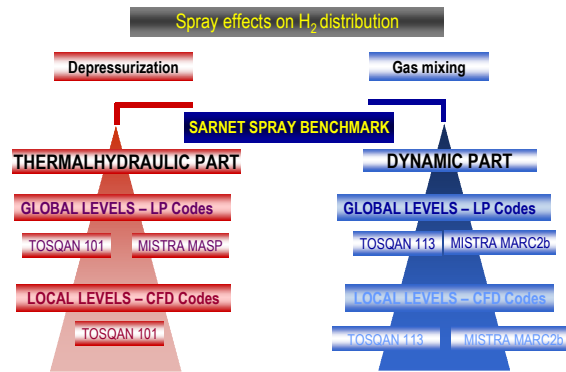
In the past, qualification of spray modeling has been performed on large-scale facilities (CVTR, NUPEC, CSE, [15]) using several spray nozzles. The present benchmark proposes the use of two recent facilities, TOSQAN (IRSN) and MISTRA (CEA) for a combined spray benchmark. The advantage of these facilities and the proposed tests in regard to previous studies are:

- the 'reduced' size of the facility, allowing a high density of instrumentation for a better analysis of the involved phenomena,

- the use of non-intrusive instrumentation, especially in the TOSQAN facility, making the characterisation of the spray droplets possible,
- a ‘separate-effect’ approach by the use of a single spray nozzle, avoiding interaction of sprays, and the possible resulting deviation in the analysis and the study of dynamical effects without any thermodynamical effects.

This benchmark is proposed in the frame of the European network of excellence, SARNET (Severe Accident Research NETwork), under the CAM (Containment) group activities. As a result, this benchmark is based on several tests. A first part, called the THERMALHYDRAULIC part, relates to the thermodynamics of sprays, i.e. the droplet heat and mass transfer modeling and the gas thermodynamical modeling. A second part, called the DYNAMIC part, relates to the gas entrainment and atmosphere mixing induced by a spray, avoiding heat and mass transfer exchanges (Figure 1).

In this paper, we will present all tests of this SARNET spray benchmark, and some preliminary calculations and study that have already been done.



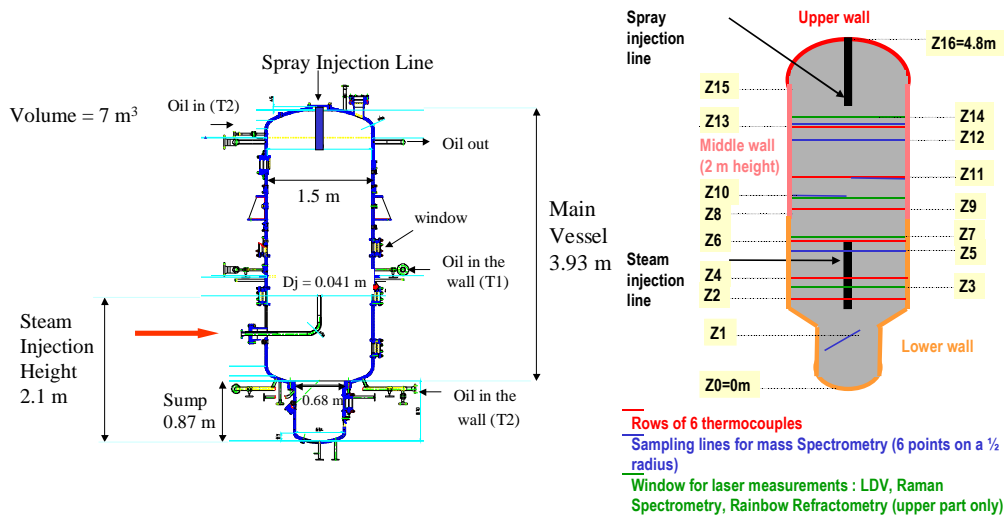
**Figure 1: Schematic of the SARNET spray benchmark and the associated tests**

## Description of the facilities

### TOSQAN

The TOSQAN facility and the associated measurement levels are presented in Figure 2. It is a closed cylindrical vessel (7 m<sup>3</sup> volume, 4 m high, 1.5 m internal diameter). The vessel walls are thermostatically controlled by heated oil circulation. The inner spray system is located 65 cm from the top of the enclosure on the vertical axis. It is composed of a single nozzle producing a full-cone water spray. This nozzle can be moved along the vertical axis in order to perform measurements at different distances inside the spray under steady-state conditions. In the lower part of the vessel, the water impacting the sump is removed to avoid water accumulation and to limit evaporation.

The available instrumentation on TOSQAN concerns mass flow-rate, temperature and pressure of the water spray injected, mass flow-rate and temperature of the water removed to the sump, mass flow-rate of injected steam and helium, gas measurements, temperature measured by protected thermocouples located on horizontal rods at 6 different heights, volume fraction measured by mass spectrometry and Raman spectroscopy, and vessel total pressure [6]. Gas temperature and volume fraction are also measured in the spray zone. For droplet measurements, techniques available are droplets velocity measured by PIV and LDV, and droplet size measured by out-of-focus visualization [7].



**Figure 2: TOSQAN facility**

### MISTRA

The MISTRA facility is a stainless steel cylindrical vessel of about 99.5 m<sup>3</sup>, 4.25 m internal diameter and 7.38 m height (Figure 3). It is constituted of 2 shells, a flat cap and a curved bottom, fixed together with twin flanges. The vessel is thermally insulated with 20 cm of rock wool.

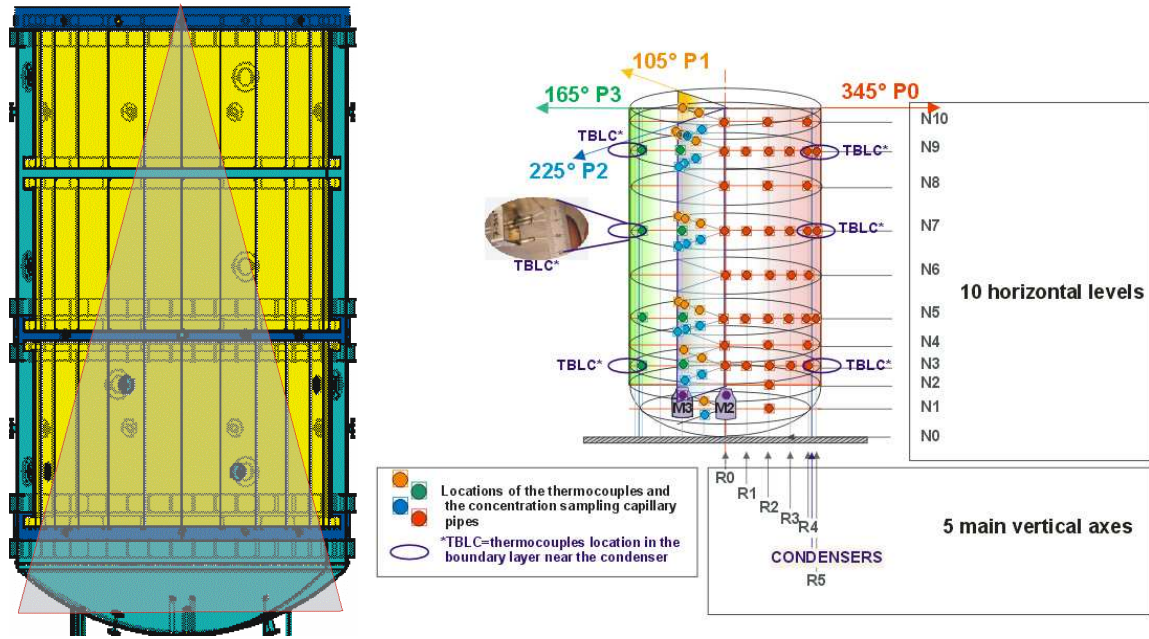
Three cylindrers (called ‘condensers’ even if no condensation occurs on them in the present tests) are inserted inside the vessel, close to the walls in order to keep them at constant temperature. A so-called "dead volume" behind these condensers exists, and during long term experiments, spurious steam condensation can occur on the vessel and bottom walls. Each condenser has its own regulation circuit designed to provide the circulating water with a most stable and uniform temperature (a wall temperature difference less than 1°C is achieved).

Gutters are installed to collect and quantify the steam condensate or droplet streams. The external parts of the condensers are insulated with synthetic foam. Spurious steam condensation or water droplets are also quantified by collecting water at different locations: along the vertical side walls, along the external part of the condensers and in the bottom. To avoid interaction of droplets with the condensers, the spray is generated by a full jet nozzle with an angle of 30°. The nozzle is fixed near the center of the flat cap at less than a few centimetres from this center (quasi-centered), the bottom of the nozzle is at few centimeters from the roof.

The measurements performed are total pressure, temperature (gas and wall), gas composition and condensed mass flow rate. They are all simultaneously and continuously recorded over the whole test period, except for gas concentration measurements that mainly proceeds with successive samplings out of the spray region.

The instrumentation mesh is located on four vertical half-planes: 105°, 165°, 225° and 345° in the main gas volume, but also in the so-called "dead volumes". The instrumental mesh grid on the half plane at 345° combines 10 vertical levels and 5 radial positions. The maximum distance between two sensors is less than 1 meter axially and 0.5 m radially. Three other half-planes are lightly instrumented to check the flow symmetry. For the off-centered injection test, the half plane at 165° allows characterization of the injection area. During the spray activation, instrumentation out of the spray jet is reliable.

Previous benchmarks associated with the MISTRA tests are presented in [11, 12, 13]. The status of the MISTRA program is given in [10].



**Figure 3: View of MISTRA facility and its main location for instrumentation.**

## Thermalhydraulic part, TOSQAN Test 101

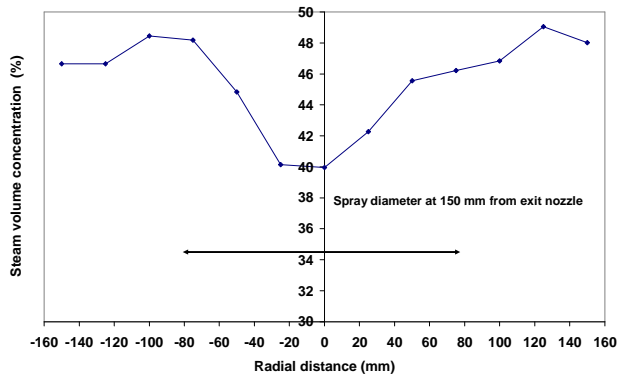
### *Description of the test sequence*

The night before a test 101, compressed air is injected into the open vessel in order to remove steam from former tests. On the morning of the test, the air injection is stopped and the vessel is closed when a thermal steady-state is reached (the relative pressure is then 0 bar). An initial pressurization is performed with superheated steam up to 2.5 bar. Steam injection is stopped and spraying starts simultaneously at a water temperature around 25°C and water mass flow-rate around 30 g/s. The transient state of depressurization starts and continues until the equilibrium phase, which corresponds to the stabilization of the average temperature and pressure of the gaseous mixture inside the vessel.

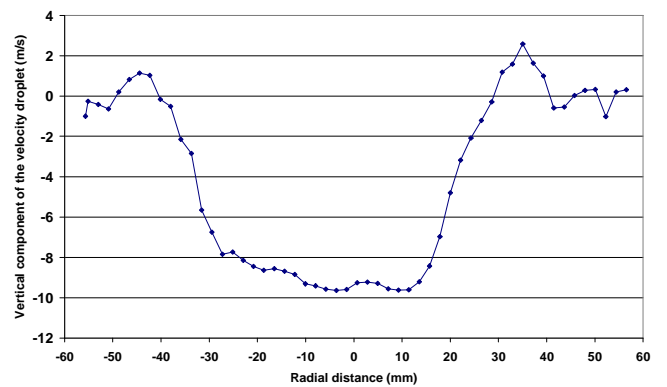
### *Main experimental results and analysis [7, 8]*

Water spray is produced by a nozzle (TG\_3.5 from Spraying System) which provides droplets of almost uniform size. Spray characterization has been performed by means of optical diagnostics in order to determine initial droplet velocity, droplet size distribution and spray angle (Figure 6). The droplet radial velocity profile measured close to the nozzle exit is presented on Figure 5. A radial profile of steam volume concentration performed inside the spray during the steady state is presented on Figure 4.

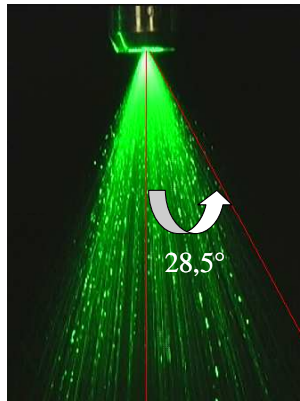
The droplet temperature measurements achieved during the thermodynamic equilibrium of a similar test (same test as test 101 but with an off-centered spray nozzle) have shown that the droplets are heated until a distance of 160 mm from the nozzle (this region is dominated by steam condensation on the droplets). The radial profile achieved in this condensation region at 150 mm from the nozzle, shows a steam decrease in the spray zone.



**Figure 4: Steam volume fraction radial profile 15 cm below the nozzle**



**Figure 5: Droplet radial velocity profile measured 5 cm below the nozzle**



**Figure 6: Laser visualization of the near field of the spray**

#### *Numerical calculations [4, 5]*

The first phase of the benchmark performed in 2004 was blind, whereas the second phase, in 2005, was open. The codes involved in this exercise were either lumped-parameter-codes or Multi-Dimensional codes: ACACIA-1D (IRSN), ASTEC/CPA-0D (IRSN), GASFLOW-MultiD (FZK), GOTHIC-MultiD (AECL), TONUS-CFD (CEA) and TONUS-LP (CEA). Only the “global analysis” of this benchmark will be discussed in this paper; a local analysis (gas temperature, gas concentration, etc) has also been performed [5] and will be continued in this SARNET spray benchmark.

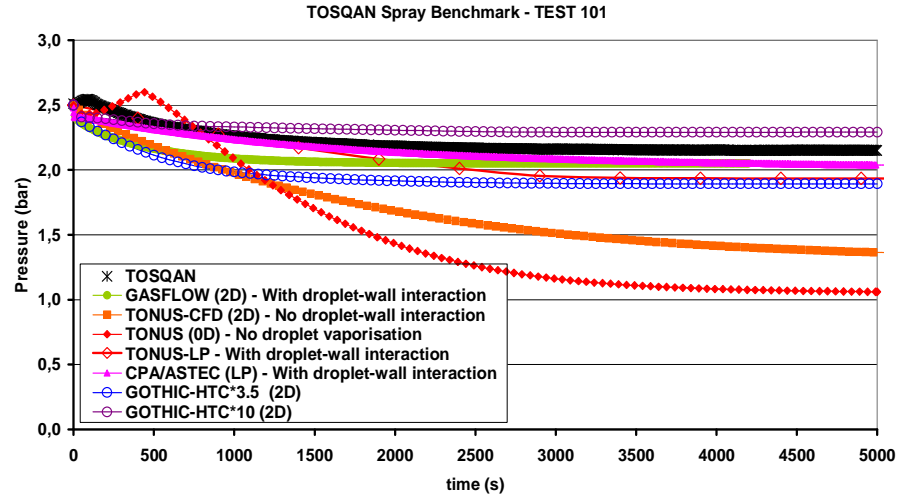
The thermodynamical global behaviour concerns the pressure variation in the TOSQAN vessel. Results for the total pressure are presented on Figure 7 and Table 1. In this table, results are given for the different models made by the code participants. The first line (Modeling 1, M1) corresponds to the blind calculations, without any droplet-wall interaction modeling. The second line (Modeling 2, M2) concerns the open calculations performed taking into account droplet evaporation.

	TOSQAN	CPA/ASTEC	GASFLOW	GOTHIC	TONUS-CFD	TONUS-LP
Modeling 1	2.15	1.20	1.56	1.36	1.36	1.06
Modeling 2		2.04	2.05	1.89	2.29	1.95
(M2-M1)/M2 *100%		41.2	23.9	28.0	40.6	15.0

**Table 1: Total pressure (bar) and associated relative difference (%) calculated by the different codes and obtained experimentally at final equilibrium**

Each code chooses a different way to take into account the involved phenomena:

- CPA: modeling M2 is performed assuming that around 10 % of the droplets are removed by evaporation;
- GASFLOW: a droplet depletion model is used for M2: one part of the steam coming from the vaporized droplets is reinjected to the gaseous mixture, and another part is removed in order to take into account the interaction between the walls and the droplets;
- GOTHIC: M2 is performed by multiplying the wall convective heat transfer coefficient HTC by a factor between 3.5 (left GOTHIC column in Table 1) and 10 (right GOTHIC column in Table 1): this parameter has a significant effect and the resulting pressure is enhanced if  $35 \text{ W.m}^{-2}.\text{K}^{-1}$  is taken for HTC (instead of  $6 \text{ W.m}^{-2}.\text{K}^{-1}$ );
- TONUS-LP: in M1, no droplet evaporation is taken into account; in M2, the injected spray flow-rate is lowered by a fraction of the real one's (14%) to simulate droplet evaporation;
- TONUS-CFD: M1 does not take into account the droplet-wall interaction and M2 uses a modified HTC as in the GOTHIC code.



**Figure 7: Time evolution of the total pressure in TOSQAN test 101 benchmark**

#### Considerations on the global behaviour

Let us consider the ideal case where no droplet wall interaction occurs, where the gas mixture is slightly superheated and wall heat losses are considered negligible. Also consider the whole vessel in a 0D approach, as one single compartment. In that case, when steady-state is reached, there is no heat and mass transfer between gas and droplets and the steam partial pressure  $P_s$  is equal to the saturation

pressure  $P_{sat}$  calculated at the droplet injection temperature:  $P_s = P_{sat}(20^\circ\text{C}) = 0.03$  bar. The steam partial pressure is close to zero and the final total pressure is close to the air partial pressure (neglecting thermal effects). However, it is found that in the TOSQAN test 101, the measured total pressure is around 2 bar, indicating that we are far away from this ideal case. This means that an external steam source has to be added in this model.

No mass balance can really help precisely this analysis: the extracted water mass flow rate is approximately equal to the injected mass flow-rate, indicating an equilibrium between, on the one side, the water mass coming from the injection and the condensation of steam on droplets, and on the other side, the water mass disappearing due to extraction of water on the bottom of the vessel, evaporation of the droplets in the gas and evaporation of the droplets on the walls.

This steam source of around 1 bar could have thus several origins: evaporation of droplets impacting the lower wall, evaporation of droplets in the gas, other. Since benchmark participants that have an evaporation modeling of droplets in the gas were not able, in the blind phase, to recover the experimental pressure curve, the assumption was made that the droplet evaporation on walls was the main source. Furthermore, the experiments show a decrease of the bottom wall temperature that could be a consequence of droplet evaporation on walls. Nevertheless, an estimation of this droplet evaporation on walls cannot be made with a high precision using the available experimental data. The TOSQAN vessel is constituted of isothermal walls controlled by heated oil circulation. During the tests, the heated oil extracted from the wall circuit has a lower temperature than the one entering the circuit. Several reasons can be proposed for this decrease of the oil temperature (heat losses, convective heat transfer, evaporation on walls). An evaporation mass flow-rate can be calculated from energy balance considering that this oil temperature decrease is completely due to droplet evaporation. In that case, the lowest evaporation mass flow-rate considering only the sump walls would be around  $4 \pm 0.5$  g/s (13% of the injected droplets), the highest one, considering the sump walls and the lower heated part of the vertical walls, would then be around  $15 \pm 0.5$  g/s.

Let us now consider the modeling approach. There are different ways to model the droplet-wall interaction in a 0D approach: convective heat transfer and latent heat transfer.

The convective heat transfer coefficient HTC has been estimated on TOSQAN tests performed without spraying (so-called ‘condensation tests’). The convective HTC depends on the geometrical configuration, which is the same in both types of tests, and on the flow regime (natural, mixed, forced convection, laminar or turbulent), which can be different in both tests. No experimental data can, at this stage, justify a factor 3 to 10 on this HTC, as used in some studies.

Concerning droplet evaporation on walls, a very simple model can be constructed if the wall heat losses are considered negligible, and if it is assumed that evaporation occurs only on walls; the following relation can be written at steady-state:

$$Q_{inj} (HL_{inj} - HL_{sat}) + \alpha Q_{inj} L = 0$$

where  $Q_{inj}$  stands for the spray mass flow rate;  $HL_{inj}$  the specific liquid enthalpy at the inlet spray temperature;  $HL_{sat}$  the saturated specific liquid enthalpy at gas temperature;  $L$  latent heat, and  $\alpha$  is the fraction of the injected spray that can evaporate. The highest value of  $(HL_{inj} - HL_{sat})$  is provided when the wall temperature is equal to the gas temperature. In that case, the fraction  $\alpha$  for test 101 is 14%. This value is the maximum value that can evaporate on walls, since a fraction of this value will evaporate directly on the droplets in the gas. A specific model should be added to distinguish between evaporation of droplets on walls and evaporation on droplets. However, for a global approach, considering the vessel as a single compartment, it does not seem necessary to make this distinction between both sources of evaporation.

As a conclusion, in order to take into account droplet evaporation in LP codes, the simplest way is to modify the inlet source.



### Local analysis

For a local analysis, using CFD or a multi-compartment approach, the global behaviour and the different sources of steam by evaporation can have an influence on the steam distribution. As a result, analysis of the energy balance and the mass sources seems to be of major importance. CFD calculations taking into account all phenomena should help for a better understanding of this test.

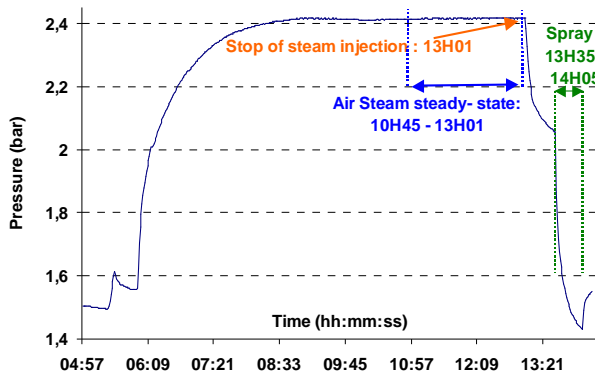
Furthermore, for the local analysis (specifically for CFD calculations) an important point could be also the way the spray injection is modelled. First calculations were made using the nozzle radius and some mean injection velocity. They have shown a spreading of the spray generally lower than the one obtained in the experiment. The reason for that was probably the injection modeling. In further studies, since the atomization process at the nozzle exit involved very complex phenomena, it is suggested to model the injected spray not as a point source, but as a droplet injection “line” (in 2D) situated at a height where experimental data are available (i.e. 70 mm from the top of the vessel rather): the experimental spray half-width (i.e. 27.1 mm) should be used instead of nozzle radius, the experimental droplet velocity profile (i.e. a flat profile of 10 m/s) instead of the mean velocity deduced from the nozzle size could be taken. Such calculations are underway.

## Thermalhydraulic part, MISTRA MASP tests

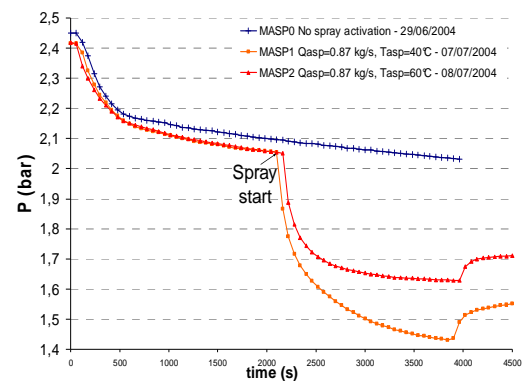
### Description of the test sequence

The spray tests MASP1 and MASP2 concern the depressurization of the containment atmosphere by spray. MASP0 is the reference case without spray (depressurization by heat losses over 3900 s).

Each MASP test starts during the steady-state of an air-steam test called M5 [14]. The M5 test consists of injection of superheated steam at 200°C in the MISTRA containment initially at room temperature and full of air. The two top condensers are kept at a temperature of 140°C (hot walls) and the bottom condensers at 80°C (cold wall where condensation occurs). The steady-state is reached when condensation rate is equal to steam injection rate (80 g/s). During the MASP tests, the condensers are kept at the same temperature as in the M5 test. After 3900 s, the gas is heated by convection with the hot walls. But this part is not as for calculation.



**Figure 8: Initial Conditions – M5 test followed by MASP1 test**



**Figure 9: Effect of spray activation and spray injection temperature on the vessel depressurization rate.**



The tests MASP1 and MASP2 are composed of two depressurization phases, the first one by heat losses, from 0 to 2100 s and the second one by spray activation during 1800 s, from 2100 to 3900 s. The droplet mass flow-rate is 0.87 kg/s and the water injection temperature is 40°C in MASP1 and 60°C in MASP2.

Results are presented on Figure 9 for the three MASP tests. In the MASP0 test, convection is driven by buoyancy: along the upper hot walls, the fluid is moving to the top, whereas along the cold bottom wall, the gas is moving down. In MASP1 and MASP2, when the spray is activated, the depressurization slope increases. The spray injection temperature has also an effect on the depressurization curve.

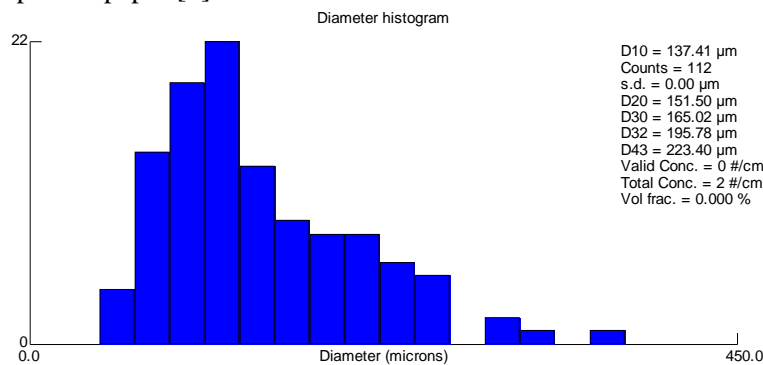
## Dynamic part, TOSQAN test 113

### *Description of the test sequence*

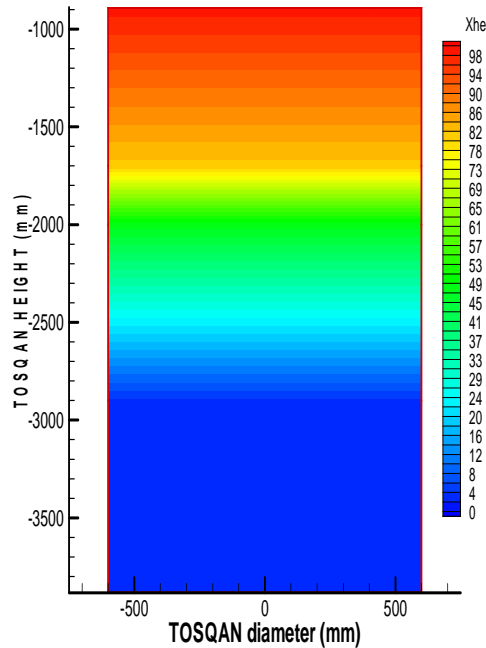
The night before test 113, compressed air is injected into the open TOSQAN vessel in order to remove helium and steam from former tests. On the morning of the spray test, the air injection is stopped. When a thermal steady-state is reached (ambient temperature), the vessel is closed (the vessel relative pressure is then 0 bar) and helium is injected at a given flow-rate (around 1 g/s). When the vessel relative pressure reaches 1 bar, helium injection is stopped. A delay of 400 s is applied before spray activation. During this time, mass spectrometry measurements are performed in order to characterize helium initial stratification and to check the repeatability of this stratification. Spray is activated (time reference  $t = 0$  s) during about 7000 s (steady-state for the mass and thermal stratifications) at 30°C and with an injection mass flow-rate of 30 g/s. Walls are insulated but not regulated.

### *Main experimental results*

Helium volume concentration measurements are performed using mass spectrometry at different levels in the vessel in order to determine the initial helium stratification before spray injection ( $t < 0$  s). The helium volume concentration field related to the initial helium stratification is presented on Figure 11. Spray droplet size distribution is presented on Figure 10. The mixing is observed after 300 s, with a mean helium volume fraction of 50% vol. Detailed results on 101 and 113 spray tests are presented in a companion paper [8].



**Figure 10: Spray droplet size distribution for TOSQAN 113 test**



**Figure 11: Helium volume fraction measured before spray activation**

## Dynamic part, MISTRA MARC2B

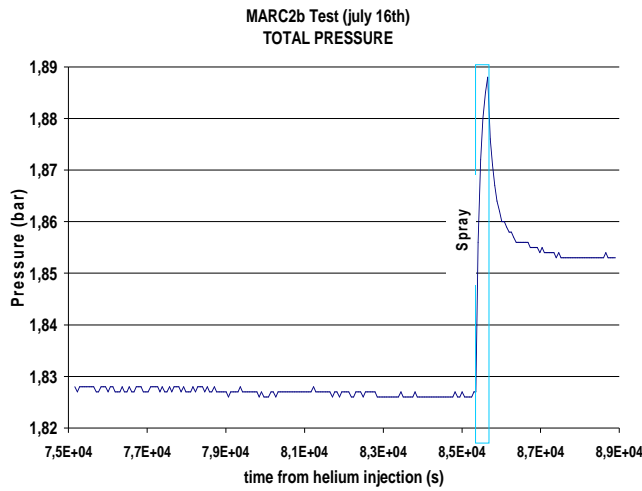
### *Description of the test sequence*

Spray is injected in a stratified mixture of helium, nitrogen and air, obtained at the end of test MARC2 [9]. This stratification is obtained by an injection of helium followed by a nitrogen injection inside the vessel initially full of air (24.3 °C, 1.01 bar). Note that this means that in the calculations, oxygen and nitrogen have to be modelled separately. The conditions before spraying are 1.828 bar for the total pressure, 24.6°C mean gas temperature, 115.6 kg of air, 6.5 kg of helium, and 46.2 kg of additional nitrogen.

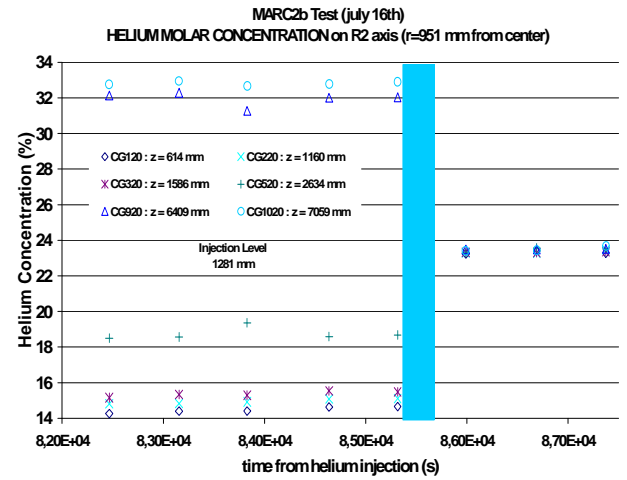
During the MARC2 test and for the initial condition of the MARC2B test, helium and nitrogen concentrations show an axial symmetry in the experiments.

The spray is injected during 300 s with a water mass flow rate of 0.90 kg/s, and a temperature of 40°C. The spray angle is of 30°, the estimated size of the droplet is around 1 mm and the injection velocity around 20 m/s.

The main results of this test are the very fast mixing and break-up of stratification during and after spray injection. The gas stratification is important before spraying: around 15%vol in the lower part and around 32 %vol in the higher part of the vessel. After spraying, a fast mixing is observed and the final average helium volume fraction is 23.4%.



**Figure 12: MARC2B Test: Effect of the spray – Spraying Conditions**



**Figure 13: MARC2b Test: Effect of the spray – Helium Molar Concentrations**

#### *Discussion on numerical aspects for the DYNAMICAL part*

The calculations of tests proposed for the DYNAMICAL part of the benchmark are underway until January 2007. These calculations, avoiding any heat and mass transfer between droplets and gas, will be used for the qualification of gas and droplet velocities models, but also for turbulence models under spraying conditions. Some of the codes participating to this benchmark have either a one-phase model, i.e. the droplet velocities are equal to the gas velocities (no relative velocities), or have a simplified turbulence model (such as a mixing length model). The results will show if a simplified CFD model, such as what is needed for reactor application, can well represent the dynamical aspects. This part is also open to LP codes that would like to improve their capabilities to calculate stratified and momentum dominated conditions.

## **Conclusion**

This paper presents four different spray tests in two facilities of different scales and under different thermohydraulic conditions. All tests are proposed for benchmarking in the frame of the SARNET European network. The TOSQAN tests have also been proposed for the CCVM matrix for the OECD members (Containment Code Validation Matrix).

Numerical calculations of TOSQAN test 101 have already been done and lead to some analysis presented in this paper. It is found that droplet-wall interaction can lead to a steam source that modifies the concentration levels in the gas mixture. This phenomenon is enhanced in the TOSQAN facility (continuously heated walls), and an open question remains: can this droplet-wall interaction be considered as negligible for other situations where walls are not heated continuously? The MISTRA MASP tests, presented in this paper, for which the bottom sump wall, where the spray droplet impact, are not heated continuously will help to answer to this question.

The two tests proposed for the spray dynamics evaluation presented in this paper will be used for CFD codes qualification of gas and droplet velocities models, but also for turbulence models under spraying conditions. This part is also open to LP codes that would like to improve their capabilities to calculate stratified and momentum dominated conditions.

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