

## Numerical modelling of liquid jets atomisation due to leakage of liquefied gas storage

Cedric LEMOFACK<sup>a,b,\*</sup>, J.M. LACOME<sup>b</sup>, J. REVEILLON<sup>a</sup>, F.X. DEMOULIN<sup>a</sup>

<sup>a</sup> CNRS, UMR6614-CORIA, Technopole du Madrillet, BP 12, Avenue de l'Universite, 76801 Saint-Etienne-du-Rouvray Cedex, France

<sup>b</sup> INERIS, Parc Technologique ALATA, B.P. N°2, 60550 Verneuil-en-Halatte, France  
lemofacc@coria.fr, demoulin@coria.fr, Jean-Marc.LACOME@ineris.fr,  
Julien.Reveillon@coria.fr

### Abstract

The objective of this work is to develop a numerical model with the aim of simulating a two phase jet resulting from a breach or leakage in a vessel or pipe containing liquefied gas. The work focuses especially on the effect of the vaporization and boiling process in the jet. To represent the flash boiling phenomena that occurs at the exit of the injector up to the end of expansion zone of the jet, the Homogeneous Equilibrium Model (HEM) have been used. Consequently, at the end of this expansion zone, gas and liquid velocities are identical and the spray is supposed to be at boiling temperature with a gas environment composed only by vapour. The velocity is considered to be driven mainly by the pressure drop, thus it is determined by the Bernoulli law at the end of expansion zone. After this zone, thanks to the thermal condition, any increase of temperature will promotes boiling. But if some air diffuses inside the spray, a non-classical vaporization process is expected. A thermodynamic equilibrium model for vaporization was thus developed. To test the model, an atmospheric two-phase jet of butane, emanating from a circular orifice is considered. The modelling results show that the calculated temperature behaviour in the spray jet by comparison with the observations is generally satisfactory. This result cannot be obtained with classical vaporization model.

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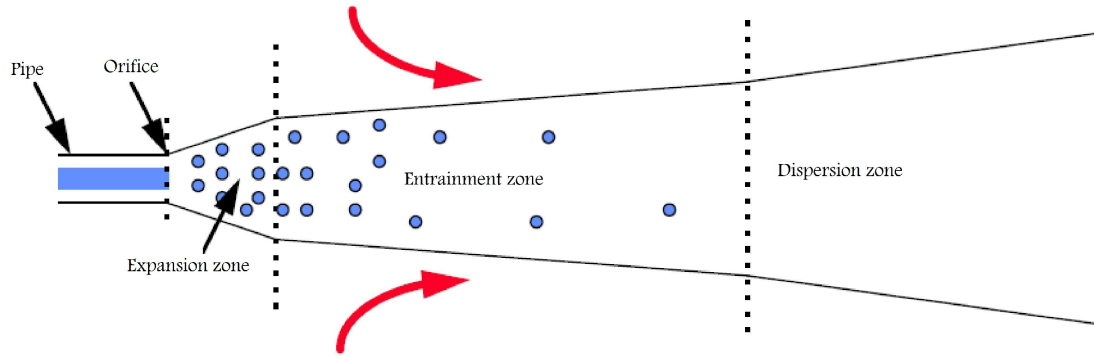
### Introduction

Experiments were carried out by INERIS with the aim to study the two-phase releases of hazardous chemicals into the atmosphere. These experiments involve to measure the main characteristics of the jet and to increase the understanding of the behaviour of sub-cooled (non-flashing) and superheated (flashing) liquid jets. It is now necessary to develop a numeric model which will include all those phenomena and will help the prediction of jet expansion. The objective of this work is to develop a numerical model with the aim of simulating a two phase flow resulting from a breach or leakage in a vessel containing liquefied gas. Basic principles of this kind of injection are summarized in Figure 1, the jet consists in 3 areas:

- The expansion zone (flash boiling, atomization): here, the fluid expand from the vessel hole pressure to the atmospheric pressure. At the end of this zone, we assume that the jet consist only in gas phase and liquid phase. Both of them are at the boiling temperature. During the expansion, jet atomization occurs and the liquid jet ends here in droplets.
- The entrainment zone (secondary break-up, droplets evaporation): the turbulent jet drives the ambient air. The energy brings by the air, of which the temperature is greater than that of the jet, is used for droplet vaporization in the two-phase jet.
- The final dispersion zone: the entrainment by the air atmosphere heats the jet and decreases its velocity up to the wind speed.

The first step of the work includes models used to describe the jet up to the end of expansion zone. These will be used as boundary conditions for the simulation of the jet from de beginning of the entrainment zone. In the second step, precisions are given on the new phenomena brought by the flashing liquid jet and the models suggested for it. Finally, results are given and discussed to see how to continue the work.

\*Corresponding author: lemofacc@coria.fr



**Figure 1.** Schematic representation of the areas of the flashing jet

### Materials and methods

To represent the flash boiling phenomenon that occurs at the exit of the injector up to the end of expansion zone, the isenthalpic Homogeneous Equilibrium Model (HEM) has been used. The model is used to determine the vapour mass fraction at the end of the zone.

The model supposes that the gas and liquid have the same velocity and the same saturation temperature due to the thermodynamic equilibrium assumption between the two phases. The mixture of the phases is homogeneous. These assumptions imply that:

- The two-phase flow is considered as a homogeneous fluid with properties at the middle of those of liquid and gas phase.
- The flow quickly tends to a thermodynamic equilibrium (no energy exchange between the liquid-gas system and the outside). So it is supposed to have this thermodynamic equilibrium during the expansion.
- Isenthalpic expansion: the enthalpy of the flow is constant (equation (1)) while its entropy decreases.

There is another HEM model with Isentropic expansion, the entropy of the flow is constant while its enthalpy decrease. This causes the fall in temperature of the system. Van den Akker [1] showed that both of the assumptions are unrealistic but fewer errors are involved with the isenthalpic expansion.

In the case of this work, the HEM model presents the advantage of vapour/liquid mass fraction estimation. This will help to determine the mass flow of each phase from the total mass flow given by the experimental data.

#### ***Isenthalpic HEM Model:***

It is considered  $h$  the enthalpy of the system,  $X$  the vapour mass fraction of gas in the jet,  $C$  the specific heat and  $T$  the temperature.

The subscripts  $i$  and  $exp$  mean the value at the interior of vessel and at the end on expansion zone.  $g$ , and  $l$  are the values in the gas and liquid phase of the jet.

$$h(T_{exp}) = (1 - X) h_l(T_{exp}) + X h_g(T_{exp}) = Cte \quad (1)$$

$$\int dh(T) = \int C_{pl} dT \quad (2)$$

From the equation (1) describing the enthalpy conservation, we introduce (2) After a derivation by  $X$ :

$$h_l(T_i) - h_g(T_i) = - \int_{T_i}^{T_{exp}} C_{pl} dT + \int_{T_i}^{T_{exp}} C_{pg} dT + \left( (1 - X) + X \frac{C_{pg}}{C_{pl}} \right) C_{pl} \frac{dT}{dX} \quad (3)$$

By supposing  $X \ll 1$  and  $C_{pg} < C_{pl}$ , we have:

$$\left( h_g(T_i) + \int_{T_i}^{T_{exp}} C_{pg} dT \right) - \left( h_l(T_i) + \int_{T_i}^{T_{exp}} C_{pl} dT \right) = -(1 - X) C_{pl} \frac{dT}{dX} \quad (4)$$

The term  $-(1 - X) C_{pl} \frac{dT}{dX}$  in (4) is equal to latent heat vaporization ( $Lv$ ) term at the right side of equation. So:

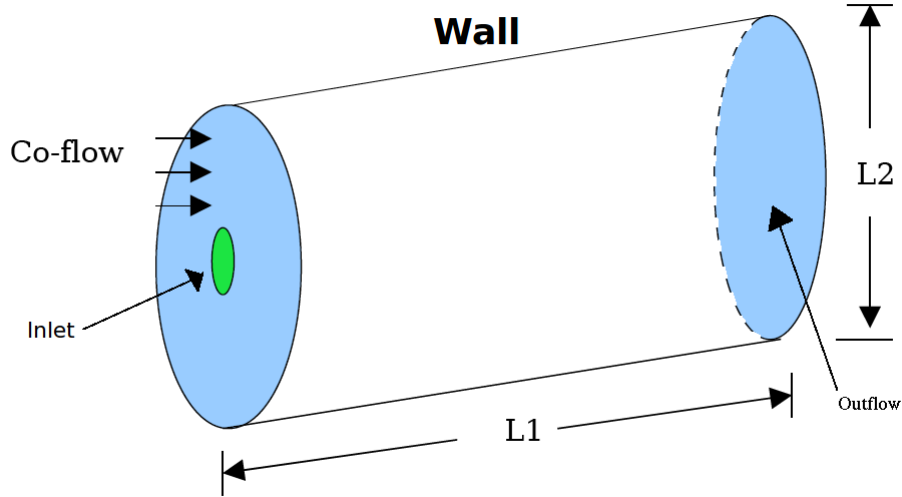
$$Lv(T_{exp})dX = -(1 - X)C_{pl}dT \quad (5)$$

The heat exchange due to vaporization is supposed greater than the heat due to warming:  $C_{pl}\Delta T \ll Lv$ . By taking account of this assumption after the integration of (5), we finally have:

$$X_{exp} \simeq C_{pl} \frac{(T_i - T_{exp})}{Lv} \quad (6)$$

At the end of expansion zone, the jet is in atmospheric pressure. So the liquid, which is in thermodynamic equilibrium with its vapour, is at its boiling temperature  $T_{exp} = T_{eb}$ .

Another issue of this work is the determination of the velocity induced by the pressure drop inside the injector and by the flash effect. The maximum kinetic energy can be estimated by the pressure drop and the variation of thermodynamic energy in the flow. Here, the velocity is considered to be driven mainly by the pressure drop, thus it is determined by the Bernoulli law. Additional velocity could be considered due to the flow expansion (liquid to gas) however there is also a reduction of velocity due to pressure loss.



**Figure 2.** Computation area

All the above work is useful to estimate values in the jet at the end of expansion zone. The simulations start at this point, since the CFD model used is the two-phase Euler-Lagrange description model. The experimental case in this paper come from the data base of the FLIE (Flashing Liquids in Industrial Environment) project [2]. The numerical software used for this study is numerical package FIRE V8.41 from AVL.

The chosen case is those of a vessel of liquid butane at  $7.78 \text{ MPa}$ . The liquid is released through a pipe and reaches the ambient air in a two-phase jet. This jet emanates from a circular orifice of  $10 \text{ mm}$  in diameter. The mass flow rate conservation between the orifice and the end of expansion zone give the diameter of this end zone :

Variable	Inlet	Coflow	Wall	Outflow
Material	butane (liquid & gas)	air (gas)	-	-
Velocity (m/s)	29.49	1	-	-
Temperature (K)	272.6	300.15	-	-
Mass flow rate (kg/s)	1.33	-	-	-
Vapour mass fraction	0.0638	-	-	-
Droplet size ( $\mu\text{m}$ )	100	-	-	-
Turbulence intensity	10	1	-	-
Lenght scale	0.005	0.1	-	-

**Table 1.** Boundary layer conditions

$D = 60.45 \text{ mm}$ . The numerical domain in which the butane is spreading is presented in Figure 2. It consists in a cylinder of  $36 \text{ m}$  in length and  $6 \text{ m}$  in diameter. To simulate a rejection of liquefied gas with wind effect, a co-flow of air surrounds the spray injection. The mass fraction of each phase is given by the HEM model. The entry values and the boundary conditions are recapitulated in Table 1. Finally, the turbulence is modelled with the  $k - \epsilon$  model and the applied gravity is  $9.8 \text{ m/s}^2$ .

**Abramzon vaporization model:**

Vaporization is based on Abramzon vaporization model [3]. By considering  $\rho$  and  $D$  the density, and the binary diffusion coefficient in the gas around the droplet,  $k$  and  $a$ , the droplet diameter and thermal conductivity,  $Sh$  and  $Nu$  the Sherwood and Nusselt number, the mass transfer rate  $\dot{m}$  is given by (7) and (8):

$$\dot{m} = \pi \rho D a Sh \ln(B_M + 1) \quad (7)$$

$$\dot{m} = \pi \frac{a k}{C_{pg}} Nu \ln(B_T + 1) \quad (8)$$

$B_M$  and  $B_T$  are the mass Spalding number (equation (9)) and the thermal Spalding number (equation (10)). They are supposed to be the same. One part of the energy available in the gas phase goes for the evaporation of liquid phase. The other part goes for heating the droplet. This is described in equation (11) below.

$$B_M = \frac{Y_{F,s} - Y_{F,\infty}}{1 - Y_{F,s}} \quad (9)$$

$$B_T = \frac{\rho_s v_s C_{pg}}{h_c} \quad (10)$$

$$h_c(T_\infty - T_s) = \rho_s v_s L v + \frac{Q_l}{\pi a^2} \quad (11)$$

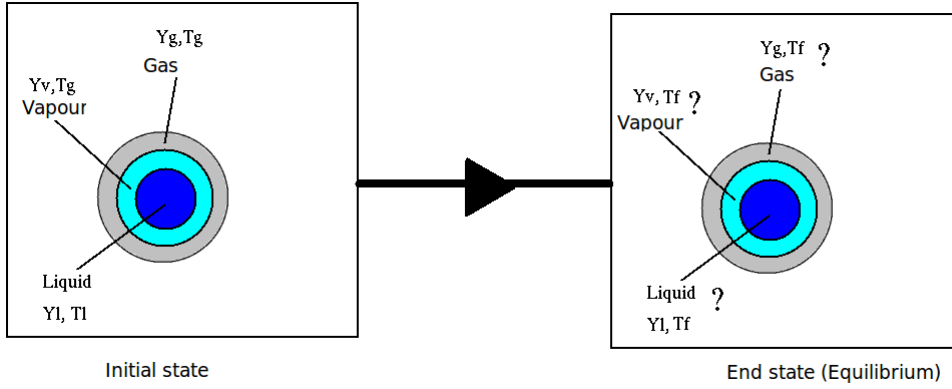
In the three equations above ((9), (10), (11)),  $Y_F$  is the vapour mass fraction of droplet material in the gas phase,  $v$  is the velocity in the gas phase and  $h_c$  is the droplet convection coefficient. The subscripts  $s$  and  $\infty$  mean

the values at the droplet surface and far from droplet. The introduction of the thermal Spalding number in (11) combined with equation (8) give the heat quantity necessary for droplet heating  $Q_l$ .

$$Q_l = \pi a k \left( \frac{h_c a}{k} (T_\infty - T_s) - \frac{Lv}{C_{pg}} Nu \ln(B_T + 1) \right) \quad (12)$$

However thermodynamic conditions at the end of the expansion zone are very particular in the case of flashing jets. Thermodynamic equilibrium assumption imposes that the liquid and gas temperature are the same and equal to the boiling temperature. Additionally, near the inlet boundary conditions of the jet droplet, environment is composed of pure vapour  $Y_{F,\infty} \simeq Y_{F,s} \simeq 1$ . Thus, this is a limit case between boiling and vaporization. As seen in equation (9), with these conditions,  $B_M$  is uncertain. However, the security brought by putting the maximum value of the both vapour mass fraction at 0.99 is not sufficient. Thus, some simulation cases have shown that the classic Abramzon vaporization model is not suitable for post flashing two-phase jet. So there is a necessity to develop another model for vaporization.

### Thermodynamic Equilibrium Model (TEM):



**Figure 3.** Initial and final state in the thermodynamic system

We propose a special procedure to solve this problem. It is considered a thermodynamic system 3 at its initial state with certain liquid mass fraction  $y_l$  and vapour mass fraction  $y_v$  in the presence of other gas like air  $y_g$ . The liquid temperature  $T_l$  differs from vapour temperature  $T_g$ . Like in HEM model, we consider thermodynamic equilibrium model at the final state. The physics assumptions here are:

- Ideal gas.
- Mass conservation (13).
- Isolated system with constant pressure transformation: enthalpy conservation (14).

$$\sum_k y_k^{initial} = \sum_k y_k^{final} = 1 \quad (13)$$

$$H_t = \sum_k H_k(T_k^{initial}) y_k^{initial} = \sum_k H_k(T_k^{final}) y_k^{final} = Cte \quad (14)$$

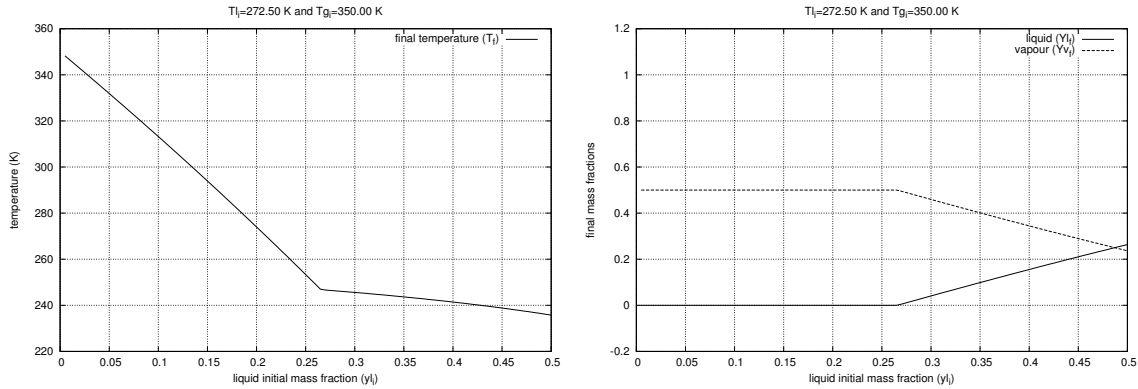
$$f(T^{final}) = H^{initial}(T_l^{initial}, T_g^{initial}) - H^{final}(T^{final}) \quad (15)$$

The first step of this method is to find the enthalpy at the initial state with de quantities  $y$  and  $T$  in (14). Knowing that the enthalpy is constant, the second step consists in finding the new values of these quantities by applying a

method for finding the zero of the function  $f(T^{final})$  (15). At the final state, thermodynamic equilibrium implies that the liquid and gas are at the same temperature.

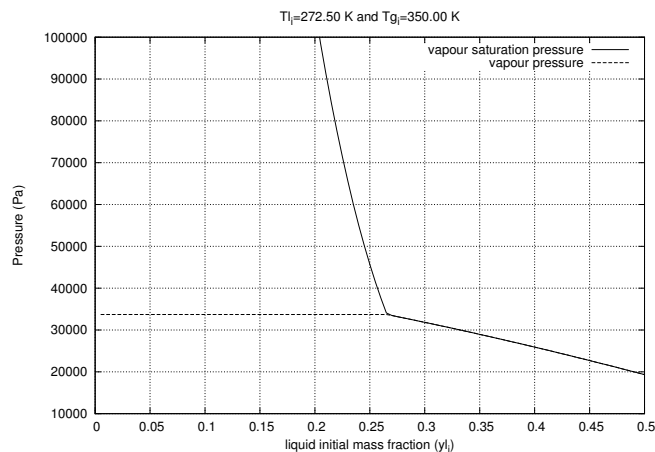
This method can be more interesting than the Abramzon model, because not only it resolve the particular problem of flash-boiling, but also it integrates the condensation phenomenon, which is supposed to occurs during the jet spreading.

The test of this model is done with the butane properties. The purpose of the test is to see if it is consistent by varying the initial quantities of  $y$  and  $T$ . In this paper we show the test of the model by varying the initial liquid mass fraction, with the liquid and gas temperature at 272.5K and 350K respectively. The total pressure is equal to 0.1 MPa.

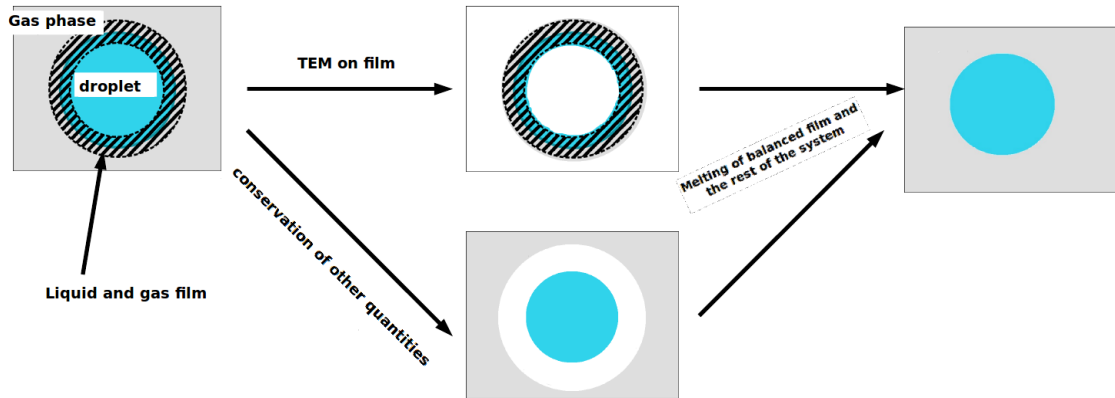


**Figure 4.** Test of the model of mass and enthalpy conservation by varying the initial mass fraction

The Figure 4 shows the final temperature (left-aligned) and the final mass fractions of liquid and vapour (right-aligned) in the system. The model is consistent with the physics. If the liquid initial amount is small, because of the great temperature in the gas compared to the liquid temperature, it evaporates completely. The temperature evolution in this case of total evaporation is linear, accordingly to the ideal gas law. But, the system come to a stage where the energy in the gas phase is not sufficient to completely evaporates the liquid. Thus, as we can see in figure 5, which compare the vapour saturation pressure of butane at the final temperature and the butane vapour pressure in the system, there is an equilibrium between the two phases when liquid remain in the system.



**Figure 5.** Comparison between the vapour saturation pressure and the butane vapour pressure in the system



**Figure 6.** Usage of the TEM model in two-phase flow module of FIRE

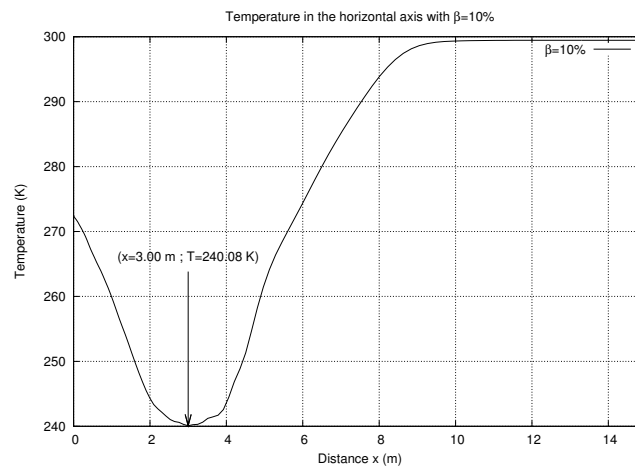
### Implementation of TEM in FIRE:

The next step is to introduce this model in the FIRE software. However, this model did not give information on how long it takes to evaporate. So, the model is completed to finally have the mass transfer rate between liquid and gas phase. This is done by adding a film of evaporation (Figure 6). It consist in taking an amount  $\beta_l$  of liquid (16) and  $\beta_g$  of gas (17) which will be applied to the model. At the current state of the work, these amounts of liquid and gas are not yet determined precisely and have the same value  $\beta$ .

$$\beta_l = \frac{m_{liquid\ film}}{m_{droplet}} \quad (16)$$

$$\beta_g = \frac{m_{gas\ film}}{m_{gas\ in\ cell}} \quad (17)$$

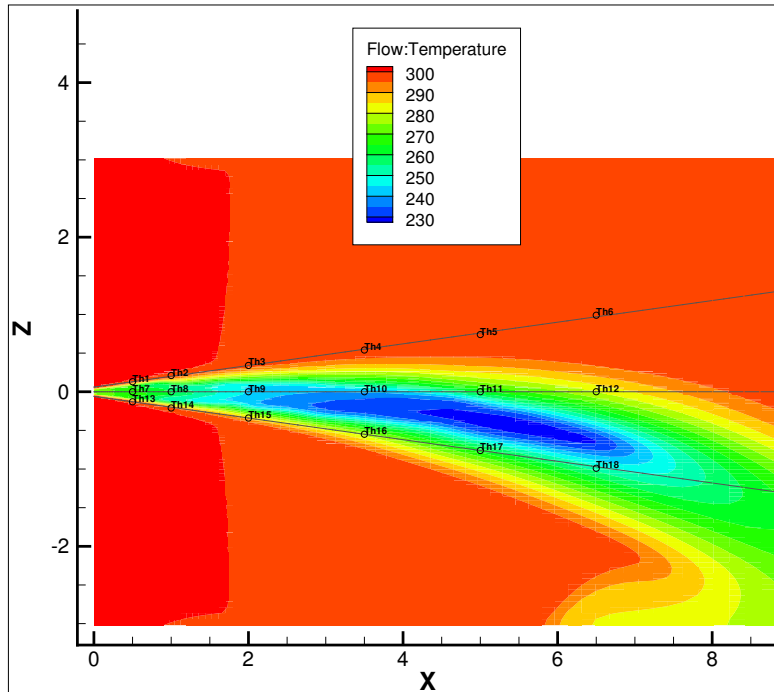
### Results and Discussion



**Figure 7.** Temperature evolution in the jet axis

It is complicated to have experimental results on the types of jets described above. But the INERIS were able to have more reliable measurements in temperature. These measurements show the same behaviour as seen on Figure 7, showing the evolution of the temperature in the jet axis with  $\beta = 10\%$ . The spray is surrounded by a hot gas

environment. However, the temperature of the spray decreases up to a certain distance. Due to the initial droplet boiling temperature, close to the injection, the vaporization process dominates the flow. Since evaporation is an endothermic phenomenon, the spray jet cools down until there is no droplet enough. Thus the spray temperature rises only once the liquid vaporization does not have enough influence in the flow.



**Figure 8.** Temperature field in a vertical plane passing through the simulated jet axis with the experimental thermocouples positions: Th1-Th6 = up axis ; Th7-Th12 = horizontal axis ; Th13-Th18 = down axis.

INERIS has done temperature measurements with thermocouples at different points on three axis (up, horizontal and down) in the jet as seen on Figure 8. The comparison of these measurements with computation results ( $\beta = 10\%$ ) in Figure 9 shows that the simulations are not far from reality. The differences can be explained by the fact that the choice of  $\beta$  and the calculations on the boundary conditions are not yet accurate.

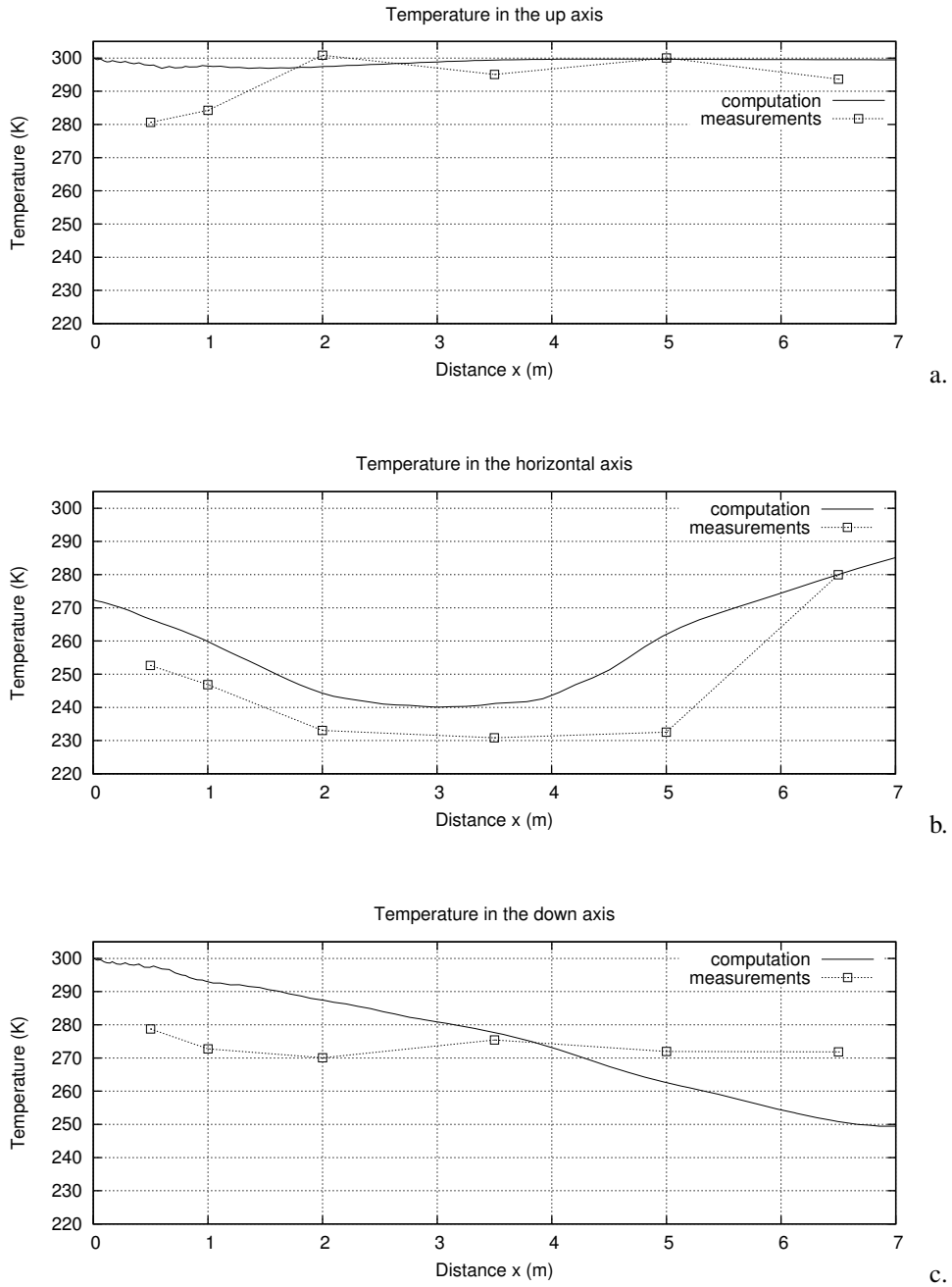
### Conclusion

The modelling results with the TEM model show that the calculated temperature behaviour in the spray jet by comparison with the observations is generally satisfactory. This result cannot be obtained with classical vaporization model. As a perspective to this work, a model is under development to estimate the value of  $\beta$  by taking account the turbulence in gas phase, the time step, the droplet area, ... Finally, the assumptions used to calculate the boundary conditions bring many lack of precisions. It would be desirable to do a CFD model of the material flow from inside the vessel to the end of expansion zone.

### References

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- [2] Bonnet, P., Bricout, P., Duplantier, S., Jamois, D., Lacôme, J.-M., Meunier, P., Éssais de rejets diphasiques à grande échelle, *Rapport d'étude N°41508, INERIS* (2005).
- [3] Abramzon, B., Sirignano, W. A., Droplet vaporization model for spray combustion calculations, *Int. J. Heat Mass Transfer* (1989).





**Figure 9.** Temperature comparison between experimental and simulation (with  $\beta=10\%$ ) results in the up (a.) horizontal (b.) and down (c.) axis.