THE SIZE OF FLAMMABLE CLOUDS ARISING FROM CONTINUOUS RELEASES INTO THE ATMOSPHERE

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The relationships defining the axial length and concentration distribution in jets and plumes and the effect of atmospheric lapse rate are reviewed. Formulae for estimating the size of flammable clouds and the quantity of material between the flammability limits are given for continuous emissions under still air conditions, when the largest clouds will be formed. Some calculated results for emissions of low molecular weight hydrocarbons are reported.

INTRODUCTION

In assessing the possible consequences of an unconfined vapour cloud explosion that might result from plant failure or emergency venting, one step is the estimation of the size of the cloud of flammable concentrations and the quantity of material therein. In considering such situations, one has a particular, although not exclusive, interest in the "worst case" that can arise.

The purpose of this paper is to briefly review the relationships concerning the various modes of dilution of the release with air, to consider how they may be applied to calculate the size and content of the largest clouds that may arise and to illustrate the matter with the results of calculations for a selection of low molecular weight hydrocarbons. The largest clouds will arise when the fewest modes of dilution are operative, but it must be recognised that the largest cloud may not be the most readily ignited. Continuous releases only are considered and it will be seen that the times required for the realisation of a steady state can be very short.

There is a considerable literature on the dispersion and dilution of material released into the atmosphere. Much of this, however, is concerned with the occurrence of comparatively dilute concentrations at considerable distances and with cases where atmospheric conditions play a more important role in dilution than the characteristics of the discharge itself. The most useful general survey of dispersion of continuous releases known to the author is that of Long (1).

In this paper only the dispersion process and the size of the resulting cloud are discussed; the cause or nature of the release and the consequences of ignition are not considered. Approximate methods have to be used but are usually adequate in view of the many uncertainties in predicting explosion damage from plant failure.

REVIEW OF RELATIONSHIPS ASSOCIATED WITH MODES OF DISPERSION

Jets

To form clouds large enough to cause pressure damage on ignition, emissions of high mass flow rate will be required and the initial velocity is likely to be high, even sonic. Unless this velocity is very rapidly lost by, say, interaction with structures, the primary dilution mechanism will be entrainment of air into the jet because of its momentum. Such a jet will persist indefinitely unless buoyancy forces are present, or until it becomes negligible and unidentifiable with respect to atmospheric turbulence. The behaviour of such jets is well established (2). The relationship describing the dilution in space is :-

$$c_{z,r} = \frac{K_1 d_o}{z} \left(\frac{M_o T_a}{M_a T_o}\right)^{\frac{1}{2}} \left(\frac{\bar{M}}{M_o}\right) e^{-\left(\frac{K_2 r}{z}\right)^2} \tag{1}$$

where $c_{z,r}$ is the volume (or molar) fraction of the emitted material at an axial distance z and radial distance r from the effective point of emission. d_o is the effective diameter of the jet after it has expanded to atmospheric pressure but before any entrainment has occurred. For a vent this will be the diameter of the vent while for a plant failure it will be related to the effective "hole" size and the internal pressure. It will be seen that the size and shape of the cloud will, for a given molecular weight and temperature, depend only on d_o

Plumes

When the material emitted has a different density to that of the ambient air, arising from differences in molecular weight and/or temperature, the resulting positive or negative buoyancy forces will lead to acceleration and the resulting movement will also cause dilution by entrainment. In the extreme case of negligible initial velocity the emission will behave as a buoyant plume from the start. In the more usual case a jet will translate into a plume after a certain distance. If the jet is moving upwards and the buoyancy forces are negative, then there will be a reversal of direction of flow at this point. In true zero wind conditions the plume would be of annular section surrounding the jet. The behaviour of plumes is well established (3,4,5). The relationship describing the dilution in space is :-

$$c_{z,r} = \frac{K_3 \dot{v}_o^{\frac{2}{3}}}{z^{\frac{5}{3}} g^{\frac{1}{3}}} \left(\frac{M_a T_o}{M_a T_o - M_o T_a}\right)^{\frac{1}{3}} e^{-\left(\frac{K_4 r}{z}\right)^2} \tag{2}$$

Jet persistence

Studies of the distance to which a jet will persist before becoming a plume indicate that the change will occur at an axial distance from the point of emission determined by the original effective jet diameter and the appropriate internal Froude number, Fr (6,7), i.e.

$$z_{tr} = K_5 Fr d_o = \frac{K_5 \omega_o d_o}{(g' d_o)^{\frac{1}{2}}} \tag{3}$$

where

$$g' = g \frac{\Delta \rho}{\rho_a} = g \left(\frac{M_a T_o - M_o T_a}{M_a T_o} \right)$$

Effect of atmospheric stability

Three separate but related characteristics of the atmospheric conditions affect dispersion. The first is the degree of turbulence, and the second is mean wind velocity. The combined effect of these can be estimated using data for the standard deviation of concentration, in both horizontal and vertical directions, for various categories of atmospheric stability (8,9). The third is the lapse rate or vertical temperature profile. If this is anything other than the adiabatic lapse rate, found in neutral conditions, then there will be changing buoyancy effects with height. As already mentioned, the three factors are not independent of each other. Inversions in which temperatures increase with height, i.e. lapse rates considerably in excess of the adiabatic lapse rate, will occur more frequently in conditions of high stability (low level of turbulence) and low wind speed, i.e. the least effective conditions for dispersion by atmospheric turbulence.

While it may be considered self-evident that cloud size will be increased if one of the possible mechanisms of dispersion is not operative, there is experimental evidence which supports this conclusion. Studies of vertical jets in cross winds produced in wind tunnels have been carried out by Hoehne and Luce (10), Pratte and Baines (11), and Keffer and Baines (12). These investigations, and particularly (10), show that the axial distance to the lower limit of flammability, and the radial spread, for jets of a variety of hydrocarbons is greatest when the wind speed is zero. It therefore follows that the cloud will be greatest in size and content of flammable material under conditions of no wind; the important atmospheric characteristic will then be the lapse rate.

The parameter used will be G, given by

$$G = \frac{g}{T_a} \left(\frac{d T_a}{dz} + \Gamma \right) \tag{4}$$

where Γ is the adiabatic lapse rate (= 0.0098 C/m)

The effect of a stably stratified atmosphere, i.e. an atmosphere with a lapse rate greater than that of a neutral adiabatic atmosphere $(G > O)$ on the height to which a plume will rise has been determined (3). The equation for the maximum vertical rise is

$$z_{max} = \frac{K_6 \dot{V}_o^{\frac{1}{4}}}{G^{\frac{3}{8}}} \left(\frac{M_a T_o - M_o T_a}{M_a T_o} \right)^{\frac{1}{4}} \tag{5}$$

Turbulent flames

As turbulent momentum controlled flames are a particular example of a jet, it is interesting to compare their lengths with those of jets where no combustion occurs.

For momentum controlled flames the well known equation of Hawthorne et al (13) is used :-

$$z_F = \frac{5.3}{c_s}\left\{\frac{T_f}{\alpha T_o}\left[c_s + (1-c_s)\frac{M_a}{M_o}\right]\right\}^{\frac{1}{2}} \tag{6}$$

A similar comparison between buoyancy controlled flames and plumes is not appropriate since the former will always have considerable positive buoyancy whereas the plumes being considered here may have low and negative buoyancy.

METHODS AND ASSUMPTIONS USED IN ESTIMATES

In order to use the basic equations (1) and (2) for jet and plume, it is necessary to assign values to the constants K_1, K_2, K_3 and K_4. For estimating the dimensions of a flammable cloud it is the instantaneous rather than the time-mean values that are required. (1) recommends that the values giving the maximum spread are used, corresponding to the greatest value of k_1 ($=9$) and the smallest value of K_2 (= 2) found. However the two constants are not independent and it can be shown for a jet that, if the radial spread of velocity and concentration were the same, then $K_2 = \sqrt{2K_1}$. The values have been chosen on this basis. For the plume again the value recommended in (1) for K_3 has been taken and K_4 estimated, assuming that the K_4/K_3 ratio is the same as for the time mean values. The values used are :-

$$K_1 = 9 \qquad\qquad K_3 = 17$$

$$K_2 = 12.7 \qquad\qquad K_4 = 13$$

The height or axial distance from the source to a concentration level of interest, such as the lower flammability limit, can readily be calculated, knowing the characteristics of the discharge, from equations (1) and (2). The volume of the envelope between the upper and lower flammable limits, and the quantity of the material that will fall within these concentration limits in the steady state can be determined by integration of these equations. To simplify this integration in the case of equation (1), the assumption is made that $\tilde{M} = M_a$. The effect of this, for gases of lower molecular weight than air, will be to overestimate the axial distances at which the upper and lower limit concentrations are reached, the former more than the latter; the opposite will be true for gases of molecular weight greater than air. For most flammable gases, the effect on axial distance or quantity within the limits will be well under 20%.

With regard to plumes it should be noted that both the experimental studies and the theoretical analyses have been concerned with systems for which the buoyancy flux, F, remains constant on dilution. This is not always the case as it can be shown that

$$\frac{F_{\infty}}{F_o} = 1 + \frac{(1-m)(n-1)}{(L-n)} \qquad, \tag{7}$$

where $\qquad L = \frac{M_o}{M_a}, \qquad m = \frac{h_o}{h_a}, \text{ and } n = \frac{T_o}{T_a}.$

Thus the buoyancy flux will remain constant if m or n equal 1. The greatest change will occur if L and n are approximately equal; however these are conditions where the buoyancy is small and plumes are not important. Since there is no satisfactory theory for systems with changing buoyancy flux, and since the characteristics of a plume depend on a fractional power of F, no correction has been applied for any change on dilution. It does, however, make the estimates for high values of m and n somewhat doubtful.

The results of the integrations for the axial length and volume of the flammable envelope and the quantity of material contained therein are :-

Jet

$$z_L = \frac{K_1 d_o}{c_L}\left(\frac{M_a T_a}{M_o T_o}\right)^{\frac{1}{2}} \tag{8}$$

$$V_{FL} = \frac{\pi K_1^3}{9 K_2^2}\left(\frac{M_a T_a}{M_o T_o}\right)^{\frac{3}{2}} d_o^3\left(\frac{1}{c_L^3} - \frac{1}{c_U^3}\right) \tag{9}$$

$$Q_{FL} = \frac{\pi K_1^3}{6 K_2^2}\frac{273}{22\cdot4}\left(\frac{M_a}{T_o}\right)^{\frac{3}{2}}\left(\frac{T_a}{M_o}\right)^{\frac{1}{2}} d_o^3\left(\frac{1}{c_L^2} - \frac{1}{c_U^2}\right) \tag{10}$$

Plume

$$z_L = \frac{K_3^{\frac{3}{5}} \dot{v}_o^{\frac{2}{5}}}{g^{\frac{1}{5}} c_L^{\frac{4}{5}}}\left(\frac{M_a T_o}{M_a T_o - M_o T_a}\right)^{\frac{1}{5}} \tag{11}$$

$$V_{FL} = \frac{5\pi K_3^{\frac{9}{5}} \dot{v}_o^{\frac{6}{5}}}{27 K_4^2 g^{\frac{3}{5}}}\left(\frac{M_a T_o}{M_a T_o - M_o T_a}\right)^{\frac{3}{5}}\left(\frac{1}{c_L^{\frac{9}{5}}} - \frac{1}{c_U^{\frac{9}{5}}}\right) \tag{12}$$

$$Q_{FL} = \frac{5\pi}{12} \frac{273 M_o K_3^{\frac{9}{5}} \dot{v}_o^{\frac{6}{5}}}{22\cdot4\ T_a K_4^2 g^{\frac{3}{5}}}\left(\frac{M_a T_o}{M_a T_o - M_o T_a}\right)^{\frac{3}{5}}\left(\frac{1}{c_L^{\frac{4}{5}}} - \frac{1}{c_U^{\frac{4}{5}}}\right) \tag{13}$$

Values of 1.39 and 1.74 for the constant K_5 in equation (3) for the axial distance to which a jet will persist have been reported for the case where initial momentum and buoyancy forces are directly opposed (6,7). For the case where momentum and buoyancy are in the same direction, the transition is a gradual one. The analysis in (6) indicates that it is essentially complete when $K_5 = 2$. (2) gives a value of 2.4 but the internal Froude number used was defined differently; this value is not inconsistent with that of (6). Since the value when momentum and buoyancy are acting in the same direction is much less critical than in the other case, a mean of the values of 1.39 and 1.74, i.e. 1.55, has been used here throughout.

The data on vertical temperature gradients in the atmosphere, as required for the estimation of the parameter G, equation (4), is rather sketchy. However any

inversion by definition must correspond to a value of G greater than $0.000334/s^2$. Data on inversion in the U.K. suggest that G values of 0.000674 ($dT_a/dz = +\infty K/m$) are not uncommon while values as high as 0.00374 ($dT_a/dz = +0.1°K/m$) are not unknown.   The value used for K_6, equation (5), is 6.65 (3).

Turbulent momentum jet flames are a particular example of jets.   From equation (6) by making the assumptions that $T_f/T_o = 8$, and that $c_s = 2c_L$, both typical for the gases considered here, and by making the assumption, corresponding to that already made for jets, that

$$c_s + \left(1 - c_s\right) \frac{M_a}{M_o} \approx \frac{M_a}{M_o}$$

equations (6) and (7) reduce to

$$\frac{z_f}{z_L} = 0.83 \quad \text{if } T_o = T_a . \tag{14}$$

Results

The more important factors influencing the size of the clouds (the envelope inside which the material is within the flammable concentration limits) have been illustrated by using the relationships given earlier for emissions of methane, ethylene, ethane, propane and n-butane at temperatures from their atmospheric boiling point to 573 K.   An air temperature of 288 K has been assumed throughout.

Figure 1 shows how the emission of ethylene at 288 K, i.e. with a small positive buoyancy in relation to air, depends on both overall mass rate of emission and velocity.   At zero velocity the emission is a pure buoyant plume.   As the velocity increases, a jet is formed of increasing distance of persistence, after which it degrades into a plume.   The total axial distance required for dilution to the lower flammable limit only decreases slowly with emission velocity until the dilution takes place wholly within the jet.   Then it decreases more rapidly as the dimensions of a jet depend only on its effective diameter which, for a fixed mass rate, will be inversely proportional to the square root of the velocity.

It will be seen, by comparing the two curves in Figure 1, that except in the case of zero buoyancy there will be a critical mass flow rate, above which even at sonic velocity dilution to the lower limit will not occur within the jet. There will be a corresponding critical effective jet diameter and plots of this diameter against temperature of emission for each of the gases are shown in Figure 2.   The curve for each gas consists of two parts, the lower temperature part representing the case where the gas will have negative buoyancy and the jet will ultimately transform into a downward moving plume and the higher temperature part in which the gas will have positive buoyancy.   At the temperature where the emission has the same density as air, the jet will persist indefinitely in calm conditions.

It will be noticed that the critical effective jet diameters will be greater than 1.3 to 1.8m except when the temperature is appreciably below the equal density temperature.   As the molecular weight increases so it becomes more likely that dilution to the lower limit will take place partly within a downward moving plume.

The effect of a stable atmosphere and the corresponding range of vertical temperature gradient on the maximum height attained by positively buoyant plumes

is illustrated in Table 1.   Two gases, both at 288 K, are considered - methane
with a large, and ethylene with a small, upward buoyancy.

TABLE 1 - Effect of atmospheric stability on height of plumes

Gas	Emission		Rate	Height for dilution to C_L in neutral atmosphere	Maximum height attained by plume in stable atmosphere		
	Temperature				(Isothermal) $G = 0.000334$	0.0007	0.001
	^{o}K		kg/s	m	m	m	m
CH_4	288		100	181	374	283	248
			1000	455	665	504	441
C_2H_4	288		100	346	175	132	116
			1000	870	311	236	206

It will be seen that, at the rates of emission considered, for methane the maximum
height will in all cases be equal to or greater than the height required for
dilution to the lower limit.   It must be remembered, however, that this latter
height required will itself be increased by atmospheric stability since this will
affect buoyancy and hence entrainment.   For ethylene however it is clear that in
none of the cases considered will there be dilution to the lower limit before
the limit of ascent is reached; at the latter point the plume will spread
laterally with a decreased rate of entrainment and dilution.   It follows from
these examples that the levels of stability corresponding to values of G =
0.000334 - 0.001 (equivalent to vertical temperature gradients of 0 - + 0.02 C/m)
can have significant effects on plume behaviour.   The effect of stable
atmospheres on the behaviour of jets is more complex and will not be considered
here; they will be less sensitive than plumes.

From equations (8) and (10) the length to the lower limit, Z_L the quantity
within the flammable envelope Q_{FL} and the mass flow rate for sonic emission
have been calculated for jets of the five gases at 288, 423 and 573 , in
terms of the effective jet diameter d_o , which determines the dimension of
the jet.   The results are shown in Table 2.

It will be seen how the length and contents decrease with increasing temperature,
due to the decreasing mass flow rate.   The importance of the term containing
the flammability limits is clearly shown, particularly in comparing Q_{FL}
for ethane and ethylene.   Values for the ratio z_s/z_L are also given for 288 K.
Their closeness to the predicted value of 0.83 (equation (13)) shows that
momentum jet flames behave similarly to jets without reaction.

The dimensions and contents of plumes cannot be described so simply as both will
tend to infinity as the density of the gas emitted approaches that of air.
However, for the gases and temperature range under consideration, it can be
said that, well below the equal density temperature, the length and contents
of a plume are less than that of a sonic jet for the same mass flow rate while
the converse is true of higher temperatures.

TABLE 2 - Dimensions and contents of flammable envelopes in jet

		CH_4	C_2H_4	Gas C_2H_6	C_3H_8	nC_4H_{10}
M_o		16	28	30	44	58
C_L	volume fraction	0.05	0.027	0.03	0.021	0.018
C_U	volume fraction	0.15	0.36	0.124	0.095	0.084
$(\dfrac{1}{C_L^2} - \dfrac{1}{C_U^2})$		356	1364	1046	2157	2945
$288^{\circ}K$ $\dfrac{z_f}{z_L}$		0.83	0.73	0.85	0.85	0.90
$\dfrac{z_L}{d_o}$		243	340	294	347	354
$\dfrac{\dot{m}}{d_o^2}$	$kg/m^2 s$	236	304	310	362	413
$\dfrac{q_{FL}}{d_o^3}$	kg/m^3	1388	4020	2980	5090	605
$423^{\circ}K$ $\dfrac{z_L}{d_o}$		200	280	243	287	292
$\dfrac{\dot{m}}{d_o^2}$	$kg/m^2 s$	189	244	252	295	337
$\dfrac{q_{FL}}{d_o^3}$	kg/m^3	782	2270	1675	2860	3400
$573^{\circ}K$ $\dfrac{z_L}{d_o}$		171	240	210	246	251
$\dfrac{\dot{m}}{d_o^2}$	$kg/m^2 s$	157	201	209	248	284
$\dfrac{q_{FL}}{d_o^3}$	kg/m^3	495	1435	1064	1810	2160

It is of interest to examine residence times within the flammable envelopes. For jets over the range 288 to 573 K the residence times are in the range 2.5 to 11s for a mass flow rate of 100 kg/s and in the range 8 to 24s for 1000 kg/s. For plumes the minimum residence times are 3s for 100 kg/s and 5s for 1000 kg/s. These residence times give a lower limit for the time required for the complete cloud to be formed; it will be seen that a very short release will be required. They also show that, if a minimum content of 1000 kg is assumed to be required for an explosion to cause pressure damage, then emission rates in the range 100 - 1000 kg/s can give rise to such clouds.

SYMBOLS USED

$\dot{m}$	=	mass flow rate (kg/s)
c	=	concentration (volume or mole fraction)
d	=	effective diameter of discharge (m)
z	=	axial length, vertical height (m)
r	=	radial distance from axis (m)
M	=	molecular weight
T	=	temperature ($^{\circ}$K)
$\dot{V}$	=	volumetric flow rate (m^3/s)
w	=	velocity (m/s)
g	=	gravitational constant (m/s^2)
ρ	=	density (kg/m^3)
Γ	=	adiabatic lapse rate ($^{\circ}$K/m)
α	=	molar ratio of reactants : products
F	=	buoyancy flux (m^4/s^3)
V_{FL}	=	volume of cloud between flammable limits (m^3)
Q_{FL}	=	quantity of material within flammable limits (kg)
K_1, K_2, etc	=	constants

Subscripts

o	=	original discharge
a	=	air
tr	=	transition from jet to plume
f	=	referring to turbulent diffusion flame
s	=	stoichiometric mixture
L	=	lower flammable limit
U	=	upper flammable limit

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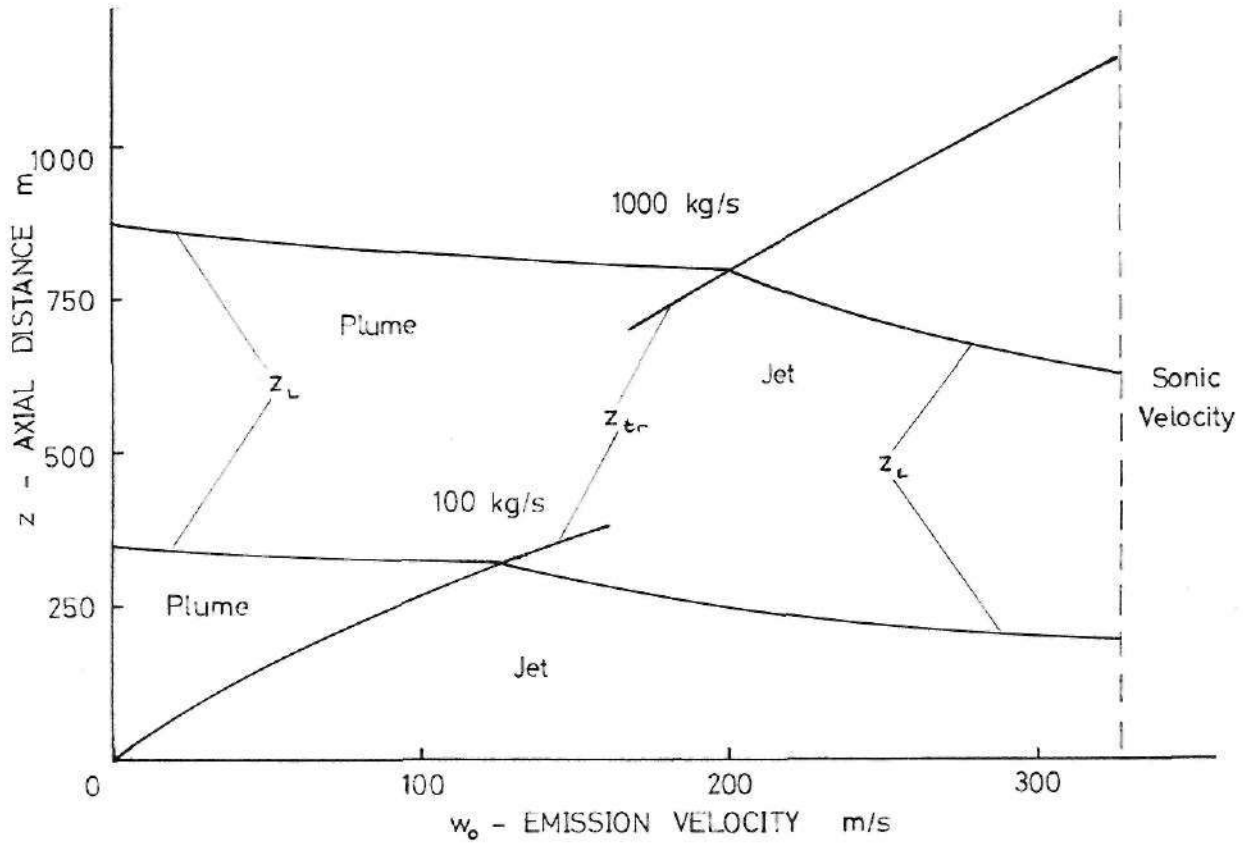   on Combustion Flame & Explosion Phenomena (1949 Williams & Wilkins) 266-288

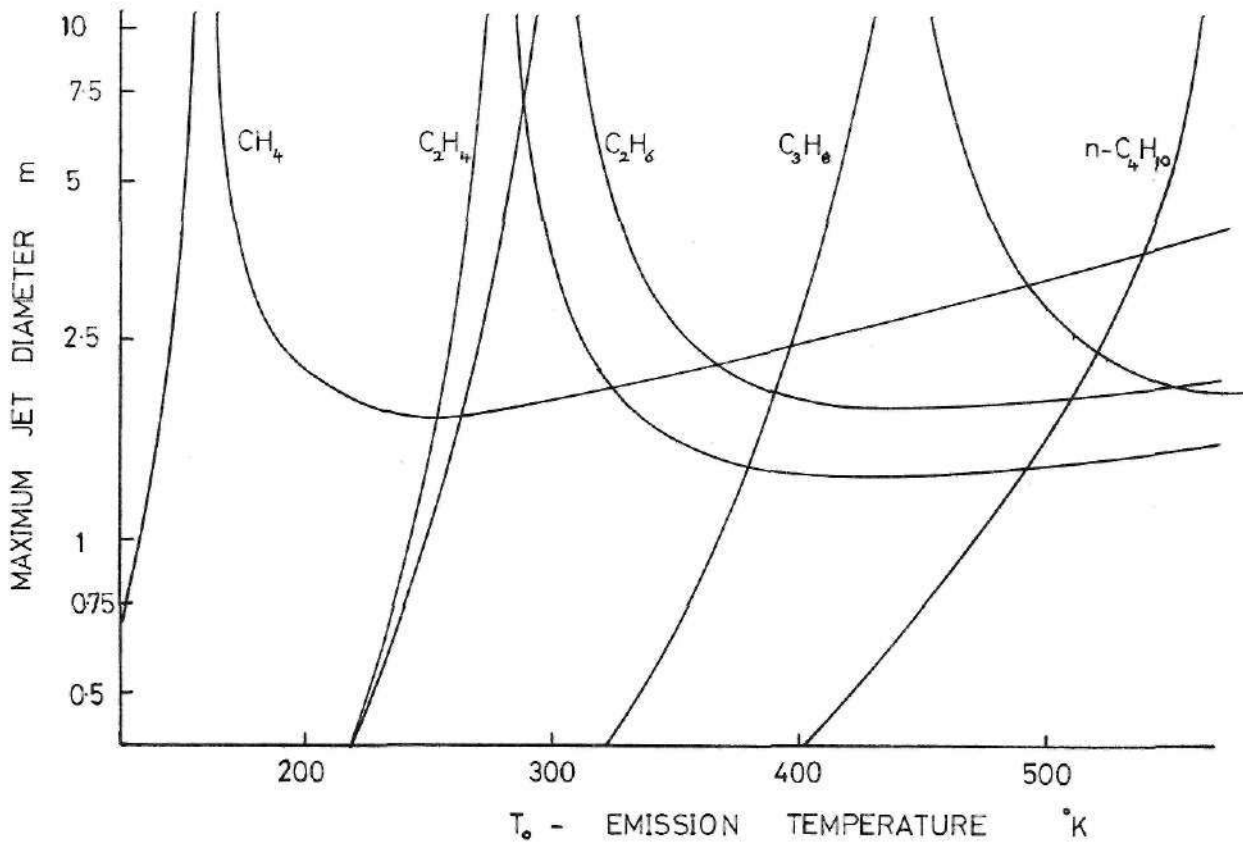Figure 1 Discharge of ethylene at 288° K into neutral atmosphere

Figure 2 Maximum jet diameter for dilution of sonic emission to lower flammable limit within jet