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# NUMERICAL MODELLING OF FLASHING LIQUID JETS DUE TO LEAKAGE OF LIQUEFIED GAS STORAGE

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## ABSTRACT

*One of the missions of the INERIS is to assess accidental risks induced by industrial activities. The use of liquid gases is very widespread in industry but a large potential hazard exists in case of accidental release. These substances can be flammable and explosive like the LPG or toxic like anhydrous ammonia. In case of an accidental leakage due to a vessel breach or a line rupture, a violently change phase could take place inside these products. This phenomenon called flashing jet are still bad understood and many strong hypothesis are often used to predict by modelling its physical consequences in the near field like thermodynamic behaviour of the whole jet, pool formation. However all these physical consequences have to be well evaluated in order to better estimate the explosive cloud or toxic cloud formation. The objective of the INERIS-CORIA work is to develop a new numerical model with the aim of simulating two phase jet resulting from a leakage in a pipe containing a liquefied gas. The work focuses especially on the effect of the vaporization and boiling process in the jet. 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.*

*Keywords : Thermodynamic Equilibrium, flash-boiling, two-phase flow, droplet, vaporization*

## 1. Introduction

### 1.1. Context

Accidental releases to the environment of pressurized liquid gases under ambient conditions could generate a large flow rate when the breach appears on the liquid filled containment. The superheated released liquid can form a two phase explosive or toxic cloud mixture. Potential consequences of these accidental releases are injuries, fatalities, destruction of installations and possible evacuation from the surrounding

area of the accident. Examples of fatal accidents ([1], [2], [3]) involving superheated liquids showed huge consequences. Predicting behaviour of the liquid-gas cloud mixtures by modelling is of direct relevance for industrial risk assessment.

At the breach level, in the case of an accidental release of pressurized liquefied gas, the product released in the ambient air is suddenly placed under temperature and pressure conditions that are such that a part of the liquid vaporizes violently. This phenomenon is generally called a "flash".

In order to calculate safety perimeters around industrial installations, one of the objectives of atmospheric dispersion research projects of INERIS is to improve models of flashing releases in realistic industrial environments.

Equivalent source term models exist for flashing release in current long range dispersion models intended to predict toxic effects or explosive cloud formation. Several factors can, however, invalidate simplified equivalent source models, especially in the very near field where many complex phenomena can occur and where obstacles can be found.

We can easily say that total mass released and the release duration are major parameters. Others parameters as the velocity, thermodynamic state, and amount and droplet sizes of imbedded aerosols of the material at the exit of the rupture are also required as inputs to the jet and dispersion modelling.

A number of experimental, theoretical and numerical studies have been carried out [5],[6],[7] to perform calculations of two phase mass flow rates. Several empirical and analytical models were developed based on hypothesis related to saturation conditions. In order to have a better use of the models, they have been compared with measured data obtained during experimental tests performed by INERIS since the 90's [8]. These comparisons allowed us to conclude that to reach a good agreement between measured data and calculating flow rate is difficult but conservative models are clearly pointed out. This issue is relevant in a risk assessment.

Recent critical review [4] of term source modelling for toxic release scenario for pressurized liquefied gases showed there is "still a significant uncertainty in the overall modeling process". Main difficulties come from modelling suspension, evaporation of aerosol and rainout.

The aim of the present work is to improve the acknowledge and the numerical modelling of aerosol evaporation.

## **1.2. Jets experiments**

In order to improve model of flashing releases in realistic industrial environments, INERIS carried out two-phase butane and propane jet releases [9] into the atmosphere and ammonia [10] jet releases in a congested environment. Indeed most leakage problems from breakages of vessel or line rupture result in the formation of jets due to difference between the internal and the external pressure. These experiments involved to measure the main characteristics of the jet and to increase the understanding of the behaviour of superheated (flashing) liquid jets.

### 1.3. Modelling objective

Basic principles of flashing jets are summarized in Figure 1. The jet consists in 3 areas:

- The expansion zone (flash boiling, atomization): Here, the fluid expands 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.

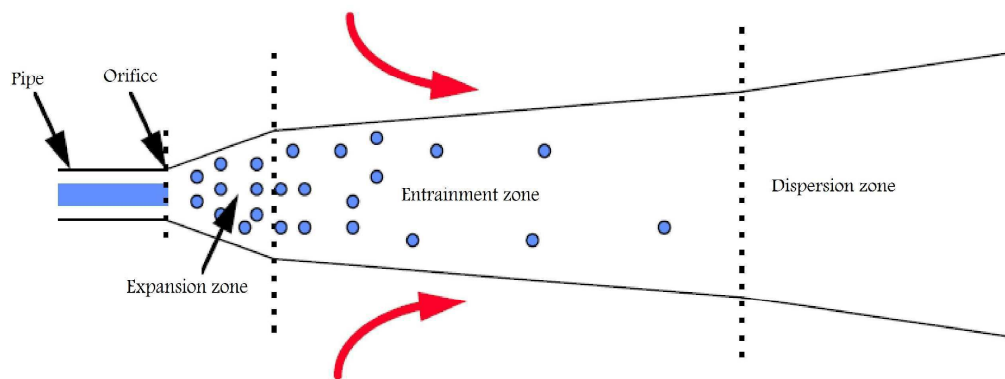


Figure 1. Schematic representation of the areas of the flashing jet

The objective of this work is to develop a numerical model with the aim of simulating thermo dynamical behaviour of a two phase flow resulting from a breach or leakage in a vessel containing liquefied gas. A focus is made on the entrainment zone where a strong decrease of temperature was measured.

This paper aims to present the first results and comparisons between modelling calculations with experimental data.

A description of approaches used to simulate thermodynamic process inside flashing jets is given in Section 2. Results and discussion are presented in Section 3.

## 2. Methods

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.

## 2.1. Expansion zone

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 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 [12] 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:

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

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

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

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

By supposing  $X \ll 1$  and  $C_{pg} < C_{pl}$ , we see that the term  $-(1-X) * C_{pl} * dT / dX$  in (3) is equal to latent heat vaporization:

$$L_v(T_b) = -(1-X) * C_{pl} * \frac{dT}{dX} \quad (4)$$

The heat exchange due to vaporization is supposed greater than the heat due to warming:  $C_{pl} * dT \ll L_v$ . By taking account of this assumption after the integration of (4), we finally have:

$$X_{exp} = C_{pl} \frac{T_i - T_{exp}}{L_v} \quad (5)$$

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.

All the above work is useful to estimate values in the jet at the end of expansion zone.

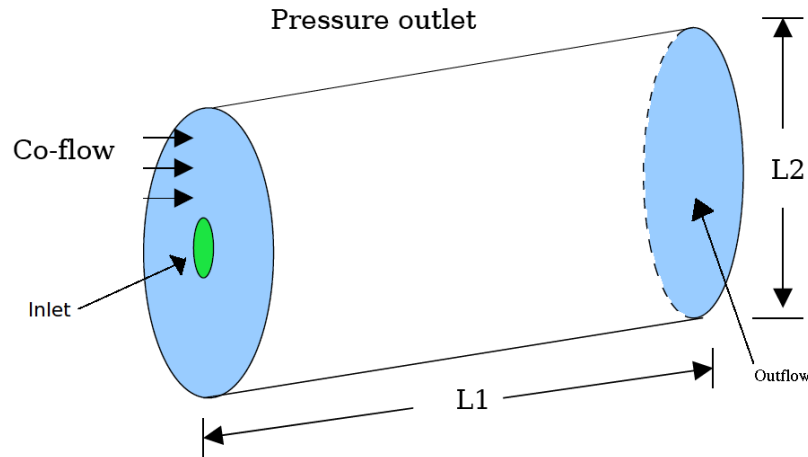


Figure 2. Computation area

The simulations start at this point, since the CFD model used is the two-phase Euler-Lagrange description model. The experimental case presented in this paper comes from the data base of the FLIE (Flashing Liquids in Industrial Environment) project

[13]. The numerical software used for this study is numerical package FIRE V8.41 from AVL.

The chosen case is whose of a vessel of liquid butane at 7.78 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 mm in diameter. The mass flow rate conservation between the orifice and the end of expansion zone give the diameter of this end zone :  $D = 60.45$  mm. The numerical domain in which the butane is spreading is presented in Figure 2. It consists in a cylinder of 36 m in length and 6 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 boundary conditions are recapitulated in Table 1. Finally, the turbulence is modelled with the K- $\epsilon$  model and the applied gravity is  $9.8 \text{ m/s}^2$ .

Table 1. Boundary layer conditions

Variable	Inlet	Coflow	Outflow
Material	Butane (liquid & gas)	air (gas)	
Velocity (m/s)	29.49	1	-
Temperature ( $^{\circ}\text{K}$ )	272.6	300.15	-
Mass flow rate (kg/s)	1.33	-	-
Vapour mass fraction	0.17	-	-
Droplets size ( $\mu\text{m}$ )	100	-	-
Turbulence intensity	10	1	-
Length scale	0.005	0.1	-

## 2.2. Abramzon vaporization model

Vaporization is based on Abramzon vaporization model [11]. 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 (6) and (7):

$$\dot{m} = \pi \rho D a S h_c \ln(B_M + 1) \quad (6)$$

$$\dot{m} = \pi \frac{a k}{C_{pg}} N u_c \ln(B_T + 1) \quad (7)$$

Usually, the mass Spalding number  $B_M$  (equation (8)) and the thermal Spalding number  $B_T$  (equation (9)) are supposed to be the same ( $B_M = B_T = B$ ). 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 (10) below.

$$B_M = \frac{Y_{F,s} - Y_{F,\infty}}{1 - Y_{F,s}} \quad (8)$$

$$B_T = \frac{\rho_s v_s C_{pg}}{h_c} \quad (9)$$

$$h_c (T_\infty - T_s) = \rho_s v_s Lv + \frac{Q_l}{\pi a^2} \quad (10)$$

In the three equations above ((8), (9), (10)),  $Y_F$  is the vapour mass fraction of droplet material in the gas phase,  $v_s$  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 (10) combined with equation (7) give the heat quantity necessary for droplet heating.

$$Q_l = \pi a k \left( \frac{h_c a}{k} (T_\infty - T_s) - \frac{Lv}{C_{pg}} Nu_c \ln(B_T + 1) \right) \quad (11)$$

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 ( $Y_{F,\infty} \approx Y_{F,s} \approx 1$ ). Thus, this is a limit case between boiling and vaporization. As seen in equation (8), 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.

### 2.3. New model: Thermodynamic Equilibrium Model (TEM)

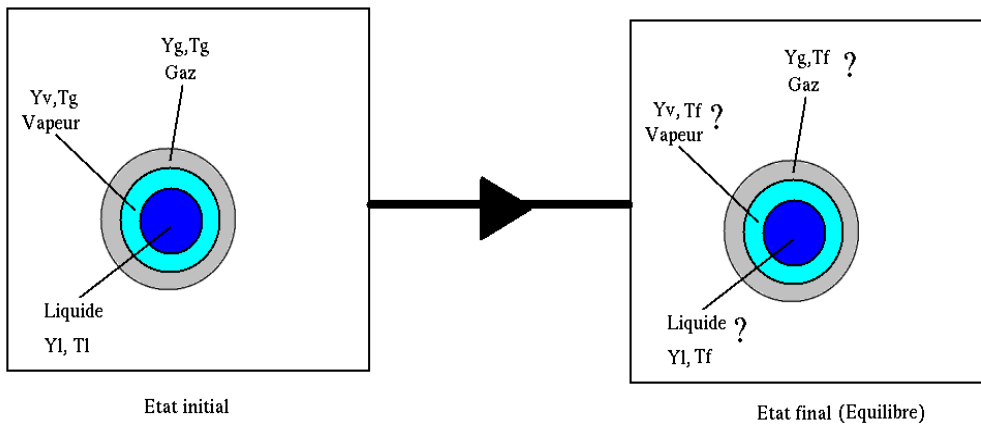


Figure 3 : Initial and final state in the thermodynamic system



We propose a special procedure to solve this problem. It is considered a thermodynamic system (see Figure 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 (12).
- Isolated system with constant pressure transformation: enthalpy conservation (13).

$$\sum_k y_k^{initial} = \sum_k y_k^{final} = 1 \quad (12)$$

$$H_t = \sum_k H_k(T_k^{initial}) * y_k^{initial} = \sum_k H_k(T_k^{final}) * y_k^{final} = Cte \quad (13)$$

$$f(T^{final}) = H^{initial}(T_l^{initial}, T_g^{initial}) - H^{final}(T^{final}) \quad (14)$$

The first step of this method is to find the enthalpy at the initial state with de quantities  $y$  and  $T$  in (13). 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  $f(T^{final})$  (14). 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 272.5°K and 350°K respectively. The total pressure is equal to 0.1MPa.

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.

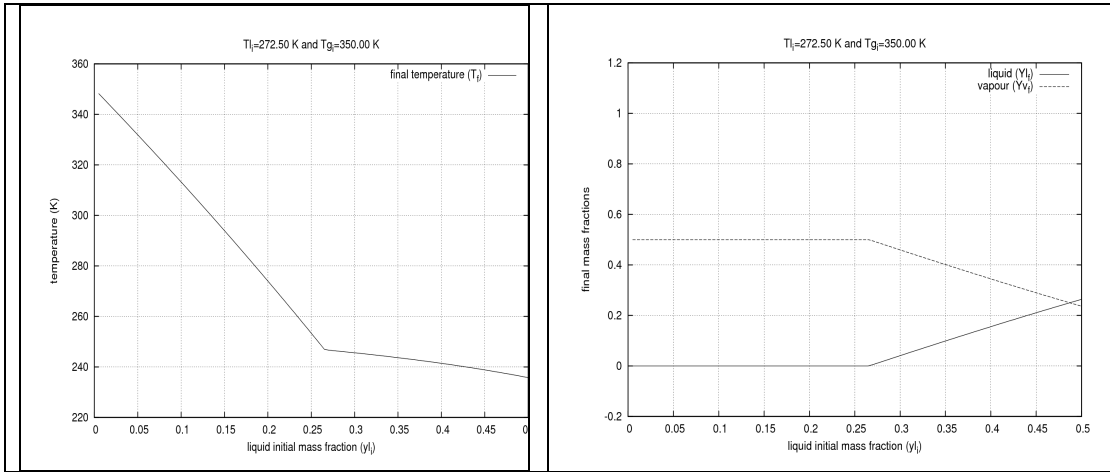


Figure 4. Test of the model of mass and enthalpy conservation by varying the initial mass fraction

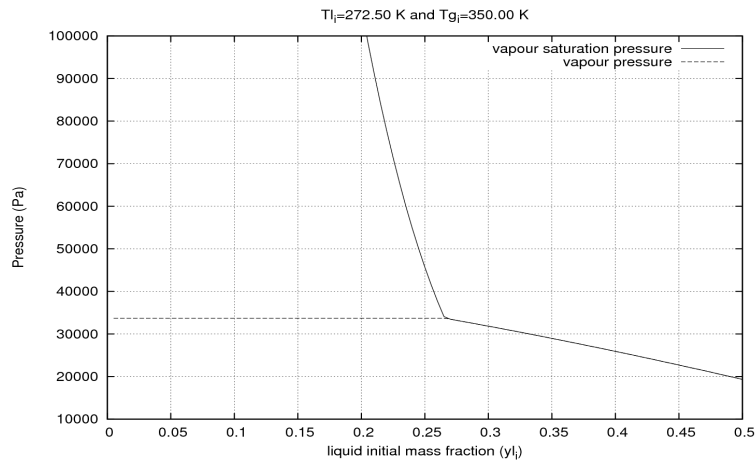


Figure 5 : Comparison between the vapour saturation pressure and the butane vapour pressure in the system

**2.4. Implementation on TEM in FIRE:**

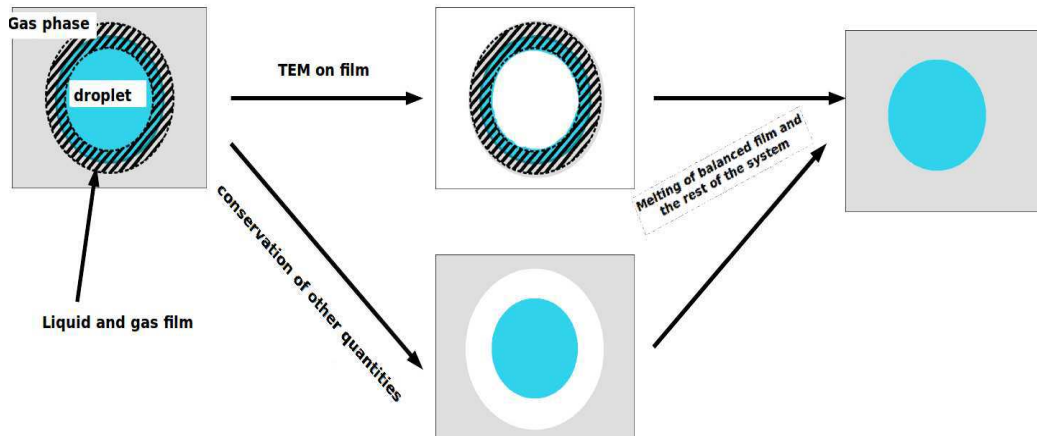


Figure 6 : Usage of the TEM model in two-phase flow module of FIRE

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 consists in taking an amount  $\beta_l$  of liquid (15) and  $\beta_g$  gas (16) 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  $\beta$ . In this paper, we will just compare the results given by taking account two different values of  $\beta$ .

$$\beta_l = \frac{m_{\text{liquid film}}}{m_{\text{droplet}}} \quad (15)$$

$$\beta_g = \frac{m_{\text{gas film}}}{m_{\text{gas in cell}}} \quad (16)$$

### 3. Results and Discussion

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  $\beta=10\%$ .

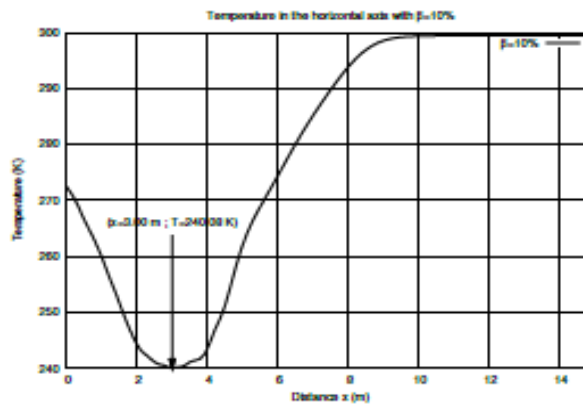


Figure 7 : Temperature evolution in the jet axis

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.

INERIS has done temperatures 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.

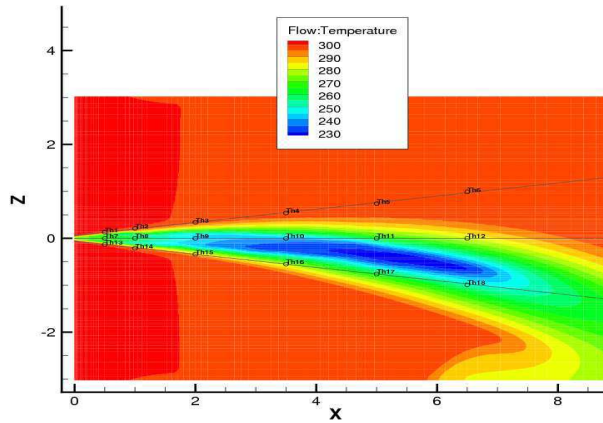


Figure 8 : Temperature field in a vertical plane passing through the simulated jet axis with the experimental thermocouples positions : Th1-Th6 = up axis; Th7-Th12 = horizontal axis; Th13-Th18 = down axis

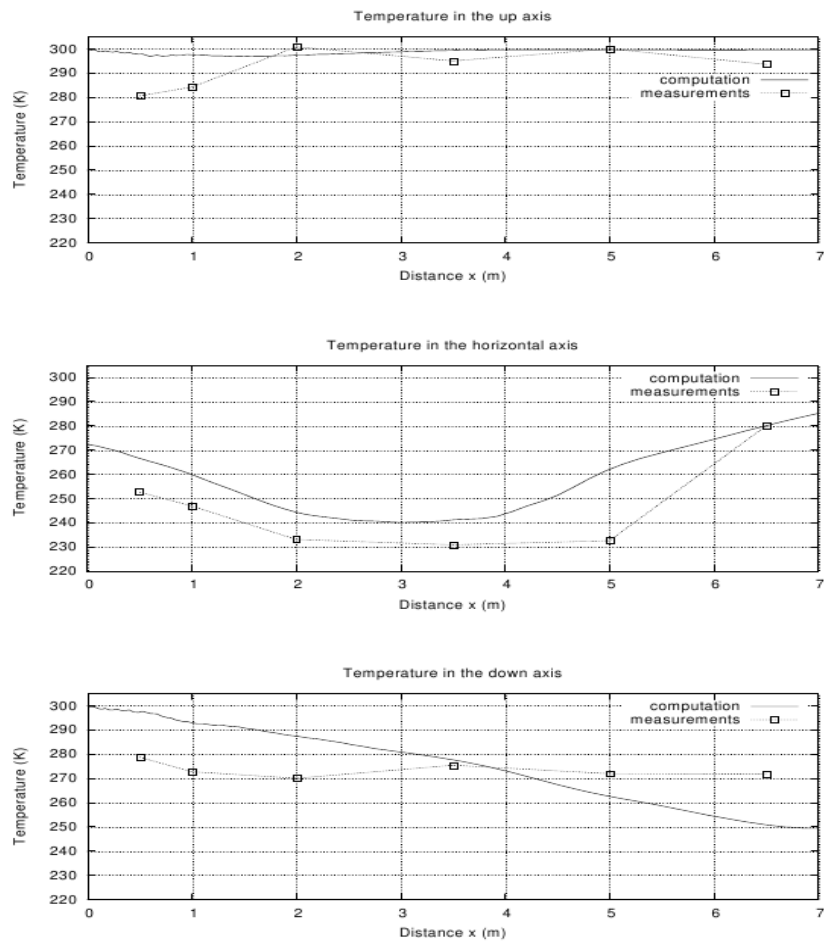


Figure 9 : Temperature comparison between experimental and simulation (with  $\beta=100\%$ ) results in the up (a), horizontal (b) and down (c) axis.

## 4. 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 calculate 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.

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