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Loss of containment: experimental aerosol rain-out assessment

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Abstract

We measured the temperature profiles and rain-out spatial distribution for flashing water jets generated from a pilot scale experimental setup. This allowed us to define the transitions between three types of jets (stable, mechanically fragmented, flashing). The present experimental data when compared to other authors' data show that the transition to flashing type occurs at lower superheat when the orifice length increases, and that homogeneous aerosol behavior could be a valid assumption for mechanically fragmented jets whereas it is not for flashing jets.

Keywords: Rain-out assessment; Flashing liquid jets; Pilot scale experiments; Aerosol; Breakup

1. Introduction

We consider the accidental release of a toxic or flammable pressurized liquid which gives rise to a two-phase jet. We would like to predict the jet mass fraction which deposits on the ground as a liquid (rain-out fraction) because this fraction does not directly contribute to the atmospheric dispersion cloud. Aerosol rain-out prediction is now far from accurate despite its role in the loss of containment event. The liquid mass flow entrained with the gas as an aerosol is often assumed (see for example [1]) to have the same value as the vapor mass flow obtained from a flash calculation. This can lead to a severe prediction error. More recent works [2–6] include a physical approach but the predictions remain unverified. A better knowledge of the initial fragmentation of the liquid phase would probably be useful.

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Nomenclature

C	growth rate constant [8,9] ($m\,s^{-1/2}$)
C_p	specific liquid heat capacity (J/kg K)
d_0	pipe or orifice diameter (mm)
D_{th}	thermal diffusivity (m^2/s)
h_{fg}	specific vaporization enthalpy (J/kg)
P_{amb}	ambient pressure (MPa)
P_0, T_0	upstream (reservoir) pressure (kPa or MPa) and temperature (K)
T_{eb}	boiling point at ambient pressure (K)
T_{sh}	shattering temperature (K)
We	Weber number (–) ($We = (\rho_{air} U^2 d)/2\sigma$)

Greek letters

ρ_f	liquid phase density (kg/m^3)
ρ_g	gas phase density (kg/m^3)
σ	surface tension (N/m)

Liquids discharged from a high pressure zone to a zone where pressure is lower than the equilibrium one have been studied by several authors like Bushnell and Gooderum [7], and Brown and York [8]. They studied the shattering temperature T_{sh}, i.e. the temperature at which a coherent jet becomes almost completely atomized.

From their experiments with water out of nozzles for $We < 12$, Bushnell and Gooderum [7] deduce that "the value of $(T_{sh} - T_{eb})/T_{sh} = 0.1$ may be approaching the upper limit of the amount of superheat that can be tolerated by a liquid jet before it shatters". "Negligible effect of the nozzle diameter and the velocity indicates that the aerodynamic forces were indeed secondary during the atomization process".

Brown and York [8] considered that the growth rate of bubbles determines the shattering effect. From Plesset and Zwick [9], and Forster and Zuber [10], the radius of a bubble follows the relation:

$$r = r_0 + C\sqrt{t}$$

where C is the bubble growth rate constant given by

$$C = \frac{C_p(T - T_{eb})}{h_{fg}} \frac{\rho_f}{\rho_g} \sqrt{\pi D_{th}}$$

They observe that "a jet of large diameter may shatter at a superheat for which a smaller jet does not shatter" (note that this observation seems to be in contradiction with the conclusions of Bushnell and Gooderum [7]). This leads them to use the Weber number (which measures the momentum exchange with air to surface tension ratio) as a parameter. They represent their experimental data for transition from a coherent to a shattered jet on a chart with We and C as coordinates. On this chart, the transition line for water is almost the same for sharp-edged and not too rough orifices. "Higher values of the Weber number permit shattering to occur with less superheat". Both Brown and York [8] and Bushnell and

Gooderum [7] used small orifices (generally less than 2 mm ID). They performed their jet's observations at a few diameters downstream.

Our objective is to enlarge their observations to situations more representative of accidental flashing liquid discharge in order to examine the validity of the assumptions in some existing models [2–6].

2. Experimental

We generated water flashing jets from a pilot scale set-up (0.230 m^3, 0.1–1.3 MPa) [11] through a 1.8, a 8 mm ID orifice (Fig. 1(a)) and a 4 m long pipe of 8 mm ID. Inlet temperature was varied from 313 to 453 K, and the sub-cooling varied from 50 to 600 kPa. Twelve capture basins (Fig. 1(b)) allowed to weigh the liquid rained out under the jet as a function of the distance from the source. A thermocouple also measured the final temperature of the jet. The 1.8 mm ID orifice gives rise to three types of jets (Figs. 2(a), 3(a) and 4(a)) which are easily distinguishable to the naked eye.

2.1. Type a jet

The jet is a superheated liquid cylinder all along its trajectory (Fig. 2(a)). There is almost no fragmentation and no dispersion of the jet (Fig. 2(b)); the second peak is due to spattering

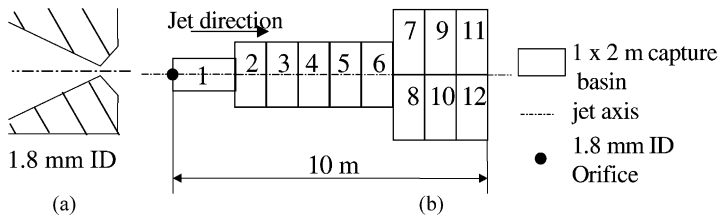

Fig. 1. Schematic representation of (a) the orifice: 1.8 mm ID, (b) the downstream area.

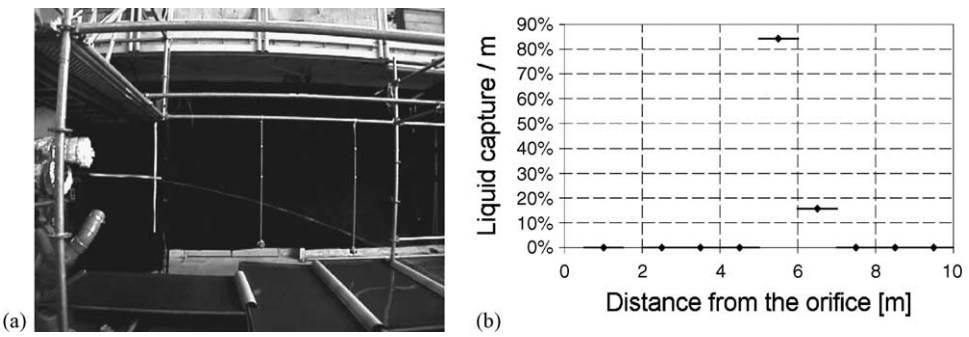

Fig. 2. (a) Jet parabolic trajectory. The three first basins can be seen. Initial storage conditions: $T_0 = 383.4$ K; $P_0 = 180$ kPa. (b) Liquid capture fraction versus distance from the orifice.

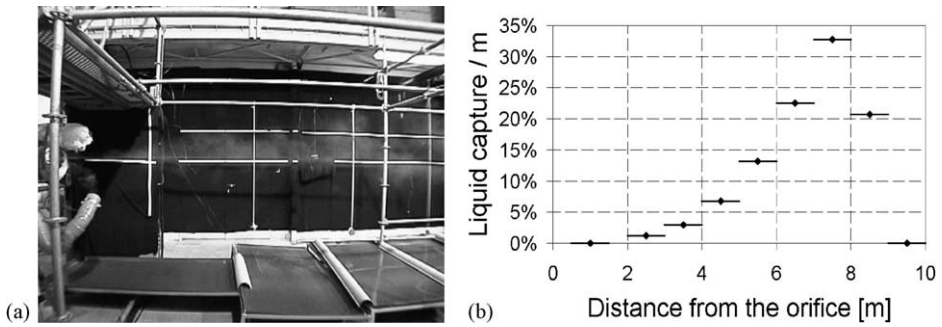

Fig. 3. (a) Vaporization along an essentially liquid jet's trajectory. Initial storage conditions: $T_0 = 383.6\,\mathrm{K}$; $P_0 = 480\,\mathrm{kPa}$. (b) Liquid capture fraction versus distance from the orifice.

from one basin to the other, except when a small obstacle is put on the trajectory of the jet which causes violent fragmentation. The distance of impact varies from 4 to 6 m when the upstream pressure is increased (Fig. 5(a)). The temperature decrease between the reservoir and the end of the jet is quite low (25–50 K) because the heat transfer area is less.

2.2. Type b jet

The liquid initial core changes progressively to a flow of droplets which "rain" in the basins (not visible in Fig. 3(a) because the droplets are too small). This fragmentation enhances the heat transfer so that some vapor can be seen along the jet's trajectory.

The liquid spreads out over 4 m or more. The mass center at impact is farther from the orifice than in the case of type *a* (6–8 m) because the upstream pressure is higher and so does the exit velocity (Fig. 5(a)).

The spreading of the jet increases with increasing upstream temperature (Fig. 5(b)), leading to a faster decrease of velocity and a shorter trajectory (Fig. 5(a)). Temperature decrease from the reservoir to the end of the jet is higher (50–85 K), because heat transfer

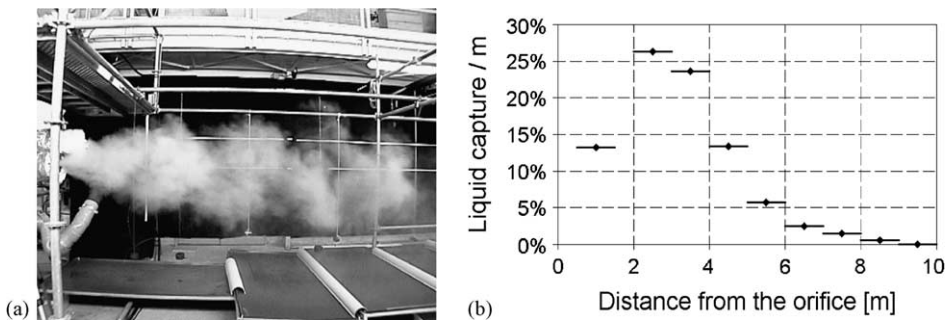

Fig. 4. (a) Immediate fragmentation of the jet. Initial storage conditions: $T_0 = 443.6\,\mathrm{K}$; $P_0 = 820\,\mathrm{kPa}$. (b) Liquid capture fraction versus distance from the orifice.

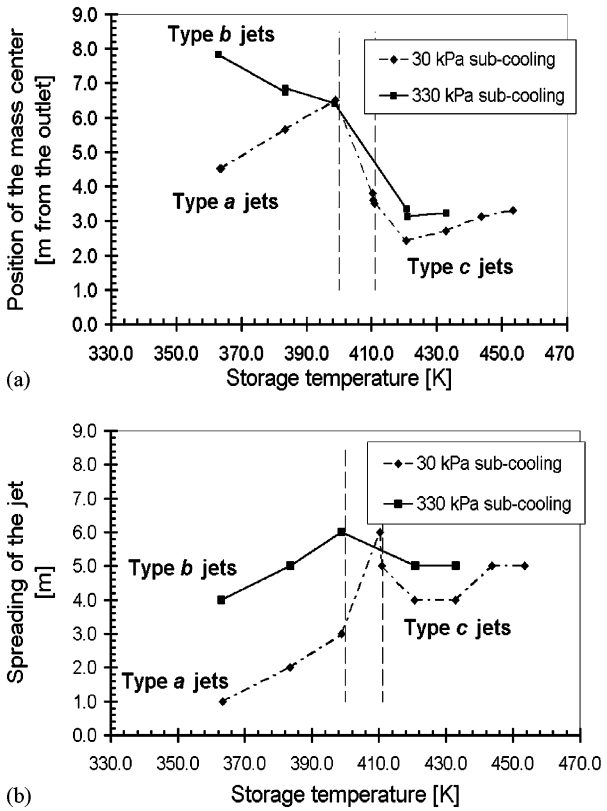

Fig. 5. (a) Mass center position of water jets. (b) Spreading of water jets (number of basins in which more than 5% of the capture liquid was deposited).

to air is more efficient when fragmentation occurs. Experimentally we do not notice any discontinuity in the transition from type *a* to type *b*. Type *b* seems to be typical of a disintegration due to momentum exchange with ambient air.

2.3. Type c jet

No liquid core can be seen anymore, disintegration takes place immediately at the outlet; it results in very fine droplets; the jet looks like a fog with a fine drizzle under it (Fig. 4(a)). The jet spreads out over 4 m or more. Jet speed decreases from the orifice, which gives a short trajectory (2–3 m) as shown in Fig. 5(a); the first few basins are the ones that are the most full. Trajectory length increases slightly with upstream pressure.

Type *c* jet behavior seems to be typical of thermal fragmentation. Mechanical fragmentation can probably no longer occur, because droplets resulting from thermal fragmentation at the orifice before air contact are small enough to be mechanically stable.

A discontinuity seems to appear while passing from type *b* to type *c* jet (Fig. 5(a)). At temperatures slightly less than the transition's lower bound, an essentially liquid jet falls at

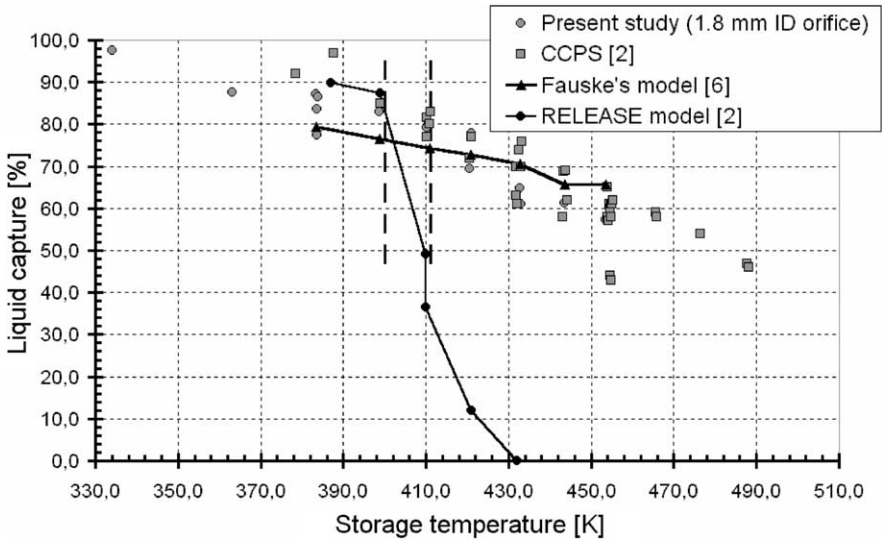

Fig. 6. Rain-out: experimental data and model results.

6 m from the exit. At temperatures just over the transition's upper bound, we observe a fog which falls at 1.5 m.

2.4. Rain-out data

Fig. 6 allows comparison of our experimental rain-out data with those obtained at the CCPS [2] with different orifices. There is a general agreement that orifice diameter does not have a crucial influence on this phenomenon. All points lie approximately on the same curve, do they come from low or high initially sub-cooled conditions: rain-out fraction is not very sensitive to initial pressure conditions.

All the above observations were obtained from experiments with the 1.8 mm ID orifice. Observations with both the larger orifice (8 mm ID) and the long pipe were qualitatively similar.

3. Discussion

As suggested by Brown and York [8], we plotted our experiments in Fig. 7 (nozzles) and Fig. 8 (pipe), using the growth rate constant C [9,10] and the Weber number as co-ordinates. Note that we use the velocity of the liquid phase (before flashing) in the definition of the Weber number for a jet out of a pipe.

Fig. 7 shows that for jets at low Weber number after an orifice whatever the diameter, the transition to flashing occurs when C is between 0.085 and 0.088 $\mathrm{m\,s^{-1/2}}$ (i.e. 38 K $<$ $T_0 - T_{\mathrm{sat}} <$ 40 K). Inside this interval thermal disintegration occurs closer to the orifice until it reaches the orifice. As observed by Brown and York [8], transition to shattering at

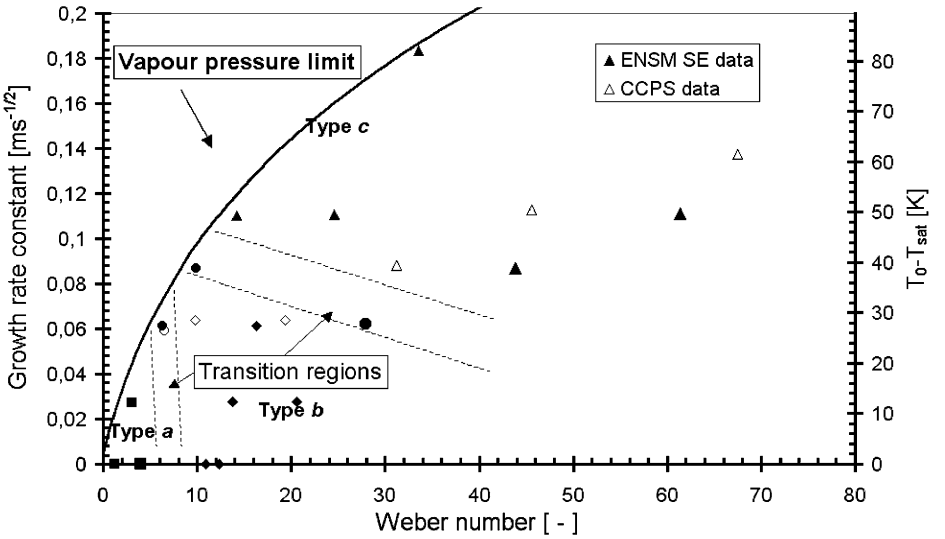

Fig. 7. Effect of Weber number and growth rate constant on type of jet breakup for 1.8 and 8 mm ID orifices (ENSM SE data), and 6.35 and 3.2 mm ID (CCPS data).

the orifice is promoted by increasing *We*, i.e. P_0. Then flash atomization takes place for lower values of *C*.

Fig. 8 shows that the same types of jets are observed for a long pipe, but the transition to flashing jets occurs at lower values of *C* ($0.02\,\mathrm{m\,s^{-1/2}} < C < 0.05\,\mathrm{m\,s^{-1/2}}$).

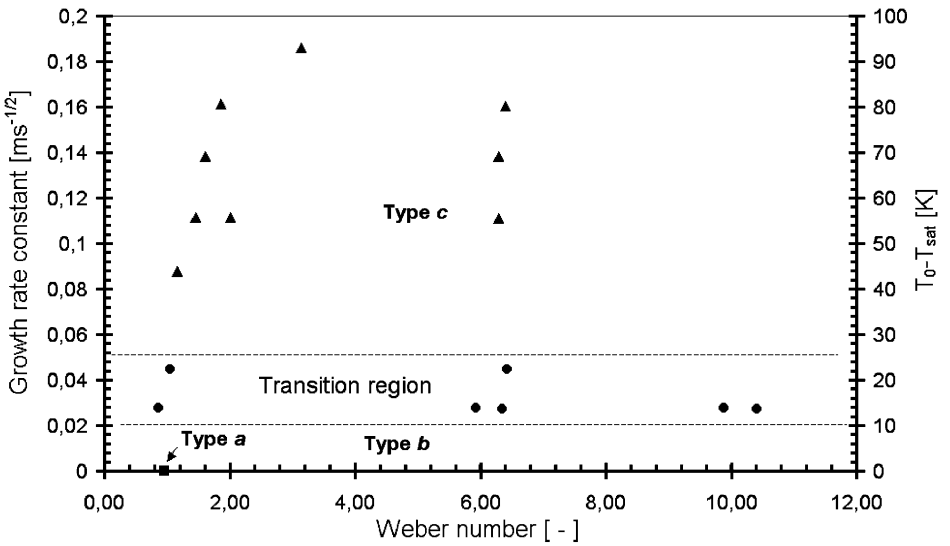

Fig. 8. Effect of Weber number and growth rate constant on type of jet breakup for a 4 m long and 8 mm ID pipe.

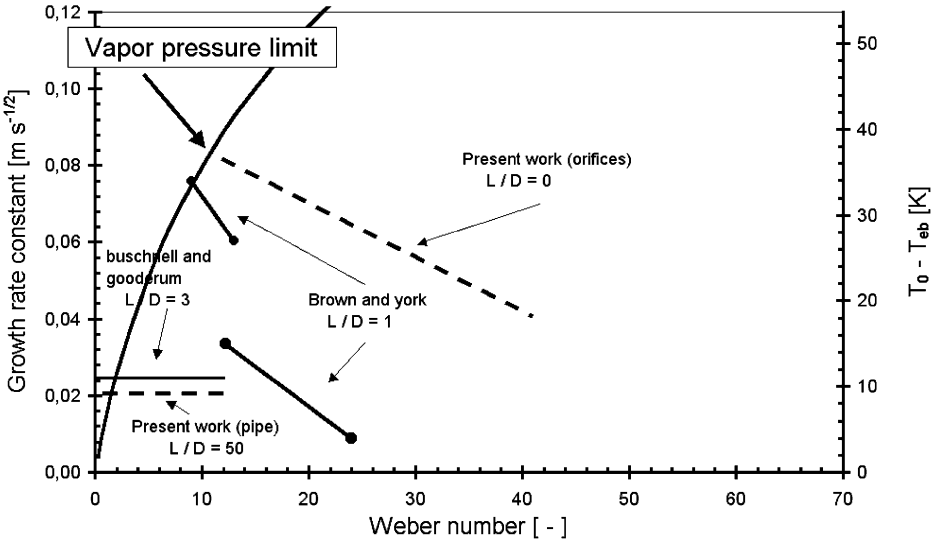

Fig. 9. Lower bound of the flashing–nonflashing atomization transition.

Fig. 9 represents the lower bound of the transition to flashing behavior as obtained by different authors. This graph reveals that there is no unique boundary. The length to diameter ratio (L/d_0) seems to influence the jet's stability. When L/d_0 tends to zero (thin orifice), an important superheat (>40 K) is necessary for flash atomization to take place, and when L/d_0 increases, the superheat necessary to obtain flashing breakup is less. For example when $L/d_0 = 3$ (Bushnell and Gooderum [7]) or $L/d_0 = 50$ (present work), the superheat needed for flash atomization to occur is about 10 K. This can probably be attributed to the nucleation sites present on the wall or the residence time in the pipe which allows vaporization to begin.

When flashing does not occur, jets are either stable ($We < 7$, type *a*) or disintegrate far from the orifice ($We > 9$, type *b*). This introduces a new transition compared to former observations (i.e., of Brown and York [8], and Bushnell and Gooderum [7]). This is because we observe our jets on a much larger scale (several meters) compared to former authors. Jets which seem to be stable at short distances progressively disintegrate due to mechanical instabilities.

It should be noticed that diameters involved in potential industrial accidents are generally 10, 100 or even 1000 times larger than the one we used. We are therefore interested in the higher Weber numbers (up to 10^4!) where type *c* jets are probably predominant.

Using $(T_{\mathrm{sh}} - T_{\mathrm{eb}})/T_{\mathrm{sh}}$ or C as the ordinate is almost equivalent when comparing jets of the same fluid (in the present study: superheated water). The question of the pertinent ordinates arises when dealing with different fluids. We can define a Weber number for flashing by comparing the kinetic energy of the bubble growing inside the liquid to the cohesive force:

$$C' = \frac{1}{2}\frac{\rho_{\mathrm{g}} u_{\mathrm{g}}^2 d_0}{\sigma}$$

In the above equation we choose to take the velocity as the liquid–vapor interfacial velocity calculated when it reaches its maximum. We neglect the initial nucleation site diameter and suppose that the bubble is centered in the middle of the initial liquid cylinder. Then we can derive the following expression for the end velocity:

$$u_{\mathrm{g}} = \frac{2C^2}{d_0}$$

where C is the growth rate constant. C' therefore becomes

$$C' = 2\frac{\rho_{\mathrm{g}} C^4}{\sigma d_0}$$

The parameter C' is inversely proportional to the exit diameter d_0. But our experiments as well as Brown and York's work [8] have shown that the exit diameter has no significant influence on the transition between flashing and mechanically fragmented jets. This tends to demonstrate that the length scale d_0 we used is not the pertinent one to describe flashing atomization. Nevertheless, we think that taking into account the cohesive force by introducing the surface tension σ into a nondimensional parameter should be a proper way to get a relevant parameter for characterizing flash atomization mechanism.

The CCPS model to predict aerosol rain-out RELEASE [2] considers parallel expansion and atomization at the orifice from which a droplet size distribution is derived. Following the approach of Wheatley [3], the model determines a critical drop size d_{c}. Droplets larger than d_c are assumed to rain-out without further evaporation. There is no attempt to model droplet trajectories or droplet evaporation rates. It is obvious from Fig. 6 that this model does not adequately fit the experimental data.

The other models that we considered [4–6] assume that the jet is homogeneous (no droplets rain out of the jet). Ambient air is entrained by the jet momentum. Continuous evaporation takes place along the jet trajectory. They differ from one another by considering either the equilibrium between liquid and vapor phases [4] or kinetically limited heat and mass transfer rates, with [6] or without [5] simplifying assumptions (dilution in air is infinite, wet bulb temperature in pure air is reached at the end of the jet, etc.).

Fig. 6 clearly indicates that the second kind of model gives better predictions: evaporation due to entrained air after initial flashing is of primary importance compared to the effect of initial size distribution on trajectory. Type *c* jet is an aerosol composed of small droplets. The thermodynamic equilibrium between the different phases will probably be an acceptable assumption. Type *b* jet is composed of larger droplets. It will probably be necessary to introduce a different temperature for each phase. In that case, a nonequilibrium model of heat and mass transfer controlled by the mean drop diameter in the jet would be appropriate.

4. Conclusion

In the introduction to the RELEASE program Johnson and Woodward [2] asserted: "the liquid release models available in 1986 could not adequately predict the complicated

processes occurring during the release of a superheated liquid". We saw here that the RELEASE model does not lead to a sufficient solution.

Our new experimental data demonstrates that different types of jets have to be considered and that some models for rain-out give reasonable predictions. We are now looking for an improvement of these models as well as the extension of their applicability to jets issued from long cylindrical ducts.

Acknowledgements

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