

THE SIZE OF FLAMMABLE CLOUDS ARISING FROM CONTINUOUS RELEASES
INTO THE ATMOSPHERE - PART 2

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Earlier work on the fuel content of flammable clouds when dispersion is either momentum controlled or buoyancy controlled is extended here to atmospheric turbulence controlled dispersion. For all three cases the dependence of cloud size on mass rate of emission is discussed and estimates of the latter which have led to UVCE incidents are given for comparison. The effective initial conditions for dispersion from choked gas releases are also considered.

INTRODUCTION

The methods usually used at the present time to assess either the likelihood or the consequences of an unconfined vapour cloud explosion (UVCE) employ simple criteria or relationships. These are based either on the total quantity of fuel that may be released or the total quantity of vapour, plus an allowance for the fine spray, that would result from the release of a liquid fuel at a temperature above its atmospheric boiling point. Study of the limited data that is available regarding actual UVCE incidents has led to a suggested minimum quantity of fuel or vapour that must be released for there to be a significant likelihood of a UVCE occurring and to suggested factors for predicting the TNT equivalent of the resulting explosion from the same quantity (1).

It is clearly desirable to have a better understanding of the factors which determine whether a UVCE can occur and its worst consequences. One factor must be the size, and particularly the fuel content, of the cloud of flammable concentrations at the moment of ignition. For releases such as occur in emergency venting or in some kinds of plant failure, they can be of sufficient duration for a steady state to be achieved. It is

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then possible in some simple cases to derive relationships between the cloud size, the mass rate of release and parameters characteristic of the controlling mode of dispersion. In a previous paper (2) such relationships were derived for the cases where the dispersion was either momentum controlled (jet) or buoyancy controlled (plume).

In this paper the scope is extended to include the size of clouds where the dispersion is controlled by atmospheric turbulence and wind speed. The relationships derived for the three modes of dispersion are then compared, particularly their dependence on mass rate of release. Next by applying realistic limits to the dispersion characteristics, the range of cloud size for a particular rate of emission can be estimated. These ranges are compared with the data for those actual UVCE incidents where it has been possible to make an estimate of the rate of emission. Finally there is a discussion of the most appropriate assumption regarding the effective initial temperature of a gas release for predicting its subsequent dispersion when the release is a choked sonic one.

It perhaps should be emphasised that the terms cloud size and fuel content refer exclusively in this paper to the mass of fuel that is mixed with air within the flammable range of concentrations. There is confusion in much of the literature when it is not made clear whether reference is being made to the total quantity of fuel released, the total quantity that would be present as vapour (or vapour plus fine spray) or the proportion of the latter that would be present in flammable concentrations.

SIZE OF CLOUDS FORMED BY ATMOSPHERIC DISPERSION

For an emission which has no initial momentum or buoyancy dispersion will result from a combination of wind velocity and atmospheric turbulence. If the concentration of the emitted material in the horizontal and vertical cross wind directions conforms to a Gaussian distribution, then the concentration at any point (x, y, z) arising from a ground level emission at $(0, 0, 0)$, the x axis being coincident with the wind velocity, will be given by

$$X_{(x,y,z)} = \frac{\dot{m}_0}{\pi \sigma_y \sigma_z \bar{u}} e^{-\frac{y^2}{2\sigma_y^2}} e^{-\frac{z^2}{2\sigma_z^2}} \quad (1)$$

or, for a point at ground level on the downwind axis,

$$\chi_{(x,0,0)} = \frac{\dot{m}_0}{\pi \sigma_y \sigma_z \bar{u}} \quad (2)$$

Pasquill (3) designated six categories of atmospheric stability (or level of turbulent mixing) designated A to F in order of increasing stability, or decreasing turbulence. On the basis of his classification graphs showing the dependence of σ_y, σ_z and $\sigma_y \sigma_z$ on downwind distance have been produced for each stability category by Gifford (4) and Turner (5). It is possible to fit the data over the range 100 - 1000m downwind with equations of the type

$$\sigma_y \sigma_z = D x^f \quad (3)$$

A problem arises because the data mentioned is based on time average measurements of concentrations over periods of some minutes. Our interest here is in the shape and size of the instantaneous cloud at the moment of ignition; this will be longer and narrower corresponding to smaller values of $\sigma_y \sigma_z$ than are given in (5). The information available suggests that it is reasonable to assume that the ratio of peak to average concentrations at any point is 2.5. The values of $\sigma_y \sigma_z$ used have therefore been divided by 2.5 before fitting them to the equations (3). The resulting values of D and f then obtained for the various stability categories are given in Table 1.

TABLE 1 - Constants for predicting the values of $\sigma_y \sigma_z$ downwind for the various atmospheric stability categories

$$\sigma_y \sigma_z = D x^f \quad \text{m}^2$$

Stability category	D	f
A	3.06×10^{-3}	2.4
B	1.38×10^{-2}	1.9
C	8.9×10^{-3}	1.8
D	6.0×10^{-3}	1.7
E	3.88×10^{-3}	1.7
F	1.43×10^{-3}	1.7

By substituting equation (3) and the values of Table 1 into equation (1), and by assuming that the crosswind isopleths are semi-elliptical in shape, it is possible to integrate through the envelope of flammable concentrations and derive a relationship for the fuel content of the flammable cloud. This is :-

$$Q_{FL} = \left(\frac{1}{\pi D} \right)^{\frac{1}{f}} \left(\frac{f}{f+1} \right) \left(\frac{\dot{m}_e}{\bar{u}} \right)^{\frac{f+1}{f}} \left(\frac{1}{X_L^{\frac{1}{f}}} - \frac{1}{X_U^{\frac{1}{f}}} \right) \quad (4)$$

For neutral and stable atmospheres D - F, which are of most interest in large cloud formation, f has the value 1.7 and equation (4) reduces to

$$Q_{FL} = \frac{0.321}{D^{0.59}} \left(\frac{\dot{m}_e}{\bar{u}} \right)^{1.59} \left(\frac{1}{X_L^{0.59}} - \frac{1}{X_U^{0.59}} \right) \quad (5)$$

Under these circumstances the length of the cloud, the distance downwind from the point of emission to the point where the concentration falls to the lower flammable limit, is given by :-

$$x_L = 0.51 \left(\frac{\dot{m}_e}{D \bar{u} X_L} \right)^{0.59} \quad (6)$$

SUMMARY OF RELATIONSHIPS FOR ATMOSPHERIC, JET AND PLUME DISPERSION

The results of the preceding section, together with those of the previous paper, enable us to predict the steady state cloud size from simple vapour emissions for the following cases.

(i) Atmospheric dispersion of an emission assumed to have no initial momentum and no buoyancy

(ii) Jet dispersion in still air of an emission with initial momentum but no buoyancy

(iii) Plume dispersion in still air of an emission with initial upward buoyancy but no momentum.

While these simple models may be regarded as remote from real conditions, it is relevant to recall that the largest clouds will be formed when the fewest modes of dispersion are effective.

In cases (ii) and (iii) as in (i) there are well established relationships for the steady state distributions both of concentration of emitted material and of velocity. The concentrations at right angles to the principal axis (either jet or plume axis or wind direction) follow quite closely a Gaussian distribution. It is possible to integrate the concentrations through the flammable envelope with sufficient accuracy if certain simplifying assumptions are made. These are :

- a) That, in the case of atmospheric dispersion, the turbulence of the air is not affected by the release
- b) That, in the case of the jet, the average molecular weight of the mixture in the region of interest equals that of air
- c) That, in the case of a buoyant plume, the buoyancy flux remains constant on dilution

TABLE 2 - Comparison of equations for cloud size

Mode of dispersion	Equation for cloud size (fuel content) kg
Atmospheric	$Q_{FL} = \left(\frac{0.321}{D^{0.59}} \right) \left(\frac{\dot{m}_0^{1.59}}{\bar{u}^{1.59}} \right) \left(\frac{1}{X_L^{0.59}} - \frac{1}{X_U^{0.59}} \right)$
Jet	$Q_{FL} = (3.40 \rho_a^{1.5}) \left(\frac{\dot{m}_0^{1.5}}{\omega_0^{1.5}} \right) \left(\frac{1}{X_L^2} - \frac{1}{X_U^2} \right)$
Plume	$Q_{FL} = \left(\frac{1.45 T_0^{1.8}}{T_a^{1.8}} \right) \left(\frac{\rho_a^{0.6} \rho_0^{0.6} \dot{m}_0^{1.2}}{\Delta \rho_0^{0.6}} \right) \left(\frac{1}{X_L^{0.8}} - \frac{1}{X_U^{0.8}} \right)$

Table 2 compares equation (5) for atmospheric dispersion with similar equations derived in the previous paper for jet and plume dispersion; the latter have been modified to use the same variables as equation (5) where possible. It will be seen that in all cases the mass rate of emission \dot{m}_0 is a most important variable, the cloud size varying with \dot{m}_0 raised to a power ranging between 1.2 and 1.59. The flammability limits are also important, a large range predictably leading to large cloud size. The other important factors depend on the mode of dispersion, the following favouring large cloud size :-

A low wind velocity and a high stability (low D) in the case of atmospheric dispersion

A low velocity of emission in the case of a jet

A low initial density difference in the case of a plume.

RESULTS UNDER REALISTIC CONDITIONS

The dependence of cloud size on the rate of emission for each of the modes of dispersion is illustrated in Figure 1, a, b and c. In each case the scales are the same and the factor peculiar to each mode has been varied over what is regarded as the maximum realistic range. Thus, in Figure 1a which illustrates atmospheric dispersion for a hypothetical hydrocarbon with $\chi_L = 0.039$ and $\chi_U = 0.176$, category D stability with a wind velocity of 10 m/s represents very vigorous dispersion conditions which are unlikely to be exceeded. At the other extreme, category F stability with a wind velocity of 1 m/s represents the least effective atmospheric dispersion conditions that are likely to be met.

In Figure 1b illustrating jet dispersion for a typical lower paraffin, the higher velocity of emission used (250 m/s) is a near sonic velocity. The lower velocity chosen (25 m/s) is such that below this jet dispersion would be unlikely to be the controlling mechanism. It should be remembered that by the time the concentration on the axis had reached the upper flammable limit the velocity would have decreased by a factor of about 10.

In Figure 1c, illustrating plume dispersion, methane at 288°K has been chosen as the most positively buoyant material that one is likely to encounter, excluding hydrogen. At the other extreme ethylene at 288°K represents the limiting density

difference below which it is considered other modes of dispersion would predominate. It can be seen by comparing Figures 1b and 1c that the considerable acceleration and velocity produced by strongly buoyant materials such as methane even with no initial momentum will result in dispersion as effective as with a sonic jet.

The three sets of calculations have been compared in Table 3, where the ranges of emission rates to produce clouds with fuel contents of 1000 and 10000 kg are given. The former may be regarded as a size below which it is hardly conceivable that a UVCE could occur. The latter represents the largest cloud that could arise from a total effective vapour release of 15 tons; the latter figure has been suggested as a limit above which an installation should be regarded as offering a major explosion hazard (1).

Considering the differences in mechanisms and the inevitably somewhat arbitrary choice of limiting conditions the ranges of emission rates necessary to produce a given cloud size shown in Table 3 are surprisingly similar. In very round terms they indicate that a minimum emission rate of about 10 kg/s is required to form a 1000 kg cloud and about 50 kg/s for a 10000 kg cloud. Real UVCE hazards frequently involve the dispersion of heavy gases near the ground and it is unfortunate that the studies of such dispersion have not yet provided relationships for the distribution of concentration permitting equations for fuel content to be derived in this case.

TABLE 3 - Calculated rates of emission to produce clouds with fuel contents (Q_{FL}) of 1000 kg and 10000 kg

Mode of dispersion	Rates of emission to give	
	$Q_{FL} = 1000$ kg	$Q_{FL} = 10000$ kg
	kg/s	kg/s
Atmospheric dispersion	6 - 100	25 - 440
Jet	13 - 110	50 - 600
Plume	16 - 110	100 - 700

RATES OF EMISSION IN ACTUAL UVCE INCIDENTS

It is of interest to compare the actual rates of emission in incidents where UVCE's have occurred with the calculated ranges. Davenport (6) has compiled an exhaustive list of such incidents with references to the original sources of information. Only in relatively few cases can a comparison be made; in many cases there is not sufficient information on which to base an estimate of the rate of emission while in others the failure was of a catastrophic kind leading to a near instantaneous release.

Table 4 gives the rates for seven incidents where an estimate has been possible. In two of the cases, East St. Louis and Decatur, the rates are the estimated maximum ones calculated from the described size of the hole created and an assumed temperature and hence pressure of the rail tank contents. The estimated total rate of emission has been corrected where appropriate to give the rate at which vapour would flash off and the latter multiplied by two to allow for fine spray. The resulting figure is called the effective rate of emission.

It is considered that the figures presented in Table 4 do not conflict with the minimum rates of emission discussed earlier. Thus two, Port Hudson and Beek, fall in the range

TABLE 4 - Estimated effective rates of emission of fuel for actual UVCE incidents

Location	Material emitted	Estimated effective rate of emission kg/s
Port Hudson	C_3H_8	23
Beek	C_3H_6	30
Pernis	Hydrocarbons	100
Lake Charles	$i-C_4H_{10}$	180
East St. Louis	C_3H_6	400
Decatur	$i-C_4H_{10}$	660
Flixborough	C_6H_{12}	1030

between the absolute minimum 10 kg/s and the rate corresponding to the cloud size at which it is suggested that a UVCE hazard must be assumed, i.e. 50 kg/s, while the remainder are well in excess of the latter figure.

It has already been pointed out that the higher the wind velocity the greater the rate of emission necessary to give rise to a cloud of a given size. The information regarding wind velocities at the incidents listed in Table 4 shows that only in the cases of East St. Louis, Decatur and Flixborough did they exceed 2.5 m/s; thus the UVCE's resulting from the lower rates of emission coincided with low wind velocities as would be expected.

THE EFFECTIVE INITIAL CONDITIONS
FROM A CHOKED GAS RELEASE

In most cases where gas escaping from a failure in a pressure vessel or pipeline presents the risk of a UVCE, it will be at sonic velocity and at a pressure greater than atmospheric at the point where it emerges. While the mass rate of release and the gas temperature and pressure can be estimated, the latter do not represent the effective initial conditions for the dispersion of the gas in air. On emergence into the atmosphere the gas will expand radially to atmospheric pressure, maintaining sonic velocity. It will be colder than its original temperature but subsequently there will be an effective increase in temperature as the kinetic energy of the high velocity gas is reconverted to thermal energy during turbulent mixing with air. These processes are discussed below in relation to the choice of the most appropriate effective initial conditions for estimating entrainment and dispersion governed by momentum or buoyancy.

The overall energy balance between the gas inside the vessel or pipe (condition 0), as it emerges (condition 1) and after it has expanded to atmospheric pressure (condition 2) can be written

$$H_0 = H_1 + \frac{U_1^2}{2} = H_2 + \frac{U_2^2}{2} \quad (7)$$

Since

$$H = \frac{\gamma}{\gamma - 1} \frac{RT}{M_0} \quad (8)$$

$$\omega = \left(\frac{\gamma RT}{M_0} \right)^{\frac{1}{2}} \quad \text{for sonic velocity} \quad (9)$$

we have

$$\frac{RT_0}{M_0} \frac{\gamma}{\gamma-1} = \frac{RT_1}{M_0} \left\{ \frac{\gamma}{\gamma-1} + \frac{\gamma}{2} \right\} = \left\{ \frac{RT_2}{M_0} \frac{\gamma}{\gamma-1} + \frac{\gamma}{2} \right\} \quad (10)$$

or

$$T_2 = T_1 = T_0 \left(\frac{2}{\gamma+1} \right) \quad (11)$$

It follows from this that the temperature and velocity after radial expansion and before entrainment will be the same as on emergence but the temperature will be significantly lower than inside the vessel or pipe.

However, on mixing with air and deceleration this energy is reconverted into thermal energy quite rapidly so that the effective temperature is, in fact, higher. Thus, by applying the principles of conservation of momentum and energy to a momentum jet, it can be shown that the average temperature of the gas/air mixture at a stage where the gas has mixed with j times its mass of air is

$$T = \frac{T_2 b \left\{ \frac{\gamma-1}{2} \left(\frac{j}{1+j} \right) + 1 \right\} + T_a j}{b + j} \quad (12)$$

where b is the ratio of the specific heat of the gas per unit mass to that of air.

If there were no significant kinetic energy effects to take into account the corresponding relation would have been

$$T = \frac{T_2 b + T_a j}{b + j} \quad (13)$$

One can therefore define an effective temperature T_3 such that

$$T_3 = T_2 \left\{ \frac{\gamma-1}{2} \frac{j}{1+j} + 1 \right\} \quad (14)$$

which rapidly tends to $T_2 \left\{ \frac{\gamma+1}{2} \right\}$ as j increases. From this and equation (11) it follows that

$$T_3 \rightarrow T_2 \left\{ \frac{\gamma+1}{2} \right\} = T_0 \quad (15)$$

It therefore appears appropriate to use the original temperature T_0 and atmospheric pressure in conjunction with the sonic velocity at $T_1 = T_2$ as the effective initial conditions.

SYMBOLS USED

- b = ratio of specific heat per unit mass of gas emitted to that of air
- D = a constant
- f = a constant
- g = gravitational constant (m/s^2)
- H = enthalpy per unit mass (J/kg)
- j = mass of air mixed with unit mass of gas emitted
- M = molecular weight
- \dot{m} = mass flow rate (kg/s)
- Q_{FL} = quantity of fuel at concentrations within flammable limits (kg)
- R = gas constant (J/°K kg-mole)
- T = temperature (°K)

- \bar{u} = wind velocity (m/s)
 w = vertical or axial velocity (m/s)
 x = horizontal distance on wind axis (m)
 y = horizontal distance at right angles to wind axis (m)
 z = vertical distance (m)
 γ = gas specific heat ratio
 ρ = density (kg/m^3)
 $\Delta\rho = \rho_a - \rho$ = density difference (kg/m^3)
 σ = standard deviation of concentration distribution (m)
 χ = concentration of emitted material in air (kg/m^3)

Subscripts

- a = air
 o = original discharge
 L = lower flammable limit
 U = upper flammable limit
 $1,2,3$ = successive stages in emission and dispersion

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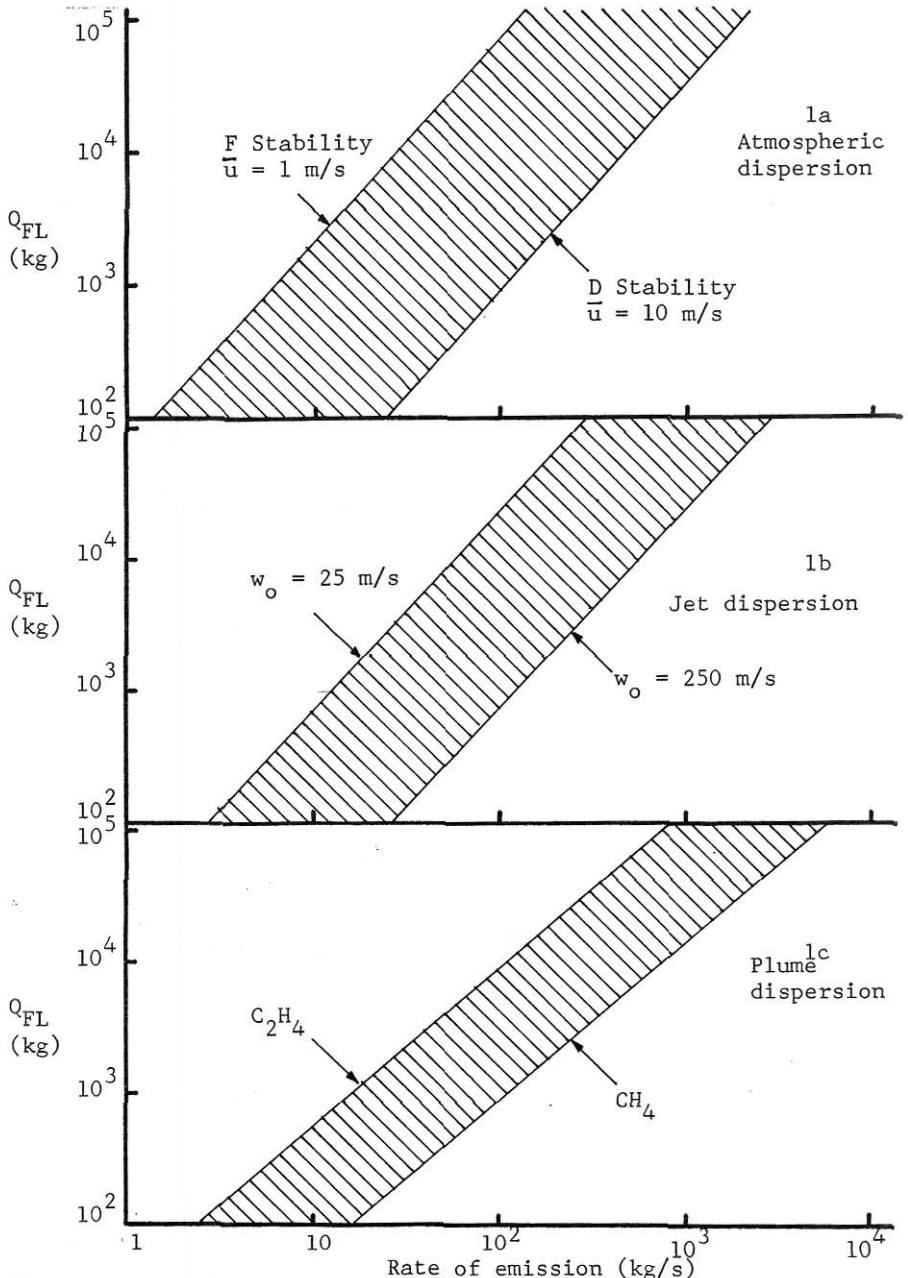


Figure 1 Dependence of cloud size on rate of emission