

## SPRAY MODEL VALIDATION ON SINGLE DROPLET HEAT AND MASS TRANSFERS FOR CONTAINMENT APPLICATIONS – SARNET-2 BENCHMARK

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### Abstract

This work is performed in the frame of the SARNET-2 network, within the Sub-Work Package WP7-2, Task 1 (spray activities). Three different elementary test series have been proposed for benchmarking and the first serie, concerning heat and mass transfer on a single droplet, is presented here. Code-experiment and code-to-code comparisons are presented. It is shown that the mass transfer terms are responsible for most of the differences and, depending on the kind of test, that the errors can either compensate together or be enhanced. Since the errors are propagating over the droplet height fall, they could be not negligible for real containment cases.

### 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 steam injection, to enhance the gas mixing in case of the presence of hydrogen and to wash out airborne radioactive aerosols. Spray modellings are thus part of containment codes. The two major thermal-hydraulic phenomena involved in spray behaviour in such applications are the thermodynamical effect of a spray (steam condensation on droplets and evaporation) and the dynamical effect (entrainment and mixing). In the past, validation of spray modelling has been performed on large-scale facilities (CVTR, NUPEC, CSE) using several spray nozzles [1]. More specific studies have been proposed in the frame of SARNET [2-4-5-6] showing that the level of spray model validation was encouraging for the use of spray modelling for risk analysis, but not sufficient, and more investigations were needed. Three different separate-effect tests, so-called elementary tests, have been proposed in the frame of SARNET-2 network, within the Sub-Work Package WP7-2, Task 1 (spray activities): heat and mass transfers (HMT), momentum transfer on industrial spray, and aerosol collection on droplet. This paper presents the description of the 9 HMT tests and the different participating organizations and associated codes. The results, in terms of code-experiment and code-to-code comparisons for all HMT tests are then presented, and an analysis of the mass flux modelling is proposed.

## 1. Description of the benchmark

### 1.1 Description of the IRSN tests

The IRSN CARAIDAS experimental set-up [8] was used to study drop evolution under representative conditions of post-accident atmosphere. The cylindrical enclosure is of 5 m high and 0.6 m inner diameter. Homogeneous conditions are obtained with gas temperatures  $T_{\text{gas}}$  from 20 to 160°C, absolute pressures  $P$  from 1 to 8 bar and relative humidities  $HR$  from a 3 up to 95 %. The drop generator is located at the top of the vessel in order to keep it at a constant temperature whatever the vessel temperature is. It produces monosized water droplets from 200 to 700  $\mu\text{m}$  diameter. Drop injection temperature  $T_d$  is set between 20 and 80°C by an electric heater. Drop diameter  $D_d$  optical measurements are performed at 3 elevations: at the top (drop generator,  $z = 0$  m), at  $z = 2.51$  m and at the bottom ( $z = 4.39$  m). The tests conditions are given in Table 1: 'evaporation' and 'condensation' tests are called EVAP-i respectively COND-i tests. Benchmark specifications are given in [7]. More details of the experiments can be found in [8].

Table 1: Mean values for the gas characteristics and for the droplet initial conditions

Test	P [bar]	T <sub>gas</sub> [°C]	HR [%]	T <sub>d</sub> [°C]	D <sub>d</sub> [ $\mu\text{m}$ ]	U <sub>d</sub> [m/s]
EVAP3	1.00	20.1	20.5	20.6	611+/-4	3.58
EVAP13	5.42	100.1	15.0	31.0	605+/-4	3.75
EVAP18	1.00	135.2	3.0	30.9	309+/-5	3.66
EVAP21	4.29	97.4	12.0	29.2	311+/-7	3.63
EVAP24	4.97	135.0	4.0	30.3	296+/-4	3.10
COND1	4.00	141.3	55.0	36.0	341+/-2	4.90
COND2	4.80	141.6	71.0	37.0	344+/-2	4.70
COND7	5.30	139.3	87.0	35.0	593+/-11	2.10
COND10	2.40	121.5	79.0	16.0	673+/-5	2.10

### 1.2 Participants and codes

The participating institutions and codes are presented in Table 2. Ten institutions have participated with 15 contributions, 10 codes and 12 spray models (2 codes have 2 options for spray modelling). Several codes have participated to the blind and open phases. ANSYS codes were used with specific sub-routines developed by the participants. ERSE company was changed to RSE on July 21, 2010.

Table 2: Participants for the blind and open calculations

Institution	Code name	Institution	Code name
KIT	KIT specific spray model	GRS	COCOSYS v.2.4 IVO
EDF	NEPTUNE_CFD v. 1.0.7	GRS	COCOSYS v.2.4 MARCH
ERSE (RSE)	ECART - standard model 4W	UJV	MELCOR v. 1.8.6 YV
	ECART -"ad hoc" model 4W*	UJD	COCOSYS v. 2.3v24
NRG	ANSYS FLUENT v. 6.4.11	UJD	ASTEC v. 2.0
NRG	SPECTRA	LEI	COCOSYS v. 2.3
IRSN	ANSYS CFX v. 12	UNIPI	FUMO
IRSN	ASTEC CPA v. 1.3 rev3		<b>10 institutions, 10 codes, 15 contributions</b>

## 2. Discussion on the results

During the tests the droplet diameter evolution was measured at two different heights. They are the basis for the following code-experiment comparison. Information on droplet velocity or droplet temperature are not available and, thus, both are subject of the code-to-code-comparison only.

### 2.1 Code-experiment comparison

The code-experiment comparison of the open exercise is presented on Figure 1 for the lowest location ( $Z = 4.39$  m). The main discrepancies are obtained for tests EVAP18, EVAP21 and EVAP24.

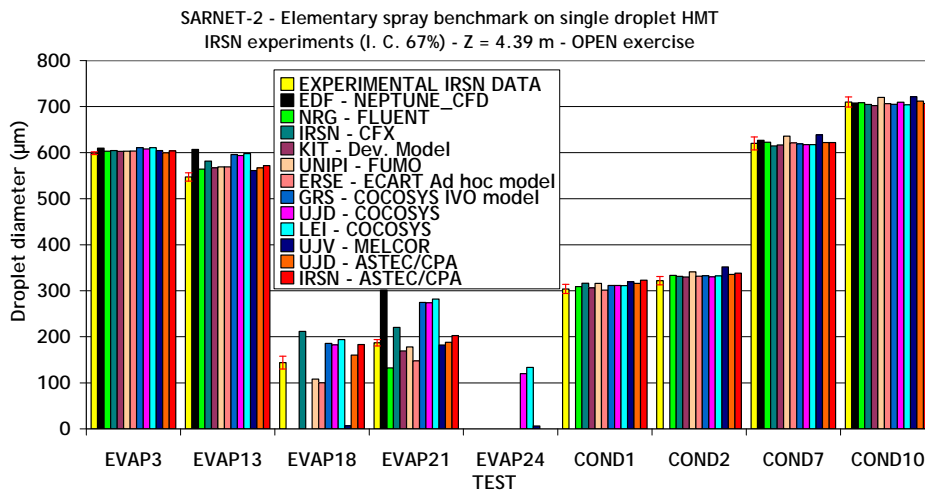


Figure 1: Droplet diameter - OPEN phase,  $Z = 4.39$  m (I. C.: interval of confidence)

In order to give a numerical value of these differences, relative differences between code and experiments are calculated (Figure 2 at  $Z = 2.51$  m and Figure 3 at  $Z = 4.39$  m). Most of the final numerical results are within a range of  $\pm 10\%$  of the measured droplet diameter, except for the three tests mentioned above.

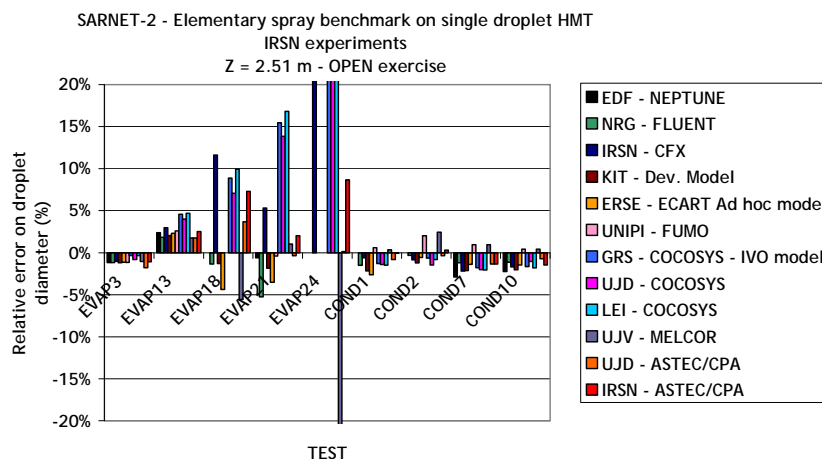


Figure 2: Relative difference between calculations and experiments - OPEN phase,  $Z = 2.51$  m

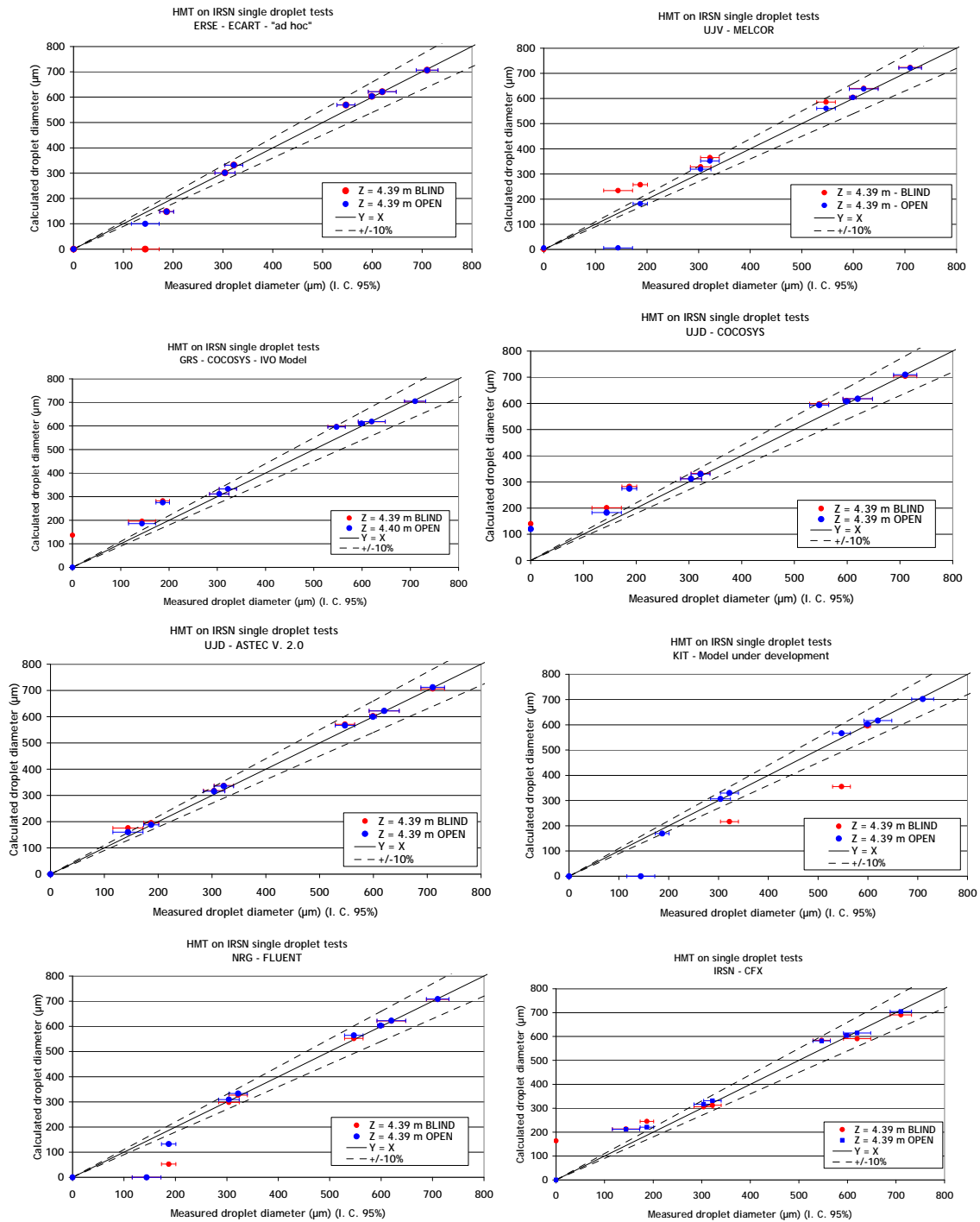


Figure 3: Code-experiment comparison (droplet size), blind and open contributions-  $Z = 4.39$  m

Differences between the open and the blind exercise are of two kinds. Large differences are obtained for three codes (KIT-model, FLUENT and CFX), for which it can be considered that the models were under development during the blind exercise (bugs or errors in the input data found after the delivery of the experimental results). Small differences for the other codes that have calculated both phases; the open phase calculations lead to more accurate results of the droplet diameter for the concerned tests, but do not allow, however, to reach a below-10% range of error (Figure 2).

Differences in the results between participants using the same codes (5 COCOSYS contributions, and 3 ASTEC/CPA contributions) are very low (not presented here) indicating a low user-effect influence for these calculations by these LP codes.

At last, CFD or Lumped-Parameter codes lead to the same kind of results, and no advantage can be drawn for one or for the other type of codes; it is worth emphasizing that CFD codes are not designed for such single droplet calculations, but that the users have managed to adapt their CFD models in such a way that the basic single droplet thermal-hydraulic behaviour of CFD codes is also tested.

As a conclusion of this code-experiment comparison, the main point that has to be considered is the differences obtained for three evaporation tests EVAP18, EVAP21 and EVAP24. Considering the tests conditions (Table 1), it cannot be seen any straight forward correlation. These tests are rather dry tests under evaporation conditions, but test EVAP13 is also such a test and its calculations do not exhibit such differences with the experiments. These three tests are also tests with lower initial droplet sizes, but other tests (COND1 and COND2) are also performed for such droplet sizes and lead to more accurate results. Droplet initial velocity is not a relevant parameter either, since these three tests are performed at intermediate values of the droplet initial velocities. The analysis of the code-to-code comparison will allow us in the next section to clarify the possible reasons of these discrepancies.

## 2.2 Code-to-code comparison

### 2.2.1 Droplet temperature

Results for droplet temperature evolutions are presented on Figure 4 for typical tests.

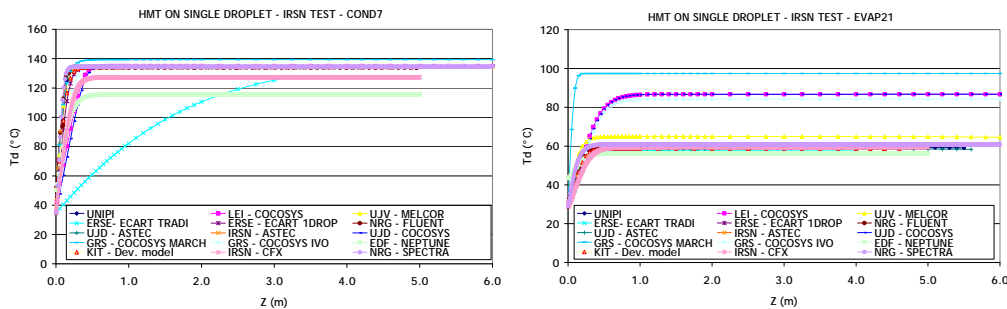


Figure 4: Droplet temperature vertical evolution for a typical condensation test (left, COND7) and for a typical evaporation test (right, EVAP21), OPEN phase, final contribution of each participant

The distance at which the droplet equilibrium temperature is reached is rather similar for all codes (generally lower than 1 m from the injection point). Concerning the equilibrium temperatures reached, they are rather similar for all codes (Figure 5). The analysis of the relative difference between the equilibrium temperature obtained by the participants and the mean value of this temperature calculated from the results of all participants is generally lower than 10%, except for COCOSYS (IVO model) and MELCOR calculations. The COCOSYS (MARCH model) and the ECART ‘traditional model’ appear to calculate even a higher final droplet temperature (not presented here).

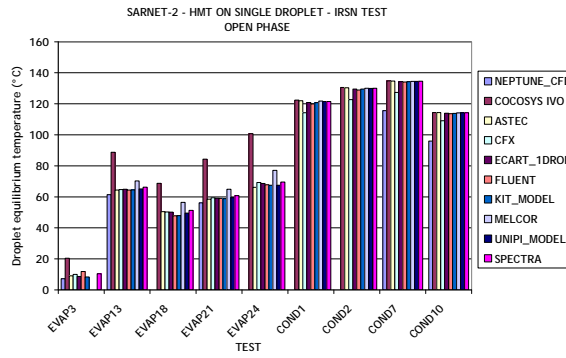


Figure 5: Droplet equilibrium temperature for the OPEN phase

### 2.2.2 Droplet size

The vertical evolution of the droplet size is presented here for typical tests on Figure 6. What is seen in test EVAP21, which is also enhanced in EVAP24 (Figure 7), is that when the rate of decrease of the droplet size due to evaporation increases, the differences between the calculations become higher.

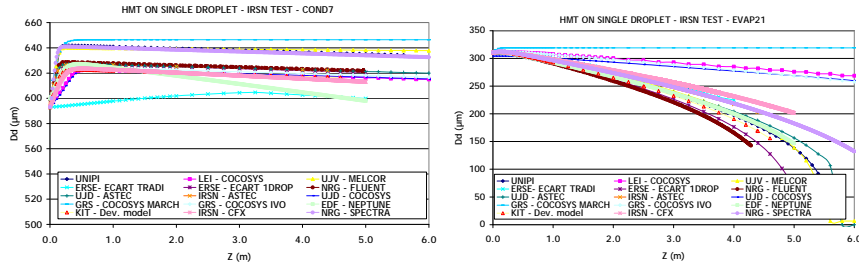


Figure 6: Droplet size evolution on the vertical axis for a typical condensation test (COND7) and a typical evaporation test (EVAP21) - final contribution of each participant

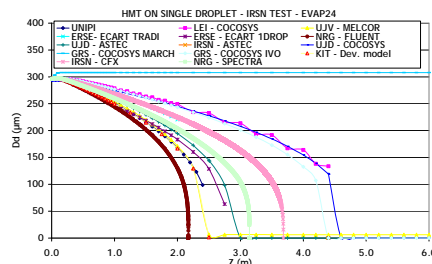


Figure 7: Droplet size evolution on the vertical axis for an evaporation test for which the droplet completely evaporates (EVAP24) - final contribution of each participant

### 2.2.3 Droplet velocity

Typical results for the droplet velocities vertical evolutions are presented on Figure 8, for COND10, the only test where the droplet velocity is accelerated and EVAP13 test, a typical test where the dynamical equilibrium is reached.

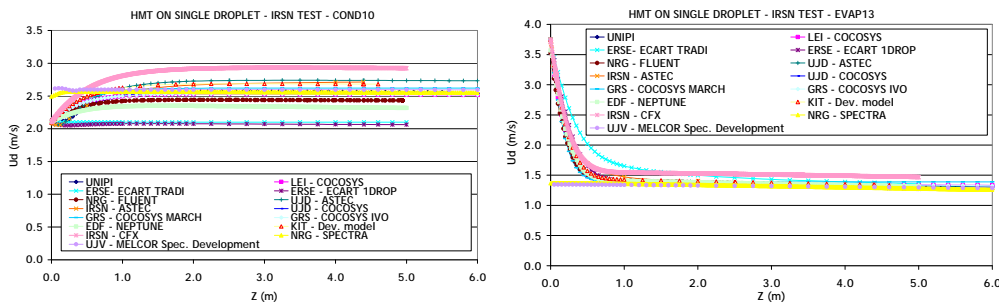


Figure 8: Droplet velocity evolution on the vertical axis for test COND10 and test EVAP13 - final contribution of each participant

The theoretical droplet settling velocity (drag and gravity forces) for each test is post-calculated using the droplet diameter obtained by each calculation at the  $Z = 4.39$  m position. The obtained value is then compared to the velocity given by the participant at the same location (Figure 9). It can be seen that the relative differences between those two values are generally lower than  $\pm 10\%$ , except for MELCOR and ECART '1 DROP'. Results for test EVAP18 show also higher values of this relative difference, but the droplet diameter changes very quickly in this test, impacting the droplet velocity.

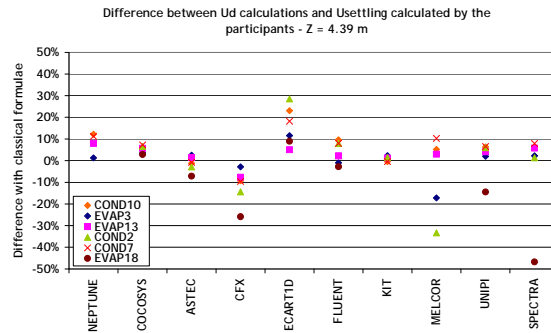


Figure 9: Relative differences between the theoretical settling velocities calculated using the droplet diameter of each calculation, and the velocities calculated by the codes (final contributions)

### 3. Analysis of the modelling

Modelling of these elementary tests requires different droplet sub-models, coupled together: energy (droplet temperature), mass (mainly droplet size) and dynamical modelling (droplet velocity). From the code-experiment as well as the code-to-code comparison, it has been shown that the droplet equilibrium temperature, as well as the droplet settling velocities (for the codes where the dynamical equilibrium is almost reached), are generally similar for most of the codes. It is thus concluded that the differences observed in tests EVAP 18, EVAP21 and EVAP24 are thus obtained because the droplet sizes calculated by all are different probably because of different mass exchanges modelling.

The suspected reason for the differences between codes concerns the expressions of the mass transfer. These expressions can be described, in a very simplified way, as a function of the droplet size  $D_d$ , the Sherwood number  $Sh_d$ , the mixture diffusion coefficient  $D_m$ , and a so-called here "density term" between mixture and droplet  $\Gamma_{d-b}$ , calculated on the basis of the so-called reference temperature  $T_{ref}$ :

$$Q_s^{mass} = \left[ \pi D_d^2 \right] \left[ \frac{D_m(T_{ref}) Sh_d}{D_d} \right] \Gamma_{d-b} \quad (1)$$

where the Sherwood number is given by a function of the Reynolds  $Re_d$  and the Schmidt  $Sc$  numbers:

$$Sh_d = A + B [Re_d(T_{ref})]^n [Sc(T_{ref})]^m \quad (2)$$

where A, B, n, and m are different constants.

These terms will be analysed on the basis of the modelling options given by few participants that have provided very detailed information on their model.

### 3.1 Coefficients of the Sherwood correlation

Several different constants A, B, n and m can be found in the literature for Sherwood correlation and are considered here as an example (see SARNET-1, Spray model report [4]): one with A = 2 and B = 0.56 (ASTEC, COCOSYS IVO, FUMO and GASFLOW), one with A = 2 and B = 0.6 (NEPTUNE), one with A = 2 and B = 0.5 (MELCOR). The constants n and m are generally: n = 1/2, m = 1/3. The relative differences between those relations are between 5 to 10% (not presented here).

### 3.2 Gas mixture diffusion coefficient

Different expressions of the diffusion coefficient can be found in the literature for a given reference temperature  $T_{ref}$  and the total pressure P. Two of them only will be considered here, just as an example: the Wilke and Lee relations (1955) and the Fuller expression (1969) described in [9]. The relative differences between the expression of Fuller and the one of Wilke and Lee are presented on Figure 10 for all calculated tests. It can be seen on this figure (left side) that these differences are around 30%. The differences in the mass flow-rate on a droplet due to the use of these two expressions are a bit higher, since the mass flow-rate on a droplet is proportional to the diffusion coefficient with a power to 1.33 (considering that the diffusion coefficient used in the Schmidt number is also used in the Sherwood number, at a power 1/3 generally). The differences in the mass flow-rate are presented on Figure 10 (right side) where it can be seen that these differences are about 40%. Such an error is constant over the whole droplet fall.

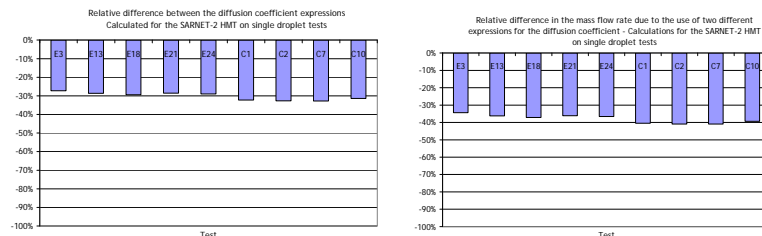


Figure 10: Relative differences between the expressions of Fuller and the one of Wilke and Lee – Left side: differences in the diffusion coefficient – right side: differences in the mass flow-rate

Two participants (GRS/COCOSYS and UNIPI/FUMO) have provided their computed diffusion coefficients. The relative differences between each of these results and any other are presented on Figure 11 where the legend should be understood as follows: legend COCOYS/FULLER\_TBULK means that it concerns the difference between COCOSYS calculation and Fuller calculations at the bulk temperature. It can be seen that this coefficient can vary significantly (above 40% for the condensation tests). This point is very important and remains one critical point in the mass flow-rate expressions.



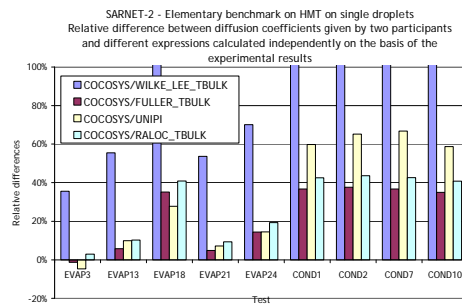


Figure 11: Relative differences on the diffusion coefficients between COCOSYS IVO model with other expressions/calculations

### 3.3 Reference temperature

A reference temperature is used for different variables: the mean kinematic viscosity of the gas mixture in the expressions of the Schmidt number, the Reynolds number and the diffusion coefficient. It should be emphasized that the kinematic viscosity can be calculated based on different reference temperatures depending if it is used in the droplet Reynolds number or the Schmidt number.

The reference temperature used in the different codes of this benchmark can be the droplet temperature  $T_d$ , the bulk temperature  $T_{bulk}$ , the mean value  $T_{film1}$  between drop and bulk temperature, or the so-called 1/3 law temperature  $T_{film2}$ , i.e. a value pondered by 1/3 of the bulk temperature and 2/3 of the droplet temperature. The influences on the droplet mass flux due to the choice of the reference temperature used in kinematic viscosity in the Reynolds number, in the Schmidt number and in the diffusion coefficient (relation of Wilke and Lee [9]) are presented on Figure 12 (the droplet characteristics used here are the ones obtained by ASTEC/CPA).

The maximum differences that can be obtained by the choice of the reference temperature are between 5 and 150% at the droplet injection location (left figures, maximum error). As soon as the droplet thermal equilibrium is reached (right figures), the error is lower than 25%. The influence of the reference temperature is higher in the diffusion coefficient expression than in the viscosity used in the Reynolds and Schmidt numbers. This result is due to the fact that the diffusion coefficient depends on a power of 3/2 on the reference temperature, and is then also on a power of (1+1/3) in the mass flux expression (the 1/3 comes from the integration of the diffusion coefficient in the Schmidt number). Using the Fuller expression for the diffusion coefficient should lead to higher differences, since the diffusion coefficient is then a function of a power 1.75 of the reference temperature.

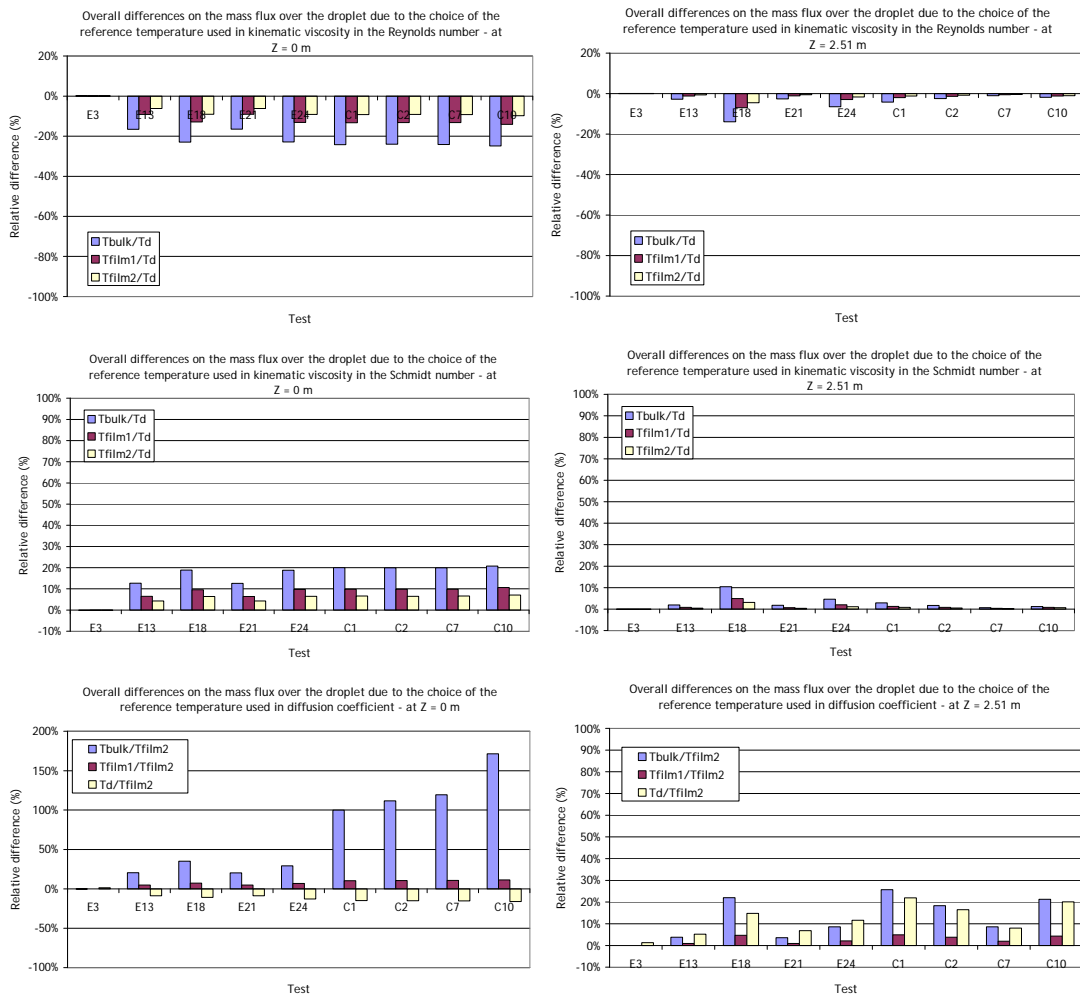


Figure 12: Influence on the mass flux due to the choice of the reference temperature used in mixture kinematic viscosity in the Reynolds number (first row), in the Schmidt number (second row) and in the diffusion coefficient (third row): left side at Z = 0 m; right side at Z = 2.51 m

### 3.4 ‘Density term’

The expressions of the so-called here ‘density term’ between mixture and droplet  $\Gamma_{d-b}$  can be different, depending on the way the Fick diffusion flux and Stefan flux is written and the assumptions that are made in the boundary layer close to the droplet. The reader will refer to [3] to get the expressions used in the different codes analysed here. The comparison is performed using the relative difference between the “density term” obtained with ASTEC/CPA and the “density term” obtained with the other codes. Results are plotted on Figure 13 (left side at Z = 0 m, and right side at Z = 2.51 m). It can be seen in Figure 13 that the differences are between 10 to 100% depending on the tests.

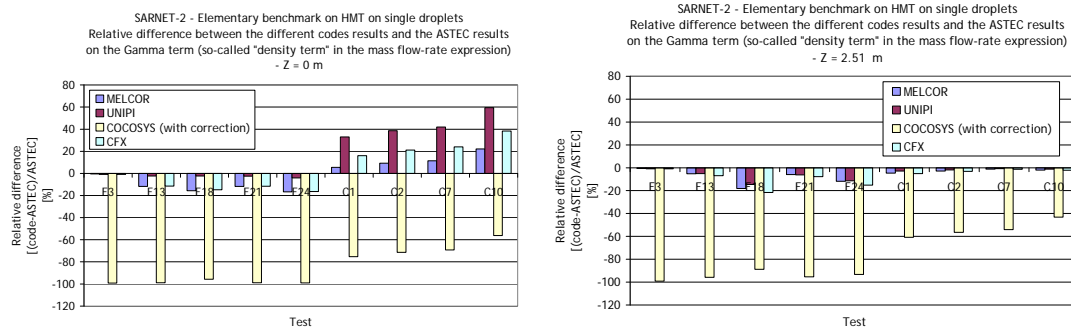


Figure 13: Relative difference between the ‘density terms’ post-calculated from ASTEC relations and the one post-calculated using the expressions given by the participants (left: Z=0 m, right: Z=2.51 m)

### 3.5 Droplet residence time and mass exchanges relative to droplet mass

From all these analysis, it can be understood that the differences in the overall mass flux term will be higher as soon as the droplet residence time is higher, and also as soon as the mass flow-rate due to evaporation/condensation is high compared to the mass of the droplet (and this can vary over the height). To illustrate this point, the average residence time at Z = 2.51 m (average value obtained on the residence time calculated from the following contributions: MELCOR, UNIPI, COCOSYS and ASTEC/CPA) obtained for all tests has been calculated and presented on Table 3. It can be seen that the test presenting the highest discrepancies between participants, Test EVAP24, is a test with a high residence time. It is less obvious to show evidence of the influence of the ratio between the mass flow-rate due to evaporation/condensation and the mass of the droplet, since this ratio depends on the height, and becomes very high as soon as the droplet size is reduced due to evaporation. As an example, the ratio between the mass flux given by ASTEC and the droplet mass at the injection location is given in the last column of Table 3 and is found to be also important for EVAP 24.

Table 3: Average residence time of the droplet and associated standard deviation at Z = 2.51 m ;  
 ASTEC mass flux at Z = 0 divided by the initial droplet mass  $m_d$

Test	Mean residence time (s) at Z = 2.51 m	Associated standard deviation (s)	$Q_s^{mass} / m_d (Z = 0)$
EVAP3	0.914	0.05	0.058
EVAP13	1.716	0.069	0.605
EVAP18	2.116	0.035	2.722
EVAP21	3.036	0.361	1.991
EVAP24	4.813	0.712	4.07
COND1	2.09	0.259	0.942
COND2	2.166	0.24	0.717
COND7	1.485	0.044	0.112
COND10	0.99	0.031	0.115

## 4. Conclusion

This work presents the results of the code-experiment comparison on HMT tests on single water droplets. The tests consist of single droplet vertical injection into a vessel pressurized with

homogeneous air-steam mixtures. The drop diameter is modified by steam condensation or evaporation depending on the gas and droplet thermodynamical conditions. Ten institutions have participated with 15 different contributions, 10 different codes and 12 spray models, as a blind and an open exercise. From code-experiment and code-to-code comparisons, it is shown that the droplet equilibrium temperatures as well as the droplet velocities are generally similar for most of the calculations, indicating a convergence in the thermal and dynamical modelling of all codes. However, even if code-experiment comparison show differences within a range of +/-10% of the calculated droplet diameter, larger differences are obtained for 3 of the 9 tests, even in the open exercise. It is concluded that these differences are due to different mass flux expressions and an analysis of this modelling is performed. Most of the codes have a similar approach to describe the droplet mass flux, but there are many choices that are made on many different parameters: diffusion coefficient expressions in a gaseous binary mixture, reference temperatures taken for the viscosity in the Reynolds and Schmidt numbers as well as in the diffusion coefficient, relations for the Sherwood number, and the so-called 'density term'. Each of them can lead to larger or smaller differences in the results, that can be enhanced as soon as the droplet and gas temperature are very different (in the injection region especially). The most influent parameters are the diffusion coefficient, the reference temperature used in the diffusion coefficient expression and the so called 'density term'. Making some lucky choices can lead to error compensation, but unlucky ones can lead to non negligible effects on the mass flow-rate over the droplet. At last, since the error is propagating over the droplet height fall, this can lead to subsequent differences, as in test EVAP24, where the droplet residence time is high and the evaporation/condensation mass flow-rate is also high compared to the droplet mass. Since the fall height in a real containment is over 30 m, these considerations could be not negligible.

## 5. References

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