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Atmospheric dispersion of jets connected with flammable and/or toxic gaseous releases

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1. Introduction

The evaluation of the rate of air mixing, with a sudden release of flammable or toxic material, deriving from ruptures of pressurized vessels, is an essential tool in hazard assessment studies and risk evaluation, particularly as the so called "domino effects" concerns. Cude (1974) treated this topic by means of a two-step approach, starting from physical considerations and making use some simplifying assumptions. Based on the law of momentum conservation and on the experimental work of Ricou and Spalding (1964), Cude firstly obtained an expression for the dispersion of a jet in calm weather conditions. He separately accounted for the jet deflection due to wind speed by means of kinematic considerations and he applied the relations so obtained, together with an appropriate plume dispersion model, either to evaluate the ground level concentration of the release or to describe the boundaries of flammable region. The major drawback of Cude's model is due to the fact that it does not consider the dynamical effects of wind speed on the air entrainment into the jet. A preliminary approach was developed by Palazzi et al., 2001, to describe the behaviour of the jet, whatever its emerging direction may be. The model, validated by means of replicated tunnel experiments, gives the boundaries of flammable clouds as well as the ground level concentrations of toxic releases, and substantially agrees with the existing ones for the limiting cases of horizontal and upward directed jets. A relatively simple model was then developed to describe the rate of air mixing with upward directed high velocity releases (Palazzi, 2002). The model was validated by comparison with a series of experimental results obtained by other researchers in wind tunnel and with the theoretical results given by existing models for jets in a calm environment and for upward directed jets in windy conditions. Considering the specific needs of the protection criteria against ignition and explosion risk, as well as of people exposure to radiating heat and/or toxic compounds, a unified short-cut method was developed by Palazzi et al. 2003. Given the release characteristics and the plant layout, the method allows, in particular, to size the vent outlet, to locate the emission on the factory plan, by calculating the safety distance from a flammable release and to compare in a very effective way the various constraints on emission height, individuating the limiting one. This work presents a more general model, suitable to describe the behaviour of anyhow directed jets, so that the potential risk connected to the various kinds of accidents, involving gaseous releases which could happen in process industries, can be quantified. The model, validated by means of replicated wind tunnel experiments, directly yields the boundaries of flammable clouds and the ground level concentrations of toxic releases.

2. Modelling

In the most general case, following an accidental release, according to Hoehne, we can distinguish three stages in release dispersion, following one another as the vertical component of jet velocity, v_z, decreases, namely: a jet controlled region, where $v_z >> u$ and the rate of air mixing with the release is mainly determined by its momentum (jet phase); a transition region, where $v_z \sim u$ and the jet deflection and the rate of air drag are maximum (transition phase); a wind controlled region, where $v_z << u$ and the release dilution is dominated by the wind (plume phase). We consider anyhow oriented releases with emerging angle: $0 \leq \theta_0 \leq 2\pi$, under the hypothesis that the release reaches the plume phase before its impact with the ground (touchdown). In this paper, both the situations of still air and windy conditions are examined in depth.

2.1 Still air conditions

According to Palazzi, 2001, under the hypothesis $x>>d$ and $\rho \approx \rho_a$, the monodimensional model based on following conservation equation:

$$mv = m_0 v_0 \quad (1) \qquad m_0 = \frac{\pi}{4} d_0^2 v_0 \rho_0 \quad (2)$$

$$m = \frac{\pi}{4} d^2 v \rho_a \quad (3) \qquad d = k_0 x \quad (4)$$

allows the attainment of following results:

$$\frac{v}{v_0} = \frac{1}{k_0} \frac{d_0}{x} \left(\frac{\rho_0}{\rho_a} \right)^{1/2} \quad (5) \qquad \frac{m}{m_0} = k_0 \frac{x}{d_0} \left(\frac{\rho_a}{\rho_0} \right)^{1/2} \quad (6)$$

$$\bar{c} = \frac{M_a}{M_0} \frac{1}{k_0} \frac{d_0}{x} \left(\frac{\rho_0}{\rho_a} \right)^{1/2} \quad (7)$$

The above-mentioned results are valid for any given starting direction of the release, i.e. with spherical symmetry. Laboratory results allowed to confirm the value $k_0 = 0.32$, according to the results presented by Cude. As an example, Table 1 shows the hazard adimensional distance, r_L/d_0, corresponding to the attainment by dilution of C_L = Lower Flammable Limit for releases of pure methane (at T_a = 298 K) and n-heptane (at T_b= 372 K).

Table 1

	T [K]	**10^3 C_L (v/v)**	**M_0 [kg kmol^{-1}]**	**ρ_0 / ρ_a**	**r_L / d_0**
methane	298	53	16	0.55	79
n-heptane	372	12	100	2.76	125

2.2 Windy conditions

We assume that air entrainment is described by following relationship:

$$\frac{dm}{ds} = m_0 \frac{k_{\vartheta,u}}{d_0} \left(\frac{\rho_a}{\rho_o} \right)^{1/2} \quad (8) \qquad k_{\vartheta,u} = k \frac{v_{r0}}{v_0} \quad (9)$$

where: $v_{r0} = |v_0 - u| = \left(v_0^2 + u - 2uv_0 \cos \vartheta_0 \right)$ (10), and $k = k(\vartheta, u)$ to be experimentally determined, with the boundary condition: $\lim_{u \to 0} k = k_0$.

Considering again eqs. (2) and (3), starting from following conservation equation:

$$mv_x = mv_{0x} + (m - m_0 u) \quad (11) \qquad mv_z = m_0 v_{0z} \quad (12)$$

following equations, are obtained, as a function of s, length described by the jet axis, i.e., curvilinear abscissa of the mass centre:

$$\frac{s}{d_0} = A\left[Sh\left(\frac{z/d_0}{A} + b\right) - \cot g\vartheta_0\right] \quad (13)$$

$$\frac{x}{d_0} = A\left[Ch\left(\frac{z/d_0}{A} + b\right) - \frac{1}{\sin\vartheta_0}\right] \quad (14)$$

$$\bar{c} = \frac{M}{M_0}\frac{u}{v_0}\frac{1}{\sin\vartheta_0}\frac{1}{Sh\left(\frac{z/d_0}{A} + b\right) - \cot g\vartheta_0} \quad (15)$$

where: $A = \frac{v_0}{u}\left(\frac{\rho_0}{\rho_a}\right)^{1/2}\frac{\sin\vartheta_0}{k_{\vartheta,u}}$ (16) $\qquad b = \ln\frac{1+\cos\vartheta_0}{\sin\vartheta_0}$ (17)

Starting from eqs. (13), (14) and (15), it is possible to obtain the coordinates of the mass centre and the release concentration, as a function of the jet axis coordinate, s:

$$\frac{z}{d_0} = A\left[\ln\left(B + \sqrt{1+B^2}\right) - b\right] \quad (18)$$

$$\frac{x}{d_0} = A\left[\sqrt{1+B^2} - \frac{1}{\sin\vartheta_0}\right] \quad (19)$$

$$\bar{c} = \frac{1}{k_{\vartheta,u}}\frac{M_a}{M_0}\left(\frac{\rho_0}{\rho_a}\right)^{1/2}\frac{d_0}{s} \quad (20) \qquad \text{where:} \quad B = \frac{1}{A}\frac{s}{d_0} + \cot g\vartheta_0 \quad (21)$$

3. Results and discussion

As an applicative example, Fig. 1 depicts the mass centre trajectory of a n-heptane jet, corresponding to three emerging angles, namely π/4, π/2 and 3π/4, for two different values of the ratio v_0/u, namely 16 and 110. In order to provide a direct comparison of the hazard areas in the different conditions, the cut-off limits for all the trajectories represented in Fig. 1 correspond to LFL. This seems to be a very useful result for practical applications, especially if compared with other complicated and time-consuming approaches, eg., CFD simulations.

Fig. 2 depicts a representation of the locus where the average concentration of a n-heptane jet is equal to LFL of the mixture release-air, for two different values of the ratio v_0/u, namely 16 and 110.and for the whole range of emerging angle $0 \leq \theta_0 \leq \pi$.

In other words, Fig. 2 shows the maximum horizontal and vertical extension of the hazardous area, in connection with the different release emerging angles.

According to the starting hypotheses (touchdown after the jet phase and constant wind velocity), the figures corresponding to downward jets, characterized by emerging angle in the range $-\pi \leq \theta_0 \leq 0$ and same values of the velocity ratio, are symmetrical to the previous ones.

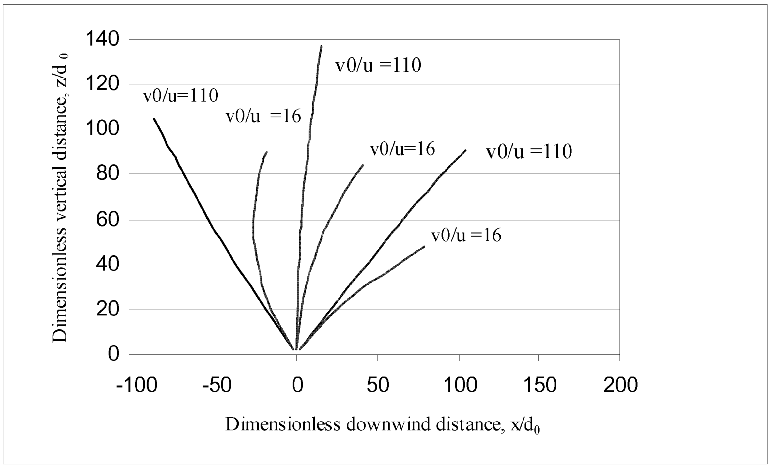

Fig. 1 Mass centre trajectory of the mass centre of a n-heptane jet for $\theta_0 = \pi/4$, $\pi/2$, $3\pi/4$ and for two different values of the velocity ratio v_0/u.

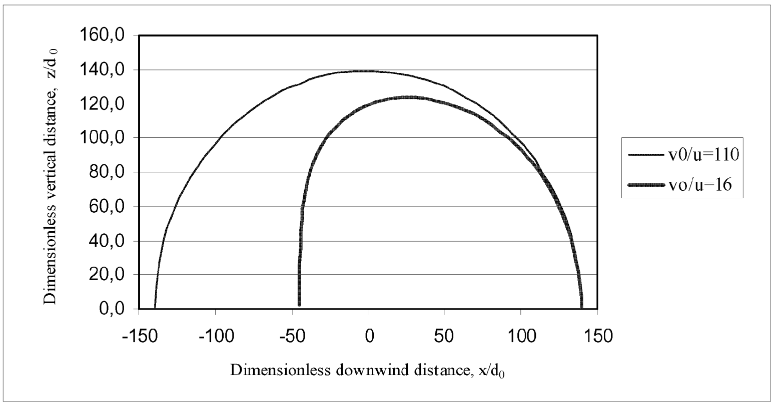

Fig. 2 Boundaries of the hazardous area, corresponding to LFL, for a n-hepatane release, considering two different values of the velocity ratio v_0/u and the whole range of emerging angle $0 \le \theta_0 \le \pi$.

In the following points, we shall discuss possible problems connected to the effective applicability of the model.

1. When dealing with a real jet, we must consider that its properties are characterized by a radial distribution in each section orthogonal to the axis and, in particular, that v=v(r) and c=c(r). Moreover, $v_a > v$ and $c_a > \bar{c}$, being the axial region of the jet mixed with the entrained air at a lower rate than the boundary region. Dealing with horizontal releases, this observation requires the need of a corrective coefficient in order to evaluate the maximum axial concentration c_a. According to Cude and, as resulting from previous experimental results (Palazzi, 2001), the axial concentration $c_a = 2\bar{c}$ (22).

2. When considering accidental releases characterized by different emerging angles, the trajectory of the jet axis is different from the centre mass one, so that it is necessary to accurately model the system by experimental runs suitable to define empirical corrective coefficient as a function of θ_0. The actual value of the entrainment constant k is connected to the jet emerging angle θ_0 and to the velocity ratio v_0/u. Previous

experimental results (Palazzi et al., 2001) confirmed the validity of eq. (9). A generalization of previous equation can be obtained in the form: $k_{0,u} = k_0 \frac{v_0 - u}{v_0}$ (23)

Experimental observations allowed characterizing the entrainment constant over the range 0< θ_0 <π/2 , according to the empirical relationship: $k = k_0 + 0.2\vartheta_0$ (24).

3. An important issue is the transition from the jet phase to the plume phase. As already remarked, during high velocity releases the dispersion mechanism modifies continuously as time proceeds, so that this behaviour requires different modelling approaches, essentially based on jet model in the first phase and on atmospheric dispersion model in the plume phase. According to Hoehne (release with $\theta_0 = \pi/2$), the plume phase starts when: $s^*_{P,\pi/2} = \frac{s_{P,\pi/2}}{\alpha} = \frac{s_{P,\pi/2}}{d_0 \frac{v_0}{u}\left(\frac{\rho_0}{\rho_a}\right)^{1/2}}$ (25).

The relative importance of the previous factors depends on the object of the quantitative risk assessment study, i.e., the evaluation of the risk connected to toxic or to flammable properties of the release. In order to develop a common, conservative framework, following assumptions were made, for any given starting jet angle θ_0 :

- starting of the plume phase when $s_p k = s_{p,\pi/2} k_{\pi/2}$ (26)
- validity of eqs. (22) and (23).

Under these hypotheses, by virtue of eq. (25), one can write:

$$s_p = 5 d_0 \frac{v_0}{u}\left(\frac{\rho_0}{\rho_a}\right)^{1/2} \frac{0.63}{k} = 3.15 \frac{d_0}{k}\frac{v_0}{u}\left(\frac{\rho_0}{\rho_a}\right)^{1/2} \quad (27)$$

3.1 Toxic release

A typical requirement is the prediction of the effectiveness of the atmospheric dispersion at some distance downwind the release, as in proximity of the source are generally available mitigation equipment e.g. water barrier, personal protective equipments etc. Gaussian dispersion is the most common method for estimating dispersion due to a release and well represents the random nature of turbulence, but its applicability is normally limited to predictions between 0.1 and 10 km. For its application, input requirements are a source emission term and the position of the point P (x_P , z_p) where the effective "plume phase" starts. From eq. (27) one can write:

$$\frac{s_P}{d_0} = 3.15 \frac{1}{k}\frac{v_0}{u}\left(\frac{\rho_0}{\rho_a}\right)^{1/2}$$ (28) and , considering eqs. (21), (18) and (19):

$$\frac{z_P}{d_0} = A\left[\ln\left(B_P + \sqrt{1 + B_P^2}\right) - b\right] \quad (29) \qquad \frac{x_P}{d_0} = A\left[\sqrt{1 + B_P^2} - \frac{1}{\sin\vartheta_0}\right] \quad (30)$$

$$B_P = \frac{1}{A}\frac{s_P}{d_0} + \cot g\vartheta_0 = 3.15 \frac{v_{r0}}{v_0 \sin\vartheta_0} + \cot g\vartheta_0 \quad (31)$$

A cautious estimate of the atmospheric dispersion downwind the point P can be easily obtained by applying a point source gaussian dispersion model, with origin in P. A more realistic description can be obtained by considering the starting dilution of the release, which on the basis of eqs. (20), (22) and (27) is: $c_{a,P} = 0.63 \frac{M_a}{M_0} \frac{u}{v_{r0}}$ (32)

and introducing the concept of a virtual point source, located upwind and such that if a release were originated at the virtual source, it would disperse and match the concentration in P.

3.2 Flammable release

The jet phase, during which the jet entrains ambient air due to shear, grows in size and dilutes, is described by the above-mentioned eqs. (13), (14) and (15), using $k=k_0$ and $c_a = 2\bar{c}$. The most hazardous situation is connected to the maximum value of X_P, i.e., $\theta_0 = 0$. In this particular condition, it results:

$$c_{a,P} = 2 \frac{M_a}{M_0} \frac{1}{k_0} \frac{v_0}{v_0 - u} \frac{d_0}{x} \left(\frac{\rho_0}{\rho_a} \right)^{172} \quad (33)$$

and, at the beginning of the plume phase, eq. (32) applies. A typical requirement is to determine the value of the velocity ratio v_0/u corresponding to the attainment of LFL before reaching the plume phase, i.e. corresponding to the condition: $C_{a,P} < C_L$ and, therefore: $0.63 \frac{M_a}{M_0} \frac{u}{v_0 - u} \leq c_L$. The corresponding "plume velocity ratio" is found using: $\left(\frac{v_0}{u} \right)_P \geq 1 + \frac{0.63}{c_L} \frac{M_a}{> M_0}$ (34). Considering, as an applicative example, two jet releases of methane and n-heptane, the resulting $\left(\frac{v_0}{u} \right)_P$ are, respectively, 23 and 16. Again, these results are in good agreement with Hoehne, 1970, who reported that in the lower part of the range $8 \leq v_0/u \leq 110$, the release exhibits typical plume phase characteristics, with predominance of dilution by normal atmospheric turbulence.

Nomenclature

c axial concentration of the jet, v/v	T temperature, K
d jet diameter, m	M molar mass, kg $kmol^{-1}$
d_0 vent diameter, m	θ_0 jet emerging angle, rad
s length of the arc of the jet axis, m	u wind speed, ms^{-1}
x downwind coordinate on the jet axis, m	v_0 release velocity, m s^{-1}
z vertical coordinate on the jet axis, m	ρ_0 release density, kg m^{-3}
m mass flow rate, kg s^{-1}	ρ_a air density, kg m^{-3}

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