## MODELLING TWO-PHASE JETS FOR HAZARD ANALYSIS

#### D.M. WEBBER

UKAEA, Safety and Reliability Directorate Wigshaw Lane, Culcheth, Warrington WA3 4NE (Great Britain)

and

J.S. KUKKONEN

Finnish Meteorological Institute, Air Quality Department Sahaajankatu 22E, SF-00810 Helsinki (Finland)

(Received January 10, 1989; accepted in revised form February 2, 1990)

#### Summary

Hazard analysis of storage or transport of pressurised chemicals requires mathematical models of the behaviour of two-phase jets. In the past different models have highlighted different aspects of the problem. Here we shall review the most important factors in modelling two-phase jets, illustrating the problems with a simple analytical model and with results from the computer code TRAUMA. Among the most important factors to be modelled are gravitational spreading, deposition of liquid, ambient air flow and 'transition' to dense gas dispersion.

#### **1. Introduction**

Reliable computational methods for estimating possible accidental release rates and atmospheric dispersion of hazardous substances are needed in hazard analysis of many types of industrial installations. Many hazardous gases are stored in liquid form in pressurised containers. Modelling the (generally) twophase release, which will occur in the event of an accidental breach of the container or pipe work, is an essential part of the total dispersion analysis. However, very few comprehensive source term models have been developed. In this paper, the source term estimation methods of continuous pressurised releases are discussed. However, phenomena inside vessels, such as pipe flow are not addressed here.

The main foundations for our considerations here were laid by Wheatley [1-3], who derived a model of a two-phase ammonia jet. This model includes the thermodynamic aspects of liquid and gaseous ammonia interacting with atmospheric water vapour, but neglects wind and gravitational effects on the jet and its interaction with any solid surfaces. The two-phase mixture is treated simply by assuming either that the liquid is all deposited in the early stages, or

that it moves coherently with the gaseous component of the jet. The model forms the basis for a computer code TRAUMA which has since been generalised to apply to substances other than ammonia.

Gravitational and wind effects on a dense, gaseous plume have been considered by Ooms and co-workers (e.g. Li et al. [4], Ooms et al. [5]). This work is very much complementary to that of Wheatley in that it models these effects in detail, but does not consider thermodynamic two-phase effects. Fauske and Epstein [6] have presented results based on a model very similar to that of Wheatley, and Havens et al. [7] have written a computerised model based on that of Ooms et al. A simple model showing how a release oriented in the downwind direction may evolve from pipe-flow to a jet to a cloud has been given by Kukkonen [8] (see also Winter et al. [9]). More detailed work on aerosol effects has been presented by Kukkonen et al. [10].

The above works, all concentrate on certain aspects of a dense jet and neglect others; they all make assumptions about what are the most important effects in various given situations. What appears to be lacking is a comprehensive, detailed model which considers all the relevant physical phenomena inherent in a fully two-phase jet in any direction relative to the wind and gravity vectors, evolving from the source to a point where the concentration is low enough to be harmless.

The question arises whether a model of such complexity is necessary. Our principal aim here is to examine the assumptions of previous models and investigate the problems inherent in them. We shall illustrate the problems in two ways: by means of a simple analytic model, and by looking at some results from the more complex computerised model TRAUMA. The analytic approach is simplistic and at first sight may seem to have little to do with two-phase dynamics. However, with suitable interpretation it gives an understanding of what are likely to be the most important physical phenomena. The conclusions from the analytic model are backed up strongly by the results from the genuinely two-phase model TRAUMA. This gives us confident estimates of the relative significance of different factors, and points the way for further model development.

#### 2. A simple analytic jet model

## 2.1 Introduction

Before examining the results of detailed models, let us reduce jet modelling to its barest essentials and see what can be learned from analytic solutions of very simple models. This will provide a context in which to interpret the results of more sophisticated models, and indicate in what areas a more detailed approach is necessary.

## 2.2 The model

We can construct the simplest possible model by ignoring the flashing depressurisation region and starting from where the jet has essentially reached ambient pressure. Let us also for the moment assume that a momentum-dominated jet is just what it says, and ignore all meteorological, gravitational, chemical, and thermodynamic effects (including phase changes in particular). The resultant model is entirely one of mass, momentum, and species conservation, appropriate to a gaseous jet or to a two-phase jet in which the liquid content is an atomised spray which is assumed not to vaporise. (This latter case may not be exactly realisable but it will give an idea of the effect of having a very dense jet.)

The equations for this simplest of all possible jet models are:

$$\frac{\mathrm{d}}{\mathrm{d}x}(CuA) = 0 \tag{1}$$

$$\frac{d}{dx}(\phi uA) = 2\pi R u_{\rm E} \tag{2}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}(\phi u^2 A) = 0 \tag{3}$$

where C is the contaminant concentration,  $\phi$  is the jet density divided by that of the ambient air, A is the jet's cross-sectional area (which is assumed circular of radius R), u is the velocity of the jet, which is in direction x, and  $u_{\rm E}$  is an entrainment velocity for which various possible models can be explored.

To complete the system of equations we need the geometrical relation

$$A = \pi R^2, \tag{4}$$

an 'equation of state'. and an entrainment model for  $u_{\rm E}$ . The two simplest possibilities for the equation of state are (a) that the contaminant has the same density as air,

$$\phi = 1 \tag{5a}$$

and (b) that the jet is an isothermal mixture of air and contaminant. In this case the concentration (in suitable units) is

$$C = \phi - 1 \tag{5b}$$

We shall look at entrainment models of the form

$$u_{\rm E} = \alpha u \tag{6a}$$

and

$$u_{\rm E} = \alpha \phi^{1/2} u \tag{6b}$$

where  $\alpha$  is an entrainment coefficient. These are the Morton-Taylor-Turner

and Ricou-Spalding [11] models discussed in detail by Wheatley [1]. These are identical in case (a), but differ somewhat in case (b). Note that  $\phi$  is the only dimensionless field in this simple model and that in principle any function of it could appear in the entrainment model. The two models above, however, will serve to illustrate its significance. We can anticipate that  $\phi$  will tend to 1 downstream and that differences will only be apparent within some distance of the source.

We shall present analytic solutions appropriate to both of these entrainment models.

One of the constants of integration in the solution of the equations will be essentially a choice of origin for x. For convenience we shall choose x=0 to be the (unphysical) singular point where A=0, and other fields may tend to infinity.

Note that this choice of origin and the structure of the equations mean that  $\alpha$  and x can only appear in the solution in the combination  $(\alpha x)$  and not separately; the size of the entrainment coefficient simply determines how rapidly the jet evolves as one goes downstream. The other constants of integration will be the conserved contaminant (or buoyancy) flux and the conserved momentum flux implied by eqns. (1) and (3).

#### 2.3 Solution for a jet of ambient density

The solution for case (a) with ambient density is:

$$R = 2\alpha x \tag{7}$$

$$u = U \cdot L[2\alpha x] \tag{8}$$

$$C = L/[2\alpha x] \tag{9}$$

where the constant U and L are velocity and length scales which are determined by conditions at the source. They are related to conserved momentum and contaminant fluxes (see below).

This is the familiar picture of a conical jet with half angle  $\beta$  given by

$$\tan\beta = 2\alpha \tag{10}$$

## 2.4 Solution for a dense jet

The solutions for the dense jet (5b) for entrainment models (6a,b) are mathematically slightly more complicated but physically similar. The conserved fluxes are the integrals of (1) and (3):

$$(\phi - 1)uA = B \tag{11}$$

$$\phi u^2 A = f \tag{12}$$

The constants B and f are buoyancy and momentum flux. We shall also define constants U and L by

$$U=f/B \tag{13}$$

$$L^2 = B^2 / \pi f \tag{14}$$

Here again L and U are the length and velocity scales of the jet, now clearly related to source fluxes (although, for reasons given above,  $L/2\alpha$  will give a better physical estimate for the downwind evolution length scale). The significance of these scales can best be appreciated by writing the above conservation laws as

$$R(\phi-1)/\sqrt{\phi} = L \tag{15}$$

$$u\phi/(\phi-1) = U \tag{16}$$

For an initially dense, two phase jet L can therefore be rather larger than the radius of the jet after the flashing depressurisation phase, and U will be close to the value of u at this point. For a jet which is not dense in the early stages L may be rather smaller than the radius at this point, and U will be larger than the actual jet velocity.

## 2.4.1 The first entrainment model

For entrainment model (6a) the solution can be written in parametric form as

$$q(1+q^2)^{1/2} + \ln[q+(1+q^2)^{1/2}] = 2\alpha x/L$$
(17)

$$p^2 = (1+q^2)^{-1} \tag{18}$$

where the dimensionless variables p, and q are defined by

$$p^2 = u/U \tag{19}$$

$$q^2 = (Au)/(\pi L^2 U) \tag{20}$$

and therefore

$$R = L(q/p) \tag{21}$$

$$A = [\pi L^2] (q/p)^2$$
(22)

$$\phi - 1 = 1/q^2 \tag{23}$$

$$\phi = 1/(pq)^2 \tag{24}$$

## 2.4.2 The second entrainment model

The model with the alternative entrainment relation (6b) is very similar. This case yields an explicit solution:

$$R = (2\alpha x) \left[ 1 + L/(2\alpha x) \right]^{1/2}$$
(25)

$$u = U \cdot [L/(2\alpha x)] [1 + L/(2\alpha x)]^{-1}$$
(26)

$$\phi = 1 + L/(2\alpha \mathbf{x}) \tag{27}$$

The above solutions for each of the entrainment models are illustrated below in Fig. 1.



Fig. 1(a). Results of the analytic models for dimensionless jet radius against dimensionless downstream distance.  $-u_{\rm E} = \alpha u$  and  $- - u_{\rm E} = \alpha u (\rho/\rho_{\rm a})^{1/2}$ .

Fig. 1(b). Results of the analytic models for dimensionless axial velocity against dimensionless downstream distance.  $-u_{\rm E} = \alpha u$  and  $- - u_{\rm E} = \alpha u (\rho/\rho_{\rm a})^{1/2}$ .

Fig. 1(c). Results of the analytic models for relative density difference against dimensionless downstream distance.  $-u_{\rm E} = \alpha u$  and  $- - u_{\rm E} = \alpha u (\rho/\rho_{\rm a})^{1/2}$ .

Fig. 1(d). Results of the analytic models for Richardson number  $(Ri=g(\phi-1)R/u^2)$  against dimensionless downstream distance. The singularity at x=0 is not in the physical region.  $u_a = \alpha u$  and  $- - u_E = \alpha u (\rho/\rho_a)^{1/2}$ .

2.5 Asymptotic downstream behaviour

In both of the above cases, sufficiently far down stream (where  $x \gg L/2\alpha$ ) the solution becomes approximately

$$R \rightarrow 2\alpha x$$
 (28)

$$u \to U \cdot L/(2\alpha x) \tag{29}$$

$$\phi \rightarrow [1 + L/(2\alpha x)] \tag{30}$$

and therefore both of the models tend asymptotically to that of Section 2.3.

## 2.6 Gravity effects

We can estimate at what point the neglect of gravity is a severe omission by considering a bulk Richardson number:

$$Ri = [g(\phi - 1)R]/u^2$$
(31)

The behaviour of this is also plotted in Fig. 1. Interestingly the velocity  $Ug = [g(\phi-1)R]^{1/2}$  which is characteristic of gravity effects is asymptotically constant (tending to  $[gL]^{1/2}$ ) downstream, and Ri therefore increases as  $u^2$  decreases. Large values of Ri as  $x \to 0$  are to do with the unphysical singularity in the density field at that point and will therefore be irrelevant to the physical region  $x > x_0$ . At large x then

$$Ri \to [gL/U^2] \cdot (2\alpha x/L)^2 \tag{32}$$

Note that this indefinite increase in Ri is a consequence of zero wind speed. The distance scale over which gravity effects become important can best be estimated by comparing the gravitational velocity scale  $U_g$  with  $u \cdot \tan \beta = 2\alpha u$ , which is an estimate of the transverse fluid velocity in the jet. That is to say that the relevant estimate of the Richardson number defined above is  $(2\alpha)^2$ , and the relevant distance scale is

$$L_{\rm g} = LU/(gL)^{1/2} \tag{33}$$

For an elevated jet  $L_g$  indicates the distance over which gravity will cause the jet to bend significantly. For a jet in contact with the ground it gives an estimate of where transverse slumping may become important and where stable stratification may be an important consideration in the entrainment process.

## 2.7 Ambient air flow

If there is an ambient wind of speed  $u_a$  (which for the moment we shall consider to be in the same direction as the jet) then the above model can only be a reasonable approximation while  $u \gg u_a$ . That is for  $x \ll L_a$  where  $L_a$  is the distance at which u reaches  $u_a$ . This is given by

$$L_{\rm a} = L[U/(2\alpha u_{\rm a})] \tag{34}$$

The ratio

$$L_{\rm a}/L_{\rm g} = [gL]^{1/2}/[2\alpha u_{\rm a}]$$
(35)

can be used as an estimate of the importance of gravity effects in the region where momentum is important. For a sufficiently large jet in a sufficiently calm atmosphere (i.e. with  $L_a/L_g>1$ ), then gravity effects will become important before the jet has lost its momentum. The existence of this possibility means that one cannot always divide jet problems simply into a momentum-dominated phase followed by a wind-advected dense gas dispersion phase.

#### 2.8 Liquid deposition

Let us now examine the possible effects of liquid drop deposition in the above models. We can consider the two extreme cases where either all liquid falls out close to the source or where none falls out at all. These cases will just correspond to different values of the buoyancy and momentum fluxes B and f in the model.

Suppose, if no deposition is assumed, that the fields take the values  $\phi_{n0}$ ,  $u_0$ ,  $A_0$  at some point  $x_0$  near the source. We shall assume that liquid drop deposition affects only the density and leaves the velocity and cross-section unaffected. The source parameters, if complete deposition is assumed, are therefore  $\phi_{d0}$ ,  $u_0$  and  $A_0$ , with  $\phi_{d0} < \phi_{n0}$ .

From eqns. (11)-(14) we can relate the various constants for the two cases:

$$U_{\rm d}/U_{\rm n} = \left[\phi_{\rm d0}(\phi_{\rm n0} - 1)\right] / \left[\phi_{\rm n0}(\phi_{\rm d0} - 1)\right]$$
(36)

$$L_{\rm d}/L_{\rm n} = \left[ \left( \phi_{\rm d0} - 1 \right) \sqrt{\phi_{\rm n0}} \right] / \left[ \left( \phi_{\rm n0} - 1 \right) \sqrt{\phi_{\rm d0}} \right]$$
(37)

This comparison together with the asymptotic state of the jet given by eqns. (28)-(30) gives an estimate of the difference (at a given downstream position) which might be made by deposition near the source. In this approximation the geometry of the jet r(x) is unaffected, but the velocity is reduced by deposition by the factor in eqn. (36). Far downstream the density is close to that of the ambient air but (significantly for gravity effects) the concentration and relative density difference ( $\phi-1$ ) are reduced by the factor in eqn. (37) if there is deposition.

The length scale in eqn. (34) over which momentum effects decrease is reduced in the case of deposition by the factor (36) but the length scale in eqn. (33) over which gravity effect become significant is increased by a factor

$$[\phi_{\rm d0}/\phi_{\rm n0}]^{3/4} [(\phi_{\rm n0}-1)/(\phi_{\rm d0}-1)]^{1/2}$$

Deposition can therefore make a difference to the relative importance of these phenomena. The postponement of the gravity effects, including both lateral spreading and suppression of entrainment, may be as important a consequence of liquid deposition as is the more direct dilution effect.

## 3. Numerical results and discussion

## 3.1 Introduction

Having looked at a simplified, analytically tractable model, we shall now examine some results from the computer code TRAUMA which was developed by Wheatley [1-3] to model the behaviour of ammonia jets. The model considers the behaviour upstream of the aperture in the container and the flashing depressurisation region as well as the isobaric jet discussed above. The thermodynamic behaviour of two-phase ammonia is fully represented, as is its interaction with atmospheric water vapour. More recently, this model has been generalised to apply to other substances.

The TRAUMA results used for this study were obtained for chlorine and ammonia releases at 20°C and 0°C, assuming total deposition or none, using both entrainment models, and for both 100% relative humidity and dry ambient air.

Where comparison is made with the simplified model of Section 2, we extract parameters from TRAUMA at an "effective source" after the jet has reached ambient pressure and, where appropriate, after deposition has occurred.

#### 3.2 Sensitivity to entrainment model

TRAUMA can use either of the two entrainment models of Section 2, which derive from Morton, Taylor and Turner [12] and Ricou and Spalding [11]. These models were derived for elevated, isothermal, gaseous, jets in quiescent air. One of the principal assumptions inherent to them is that the turbulence generated by the discharge dominates that in the ambient air.

As we have seen the entrainment formulae differ by a factor  $\phi^{1/2}$ , where  $\phi$  is the jet to air density ratio. In principle any function of  $\phi$  could be introduced into the entrainment model without invalidating the simple dimensional arguments upon which such models are based. The two models considered do, however, give some idea of the dependence on this factor. The largest differences between model predictions are given in cases with considerable jet density (which are usually cases with low jet temperature and with significant airborne liquid fraction). The Ricou–Spalding formula gives a somewhat higher entrainment rate (for the same  $\alpha$ ) when the jet density is larger than ambient air density, but the difference is reduced, as expected, as one goes downstream.

The difference between the two models is higher for substances with a large latent heat of evaporation (such as ammonia), as the jet temperature may be lower in that case. A high value of relative humidity (and a large mass of entrained air compared to the substance mass) decreases this difference, as the condensation of water vapour releases energy and heats up the jet.

We have looked at a number of examples using each model over a range of conditions and find that the relative difference in concentration values is typically no greater than 10% in regions of interest.

#### 3.3 Sensitivity to liquid deposition

The description for estimating deposition should include estimation of aerosol dynamics. A certain fraction of droplets will evaporate before gravitational settling takes place, and others may deposit on the ground. The problem is therefore one of estimating the competing processes of evaporation and settling. The magnitude of the jet-borne fraction depends in particular on container pressure and the physical and chemical properties of the substance, which determine the stability of the droplets in the flow field encountered.

In TRAUMA the stability of droplets is calculated by using a criterion derived from laboratory experiments on the break-up of liquid phase jets. The criterion compares the disintegrating forces due to the flow field to the restoring force of surface tension of the droplet. The gravitational settling velocity of the largest stable drop is then compared with the axial velocity of the jet. If the droplet 'trajectory' falls out of the jet, a total deposition of the liquid phase is assumed, otherwise, no deposition is assumed.

The aerosol considerations of TRAUMA are certainly oversimplified. In particular, the velocity scale used in calculating the drop Weber number is that corresponding to the axial velocity after the initial depressurisation of the jet. This may be very high (predictions in the range 20 to 200 m/s are not uncommon) and therefore we find a fairly small 'largest stable drop' and a relatively small gravitational settling velocity. This procedure may underestimate the deposited mass fraction. On the other hand the effect of evaporation on reducing droplet size is neglected in TRAUMA, which tends to lead to an overestimate of the deposition rate.

We therefore believe it prudent to make estimates with and without deposition in any cases of practical interest. Accordingly we have studied this, in the context of TRAUMA, by comparing numerical results for a number of cases, where either a total deposition or no deposition was assumed to take place.

The most direct effect of deposition is the reduction of the mass of contaminant in the jet. If the vapour fraction after depressurisation is v, then the theoretical maximum deposited substance mass is 1-v of the total mass. The fraction v may be typically 20%, and therefore we might have a five-fold reduction of the substance mass flow rate due to deposition of liquid.

In the example calculations for chlorine and ammonia at ambient temperatures ranging from  $0^{\circ}$ C to  $20^{\circ}$ C, the concentration values at distances 50-100m were larger by a factor of 2 to 4 in the cases with no deposition compared to the values in the cases with total deposition. The results were very close to what is expected from the simple considerations of Section 2, despite some interesting thermodynamic differences. (The jet temperature is higher in the case with deposition, as the evaporation of substance liquid always cools the jet.)

## 3.4 Sensitivity to ambient air humidity

The effect of water vapour condensation on the temperature evolution of the jet is taken into account in the model TRAUMA. The effect of ambient air humidity is largest in the dispersion regime, where the mass of entrained air is large compared to the mass of substance and the relative humidity of ambient air is near its maximum value. Consequently, the effect of moisture is larger at large distances. In this analysis distances larger than 100 m were not considered, as the model does not take into account gravity spreading. The moisture effects are somewhat larger, if the ambient temperature is high, as in that case the absolute humidity (mass of water in the air per unit volume) is larger.

Example calculations were made for a number of different cases including pipe flow releases with a moderate mass flow rate as well as ruptures in container wall with a very large mass flow rate. Each of the cases was calculated assuming no ambient humidity and 100% relative humidity, respectively. The temperature of the jet is higher in the cases with humidity. The difference in the temperature values in the cases with humidity and no humidity was in the range 0 to 20°C. The corresponding difference in the density of the jet is less than 10%, as is the difference in concentration.

We must interpret the significance of these effects with care, as the jet code TRAUMA is only capable of giving the direct effects of thermodynamic changes on the jet itself. The difference in density, caused by condensation of atmospheric moisture may affect the magnitude of gravitational effects (cloud spreading and entrainment suppression) downstream. This latter effect is not taken into account in the model calculations.

The enthalpy change in forming the water solution for ammonia is also taken into account (Wheatley, 1987a) but for most substances which do not interact with water to form distinct chemical species, the solution enthalpy is negligible. Ammonia and hydrogen fluoride are two notable exceptions; they do not form distinct chemical species (e.g.  $NH_3 + H_2O \rightleftharpoons (NH_4)^+ + (OH)^-$ ) but their enthalpy of solution is significant. The formation of a solution is an exothermic process.

The effect of the solution enthalpy for ammonia was also studied numerically. The maximum amount of heat is released in this process in the cases where the mass of substance in liquid form and the mass of water are largest. A number of cases were calculated, alternatively taking into account the solution enthalpy and neglecting it. In all the calculated cases the difference in the concentration values (with solution enthalpy and without it) was less than 1%.

#### 3.5 Sensitivity to transition criterion

The question of when a jet becomes a cloud is not entirely straightforward, as discussed in Section 2. A jet is essentially defined as a flow where momentum is the predominant phenomenon determining the flow. One often therefore encounters the idea that the jet ends when its velocity roughly matches that of the ambient flow. However, as we have seen, the effects of gravity may become important before the momentum of the jet is negligible (relative to the ambient flow). Furthermore the jet may behave in an un-jet-like way if it encounters a solid surface. Even a horizontal neutrally buoyant jet will encounter the ground at some point unless it is released high above the ground.

To back up the conclusions of Section 2 with some concrete examples we have looked at the consequences of assuming different transition criteria in TRAUMA. The possibilities we considered were:

- (i) comparing the advection velocity of the jet and the wind velocity;
- (ii) comparing energy scales of gravitational settling and momentum driven flow;
- (iii) comparing lateral spreading velocities due to gravity spreading and momentum driven flow.

A number of example calculations were made by using these three criteria, and we shall present the results here in the context of the analysis given in Section 2.

Calculations in TRAUMA are terminated when the jet reaches a prescribed wind velocity (criterion (i)). This is often the last of the criteria to be satisfied.

To relate the results of TRAUMA to the model above, we extracted the jet area, density, and velocity at a point immediately after the jet had reached ambient pressure, and, where appropriate, after deposition had been assumed to occur. The value of *B*, *f*, *L*, *U*,  $L_g$  and  $L_a$  obtained from these are given for some typical runs in Table 1.  $L_a$  is based on a wind velocity at the yet height of 5 m/s, and  $L_g/2\alpha$  is given with  $\alpha = 0.08$  (see Wheatley [1]).

#### TABLE 1

Parameters	from some of	the	TRAUMA	runsª	described	in	Section	3
1 at ameters	from some or	une	IRAUMA	runs	described	111	Section	•

R	un	Den- sity ratio Ø	Veloc- ity u	Area A	Radius R	Buoy- ancy flux B	Momen- tum flux f	Veloc- ity scale U	Length scale L	Grav- ity scale L <sub>g</sub>	$L_{\rm g}/2lpha$	Ambient momen- tum length- scale $L_{a}$
1	Cl <sub>2</sub> 20°C	6.99	68.0	0.0307	0.0988	12.5	992.0	79.4	0.224	12.0	75.0	22.2
2	$Cl_2 20^{\circ}Cd$	2.64	68.0	0.0138	0.0663	1.54	168.0	110.0	0.0669	9.08	56.8	9.2
3	Cl <sub>2</sub> 0°C	7.53	50.0	0.00809	0.0507	2.63	151.0	57.5	0.121	6.39	39.9	8.7
4	$Cl_2  0^{\circ}C d$	2.462	50.0	0.00266	0.0291	0.194	16.3	84.0	0.0271	4.41	27.6	2.85
5	$NH_30^{\circ}C$	4.052	103.0	0.00379	0.0348	1.196	164.0	137.0	0.0527	10.0	62.8	9.0

<sup>a</sup>On the left hand side of the table the released substance, and liquid storage temperature are given. The symbol "d" shows where complete liquid deposition was assumed. The density, velocity, and jet radius were taken at the point after the flashing region and where the jet has reached ambient pressure.

The units for u, A, R, B, f and the various scales are SI. Their dimensions are given in the index of notation.

The analysis of Section 2 indicates transition points according to the various criteria to be of order

(i)  $L_{\rm a}$ ; (ii)  $L_{\rm a}/2\alpha$ ; (iii)  $L_{\rm g}$ 

For those situations considered in Table 1 where no significant deposition is assumed,  $L_{\rm a}$  is of order  $L_{\rm g}$  or larger, confirming that gravitational effects will be expected to become important before momentum effects become negligible. For air speeds lower than 5 m/s this effect will be more prominent still.

Examining the results of TRAUMA in detail, we find that transition distances obtained by applying each criterion are of the order of, but a little greater than, the respective length scales. Typically the transition distances given by criterion (i) are 30 to 50 m depending on the wind velocity, and the transition distances given by criterion (ii) are approximately 40 to 60 m. However, the transition distance given by the criterion (iii) is smaller, approximately 6 to 10 m.

The main conclusion of these calculations is that gravity effects may indeed be significant at small distances, as was concluded in Section 2 from the general length scales of the problem.

The main part of the fluid dynamics of present jet models is based on experiments on 'airborne' jets (jets which do not touch the ground). The jet evolution may be significantly changed, when we have a high-density jet dispersing near ground level. In particular, the lateral spreading velocity of such jets will most likely be substantially larger than predicted by currently available models.

#### 4. Conclusions

One of the main objectives of this study has been to provide information on the importance of different factors to get a firm basis for further model development. The results derived from the analytic calculations and sensitivity analyses are in some cases complementary, but also lend mutual support. The most important factors for future modelling efforts are gravitational spreading, deposition of substance liquid fraction, ambient wind and the transition to dense gas dispersion.

The set of jet equations which we have examined for species, mass, and momentum conservation can be solved entirely analytically for both Ricou-Spalding and Morton-Taylor-Turner entrainment models. Despite the manifest simplicity of the model, these analytic results give very useful insight on the effect on the jet evolution of entrainment models, gravity, ambient air flow, and liquid deposition. In particular, the analytic model gives explicit estimates of length scales over which gravity and wind effects will be significant. These are supported in the presence of more complex thermodynamic effects by the code TRAUMA.

The sensitivity analyses have shown that, the effect of different entrainment models and the effects of water vapour do not have larger direct effect than about 10% each in the concentration values. The enthalpy change in forming the water solution appears only to have a very small effect on the concentration, even for substances with a high enthalpy of solution. However, a proper account of gravity effects in the jet and the subsequent 'cloud' dispersion phase will emphasize the significance of these effects.

Further, the sensitivity analyses have shown that liquid deposition may cause a direct decrease in concentration by a factor of 2 to 4 in typical conditions.

It has also been shown that the choice of transition criterion to a heavy gas dispersion model may have a substantial effect on predictions. Analytic and numerical calculations have shown the existence of a region where gravity effects have become significant, but where jet momentum effects have not decayed. This has important consequences for the way in which one models the transition from jet to cloud. Gravitational effects may be substantial even at small distances from the source.

The significant transition may in fact be where the jet makes contact with the ground. Upstream of this point momentum will be important and gravity effects will possibly bend the jet trajectory. Downstream of this point a cloud must be modelled with momentum, but gravity effects cause lateral spread and suppression of entrainment, as air can no longer be entrained from below. Ground friction will also be important in this regime.

Jet experiments on hazardous cryogenic substances have been conducted in the Nevada dessert, most recently on hydrogen fluoride, reported by Blewitt et al. [13]. In these experiments a horizontal jet was set up close to the ground, which contained a large airborne liquid droplet injection. Concentration measurements were made some hundreds of metres downwind. The interaction of the jet with the ground is clearly significant in these experiments, requiring an understanding of both 'jet' and 'cloud' phenomena.

In order to conduct safe, small scale experiments, it may be preferable to create a jet by heating a less volatile, less hazardous substances (such as a Freon) to engineer the pressurised release conditions. It may be, in such a case, that the different thermodynamic situation affects the later gravitational behaviour of the jet, and any such experiment where gravity effects are considered may need to be interpreted with care.

Experiments on two-phase jets over a distance sufficient to exhibit the gravity behaviour would be very welcome. Horizontal jets are of special interest, as a starting point which may expose the shortcomings of current two-phase modelling. High-density (low-temperature) jets dispersing at ground level are important for obtaining information on the gravity spreading rates of jets.

#### Acknowledgement

The work presented here was funded in part by the Health and Safety Executive and in part by the Commission of the European Communities under the Major Technological Hazards programme.

# Notation

Α	Cross-section of jet	(L <sup>2</sup> )
B	Buoyancy flux (normalised)	$(L^3/t)$
C	Concentration (normalised)	(_)
f	Momentum flux (normalised)	$(L^{4}/t^{2})$
g	Gravitational acceleration	$(L/t^2)$
$\overline{L}$	Jet length scale	(L)
$L_{ m a}$	Length scale for momentum decay	(L)
$L_{g}$	Length scale for gravity effects	(L)
$p^{\check{2}}$	Dimensionless velocity variable	(-)
$\bar{q}^2$	Dimensionless volume flux variable	(-)
Ŕ	Jet radius	(L)
Ri	Bulk Richardson number	(_)
u	Axial jet velocity	(L/t)
U	Jet velocity scale	(L/t)
$u_{\rm a}$	Ambient air flow velocity	(L/t)
$U_{g}$	Velocity scale for gravity effects	(L/t)
x	Downstream distance	(L)
Greek		

# $\begin{array}{lll} \alpha & \text{Entrainment coefficient} & (-) \\ \beta & \text{Jet half angle} & (-) \\ \phi & \text{Jet density divided by air density} & (-) \\ \rho_{a} & \text{Ambient air density} & (M/L^{3}) \\ \rho & \text{Jet density} & (M/L^{3}) \end{array}$

## Subscripts

- 0 initial value
- n with no liquid deposition
- d with total liquid deposition

## References

- 1 C.J. Wheatley, Discharge of liquid ammonia to moist atmospheres Survey of experimental data and model for estimating initial conditions for dispersion calculations, UKAEA Report SRD/HSE/R410, London, 1987.
- 2 C.J. Wheatley, A user's guide to TRAUMA A computer code for assessing the consequences of accidental two-phase releases of  $NH_3$  into moist air, UKAEA Report SRD/HSE R394, London, 1987.
- 3 C.J. Wheatley, A theoretical study of  $NH_3$  concentrations in moist air arising from accidental releases of liquefied  $NH_3$ , using the computer code TRAUMA UKAEA Report SRD R393, London, 1987.

- 4 Xiao-Yun Li, H. Leijdens and G. Ooms, An experimental verification of a theoretical model for the dispersion of a stack plume heavier than air, Atmos. Environ., 20 (1986) 1087-1094.
- 5 G. Ooms, A.P. Mahieu and F. Zelis, The plume path of vent gases heavier than air, In: C.H. Buschman, First Int. Symp. Loss Prevention and Safety Promotion in the Process Industries, The Hague, 1974, Elsevier, Amsterdam, p. 211.
- 6 H.K. Fauske and M. Epstein, Source term considerations in connection with chemical accidents and vapor cloud modeling, In: J. Woodward (Ed.), Proc. Int. Conf. Vapor Cloud Modeling, Am. Inst. Chem. Eng., New York, NY, 1987, p. 251.
- 7 J.A. Havens, T.O. Spicer and D.E. Layland, A dispersion model for elevated dense gas jet releases, ibid, p. 568.
- 8 J. Kukkonen, Modelling of discharges and atmospheric dispersion of toxic gases, Finnish Meteorological Institute: Publications on Air Quality No. 1, Helsinki, 1987.
- 9 S. Winter, K. Nyren and E. Karlsson, Uppkomst och utbredning av explosiva eller giftiga gasmolin, FOA Report E 40011, 1984.
- 10 J. Kukkonen, T.Vesala and M. Kulmala, The interdependence of evaporation and settling for airborne freely falling droplets, In: Proc. European Aerosol Conf., 30 Aug.-2 Sept. 1988. Lund, Sweden. J. Aerosol Sci., 20 (1989) 7-22.
- 11 F.P. Ricou and D.B. Spalding, Measurements of entrainment by axisymmetrical turbulent jets, J. Fluid Mech., 11(1961) 21-32.
- 12 B.R. Morton, G.I. Taylor and J.S. Turner, Turbulent gravitational convection from maintained and instantaneous sources, Proc. R. Soc., A234 (1956) 1-23.
- 13 D.N. Blewitt, J.F. Yohn, R.P. Koopman and T.C. Brown, Conduct of anhydrous hydrofluoric acid spill experiments, In: J. Woodward (Ed.), Proc. Int. Conf. Vapor Cloud Modeling, Am. Inst. Chem, Eng., New York, NY, 1987, p. 1.