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Scaling rules for reduced-scale field releases of hydrogen fluoride

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Abstract

The potential consequences of an accidental release to the atmosphere of hydrogen fluoride in large quantities are severe, but risk-assessment studies are presently constrained by being unable to predict very reliably the released gas cloud behaviour. Due to a variety of complex thermodynamic and chemical interactions, a dispersing gas cloud may be heavier or lighter than air in different stages of its dispersion. If cloud buoyancy is significant then the reduced ground level concentrations due to the plume rise may be a major mitigation factor in any risk assessment. Atmospheric water vapour plays an important part in the development of cloud buoyancy and the borderline conditions lie around 10°C and 75% humidity, typical of Northern European weather conditions. The only effective way of investigating these phenomena is with releases of hydrogen fluoride in the field under appropriate meteorological conditions. However, full-scale simulations are costly, time consuming and hazardous. A reduced-scale simulation greatly reduces these problems, but needs to be correctly scaled. The report considers these scaling requirements and shows that, within some constraints, they can be successfully achieved. As an example, a one tenth scale field experiment reduces the required released quantities from tonnes to kg. The required windspeeds reduce to about one half of the full scale, which is acceptable while placing some constraints on the lowest scalable windspeeds. It is more difficult to investigate stratified flows as a reduced-scale experiment atmospheric stratification appears less severe than its full-scale equivalent. © 1997 Elsevier Science B.V.

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1. Notation

The notation follows a general rule, where appropriate, that full-scale parameters are upper case and model-scale parameters are lower case. Where this is so, upper and lower case parameters are given together without further comment.

a, A	Source discharge opening cross-sectional area.
c_p	Specific heat of air.
d, D	Droplet stop distance (Eq. (31)).
F_r	Froude number $(U^2(gL)^{-1})$.
f, F	Frequency in atmospheric turbulence spectrum. F is also buoyancy flux in Eqs. (44) and (45).
g	Acceleration due to gravity.
h, H	Windspeed reference height.
h_f, H_f	Surface heat flux.
l, L	Characteristic length scale for dispersing releases.
L_p	Briggs' lift-off parameter (Eq. (43)).
m, M	Mass of material released.
m_f, M_f	Discharge momentum flux.
q, Q	Volume release rate of a continuous release. Q is also heat release in Eqs. (45) and (46).
S_c	Model scale as a fraction, i.e. $S_c = 0.1$ for a scale of 1/10.
t, T	Time scale of dispersing cloud. Subscript r refers to the release time.
u, U	Windspeed at reference height indicated by the subscript. Thus, U_H is the full-scale windspeed at height H above the ground.
u_*, U_*	Friction velocity appearing in the usual logarithmic rough-wall velocity profile equation:

$$\frac{U}{U_*} = \frac{1}{\kappa} Ln\left(\frac{Z}{Z_0}\right) \tag{1}$$

u', U'	Longitudinal turbulence intensity (i.e., the standard deviation of the fluctuating velocity component).
v, V	Volume of HF released (as vapour at ambient conditions).
v_f, V_f	Droplet falling speed.
w, W	Source discharge velocity.
z, Z	Height above ground.
z_0, Z_0,	Aerodynamic roughness height appearing in Eq. (1).
$\Delta\theta$, $\Delta\Theta$	Atmospheric temperature difference from the ground to the reference height.
ρ	Gas density; ρ_a = air density; ρ_g = release gas density at ambient conditions.
$\Delta\rho$	$\rho_g - \rho_a$.
κ	Von Karman's constant, taken as 0.4.

2. Introduction

Anhydrous hydrogen fluoride is used and stored in large quantities (up to 100 te), especially in the petroleum industry where it is used in alkylation plant for producing additives for lead-free petroleum spirit. The dispersion of accidental releases of anhydrous hydrogen fluoride (HF) is presently a matter of great concern in risk assessment as even at exposure levels of a few tens of ppm it can cause permanent health effects. There is particular difficulty with flashing releases of HF stored under high pressure and/or temperature, where the earlier stages of the gas cloud's dispersion show complex chemical and thermodynamic behaviour as it mixes with humid air. The HF molecule is lighter than air, but the molecules may oligomerize (that is, partially polymerise) at release, increasing the molecular weight beyond that of air, though the oligomers will decompose again over short time scales. At the same time the continued evaporation of liquid HF droplets generated in the release cools the cloud, further increasing its density. In addition there is an exothermic reaction with atmospheric water vapour which reduces the cloud density. As a result the overall density of the cloud may be lighter or heavier than air depending upon a number of factors, including the form of the release, the rate of dispersion of the cloud and the atmospheric temperature and humidity. These effects cannot be considered independently as there is an interaction between them which affects the overall cloud behaviour. Some of these problems are discussed in [9,6,14].

The variation in density in the cloud as it disperses, especially whether it may pass from being negatively to positively buoyant, may be critical to some risk assessment studies as a mitigating factor. If the cloud develops sufficient positive buoyancy for the bulk of it to become airborne, concentrations of HF at the ground may be significantly reduced. At present the available information on these complex forms of cloud behaviour is insufficient to construct reliable numerical models for risk assessment calculations. Some sort of physical simulation of the process is required to investigate the problems further.

Unfortunately, the correct molecular and thermodynamic behaviour in a dispersing cloud can only be obtained by using HF as the released gas. There is no suitable safe surrogate material with the appropriate thermodynamic and chemical properties that can be used in either field experiments or small-scale wind tunnel experiments. Also, it must be discharged in a similar way to the full scale in order to generate the correct proportion and size distribution of HF droplets within the cloud. Furthermore, the dispersion must be into an atmosphere at the correct temperature and humidity.

The major US field trials, the Goldfish series of experiments, were carried out over a desert site in conditions of very low atmospheric water content. Thus, they did not show the development of buoyancy in the gas cloud. Sites permitting such large releases are rare and it is probably impracticable to carry out a similar field trial in a humid atmosphere with a large release approaching the scale of a real accident, which may involve up to 100 te of HF, due both to problems of cost and time and to the hazardous nature of HF on a site of limited dimensions. A very small-scale laboratory wind tunnel model would be a very convenient alternative form of experiment, but again for reasons of safety and the scaling problems of using HF in a humid atmosphere, this is not feasible either.

One possible option is to use a reduced-scale release in the field, using similar scaling principles to those of wind tunnel models but at larger scales. In this case many of the scaling problems associated with a very small-scale wind tunnel model are removed, but the advantages of using the correct material in a humid environment remain. The smaller scale significantly reduces cost and hazard problems and makes a field experiment practicable on a smaller site. This type of experiment can be used either as a convenient vehicle for examining the chemical/thermodynamic/mixing problem or, far more usefully, as a direct small-scale simulation of a large release. Releases of HF in the range 1–100 kg (limited mainly by the size of the site available) result in only limited hazards which can be kept under effective control. The main problem is whether such a release can correctly scale to simulate a much larger accident involving tonnes of material.

The present paper considers the scaling rules that must be applied to a small-scale field release of buoyant (either positively or negatively) material in order to simulate a larger release. The general principles are similar to those used for reduced-scale wind tunnel dispersion modelling, where the dispersion of buoyant flows is routinely successfully modelled at scales typically between 1/100 and 1/1000. In a small-scale field experiment larger scales can prevail, down to 1/100 at the smallest, so some of the constraints that occur with wind tunnel models are relieved. However, another major difference is that in a wind tunnel model the wind environment is under complete control while in the field it is a given quantity with frequencies of occurrence of particular windspeeds, directions and stratifications. Small-scale modelling in the field imposes some constraints on required windspeeds and levels of stratification; these must be within reason for this approach to succeed.

An initial experimental programme of field releases of HF, based on these premises, has been carried out at the UK Defence and Evaluation Research Agency's Protection and Life Sciences Division, Porton Down, for the UK Health and Safety Executive.

3. Scaling

3.1. General

As noted in the introduction, the general principles of setting up a reduced-scale field experiment are similar to those used in scaling wind tunnel model experiments, except that there are constraints over windspeeds when modelling in the field. It is not proposed to cover the modelling principles in detail here as they are available from other sources. There are detailed reviews in [12,13] and specific discussions of modelling heavy gas releases in [4,8]. Only the important parameters for a reduced-scale field experiment are discussed here. For example, there is always some concern over the effects of reduced Reynolds numbers in small-scale wind tunnel experiments. However, at the relatively larger scales of a field experiment this is no longer of much practical importance.

A neutrally stable atmosphere is considered in the first instance. Modelling of stratified flows is considered later.

The initial consideration here is with a release of a fixed quantity of material over a finite time. The release time may be anything between so short as to be instantaneous and so long as to be effectively continuous. This is the most likely form of a real accident and is similar to that used in the field experiments. The relationship with scaling rules for continuous releases is considered later, but they do not differ in substance from those described initially.

3.2. Length scales

The characteristic length scale (l, L) for the release is defined in terms of the volume of vapour released (at ambient conditions), as

$$L = V^{1/3}, \tag{2}$$

in the full scale and, similarly,

$$l = v^{1/3}, \tag{3}$$

for the model.The characteristic length scale of the approach flow is assumed to be defined by the aerodynamic roughness height (z_0, Z_0), appearing in the usual rough-wall velocity profile equation,

$$\frac{U}{U_*} = \frac{1}{\kappa} Ln\left(\frac{Z}{Z_0}\right), \tag{4}$$

for the full scale, and

$$\frac{u}{u_*} = \frac{1}{\kappa} Ln\left(\frac{z}{z_0}\right), \tag{5}$$

for the model scale.

The assumption that z_0 is the sole controlling parameter of the approach flow is considered in more detail in Section 3.7, which considers the scaling of atmospheric turbulence.

Lengths must scale directly in the model, so that

$$\frac{l}{L} = \frac{z_0}{Z_0} = \frac{h}{H} = S_c. \tag{6}$$

Where S_c is the model/full-scale length scaling factor. Note that the reference height for the approach windspeed, h, H, reduces with the scale. It must also be noted that a strict scaling of the aerodynamic roughness height is not necessary for an acceptable model. The turbulence in the approach flow is its most important feature for a dispersion model and this changes only slowly with changes in the aerodynamic roughness height. Scale errors in z_0 of a factor of two, for example, would be of limited significance.

Since we are considering a release of the same material in the model as in the full scale, there is a direct equivalence between the volume of material released and its mass. So that,

$$\frac{v}{V} = \frac{m}{M} = \left(\frac{l}{L}\right)^3 = S_c^3. \tag{7}$$

It can be seen that there is a substantial reduction in the released mass of material required in the model even at moderate scales. Thus, for example, at an assumed scale of

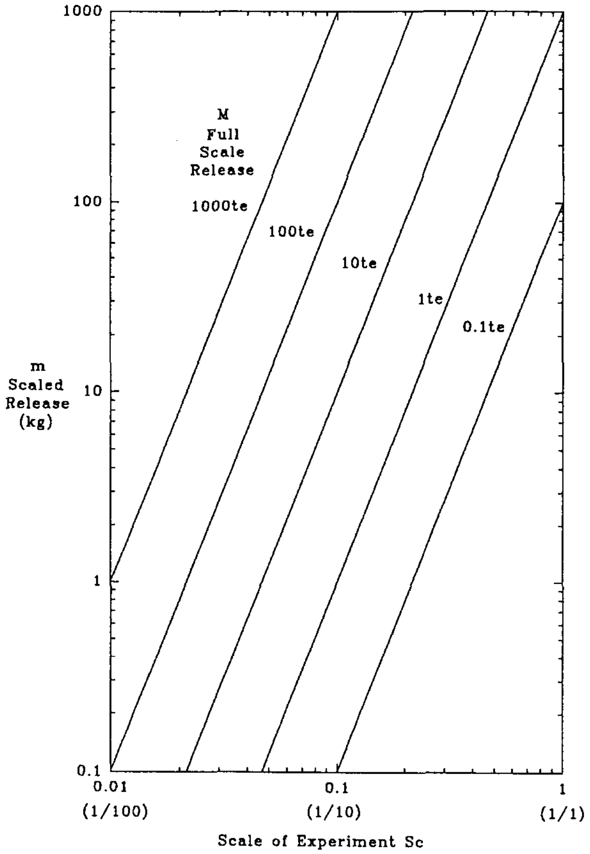

Fig. 1. Released mass of gas in a scaled model for various scales and full scale released masses.

1/10 ($S_c = 0.1$) releases of kilogrammes in a model are the equivalent of tonnes at full scale. Fig. 1 gives a plot of the release mass required to model various full-scale releases at different scales. For the field experiments at Porton Down, the maximum tolerable release quantities are less than 10 kg. At the assumed scale of 1/10 these correspond to full-scale releases of up to 10 te, which is well within the range of practical interest.

3.3. Velocity scales

For buoyant flows, whether positively or negatively buoyant, the formal requirement for correct scaling is that both the density ratio,

$$\frac{\rho_g}{\rho_a}, \tag{8}$$

and the Froude number, F_r, where

$$F_r = \frac{U^2}{gL}, \tag{9}$$

should retain identical values at full scale and model scale.

Another scaling parameter commonly encountered in modelling buoyant flows is the Richardson number, R_i, where

$$R_i = g\frac{\rho_g - \rho_a}{\rho_a}\frac{L}{U^2}. \tag{10}$$

In fact, scaling with Richardson number is a degenerate form of satisfying Eqs. (8) and (9) separately that is strictly only valid for small density differences. If Eqs. (8) and (9) are satisfied then the Richardson number is automatically correctly scaled.

In the present case the same material is to be released at model scale as at full scale, so that the density of the release remains fixed and Eq. (8) is satisfied. Eq. (9) is satisfied if

$$\frac{u_h}{U_H} = \left(\frac{l}{L}\right)^{0.5} = S_c^{0.5}. \tag{11}$$

So that the windspeed over a model must be lower than at full scale. It is perhaps more appropriate for a field experiment to express this in the form 'whatever windspeed occurs over the model is equivalent to a higher windspeed at full scale'. This is a constraint on setting up a reduced-scale field model as there is great interest in releases at low windspeeds, where plume concentrations are highest and buoyancy effects at their greatest. The frequency of occurrence of relatively low windspeeds over the site therefore governs the lowest equivalent full-scale windspeed that can be readily modelled.

There is some difference of opinion as to whether U or U_* (the friction velocity in Eq. (1)) is the most suitable reference windspeed for scaling heavy gas releases. U_* is often preferred as a 'natural' parameter occurring in the atmospheric boundary layer equations, though the present authors prefer the windspeed at a height near the top of the gas cloud as it avoids some difficulties in dealing with the effects of surface roughness on gas cloud dispersion. In the present scaling exercise the choice is not important as the ratio U/U_* remains constant at all scales as long as the ratio H/Z_0 is also scaled, which is the case in the present study. In the following discussion U and U_* are therefore used a little arbitrarily as seems convenient.

The constraint on windspeed is not as severe as appears from Eq. (11) due to the reduced reference height for the windspeed when the scale is reduced (Eq. (6)). As windspeeds are lower closer to the ground, this provides some compensation for the reduction in the reference windspeed at reduced scales required by Eq. (11). A convenient way of accounting for this is to calculate the change in windspeed required, at a fixed height, for different model scales. This is also desirable for assessing the frequency of occurrence of the required windspeeds since meteorological measurements are usually made at fixed heights.

If the required model windspeeds are referred back to the full-scale reference height

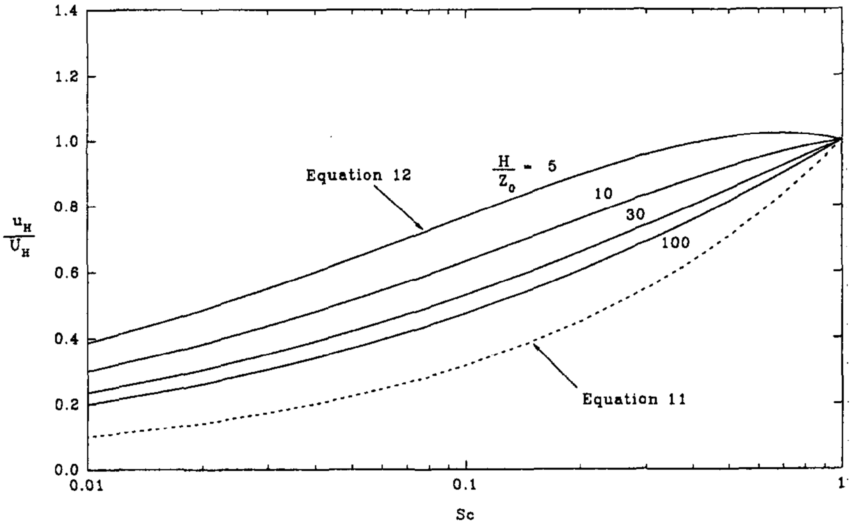

Fig. 2. Wind speed reduction required over a small scale release, referred to the same reference height as the full scale, for different surface roughnesses.

(that is, H, so that the relevant windspeed is u_H) some manipulation of the basic equations gives an expression for the required ratio of model to full-scale windspeeds, u_H/U_H, at this fixed reference height. This is,

$$\frac{u_H}{U_H} = S_c^{0.5} \cdot \left(1 - \frac{Ln(S_c)}{Ln\left(\dfrac{H}{Z_0}\right)}\right). \tag{12}$$

The equation gives the velocity ratio in terms of the full-scale values of the windspeed reference height, H, and aerodynamic roughness height, Z_0. However it assumes that the model values are correctly scaled, to h and z_0 respectively. This expression is shown plotted in Fig. 2 as the required velocity ratio as a function of model scale for a range of values of H/Z_0. Also shown on Fig. 2 is the simple square root relationship of Eq. (9) if the reference height changes with the scale, so that the degree of compensation obtained due to the reduced windspeeds nearer the ground can be observed. It can be seen that the degree of compensation increases as the model scale reduces, simply because the true velocity reference height reduces with the model scale.

Expressed on this basis there is a significant alleviation of the required reduction in windspeed over a reduced-scale model. As an example, we can consider the 1/10 scale model discussed previously. Eq. (11) requires that the windspeed over a model should be about one third of that at full scale, though at the reduced reference height. If the full-scale reference height is 10 m and the full-scale aerodynamic roughness height 30 cm (equivalent to the relatively sparsely developed edges of an urban area), Eq. (12) shows that the windspeed over the model at 10 m height needs to be only about half that at full scale.

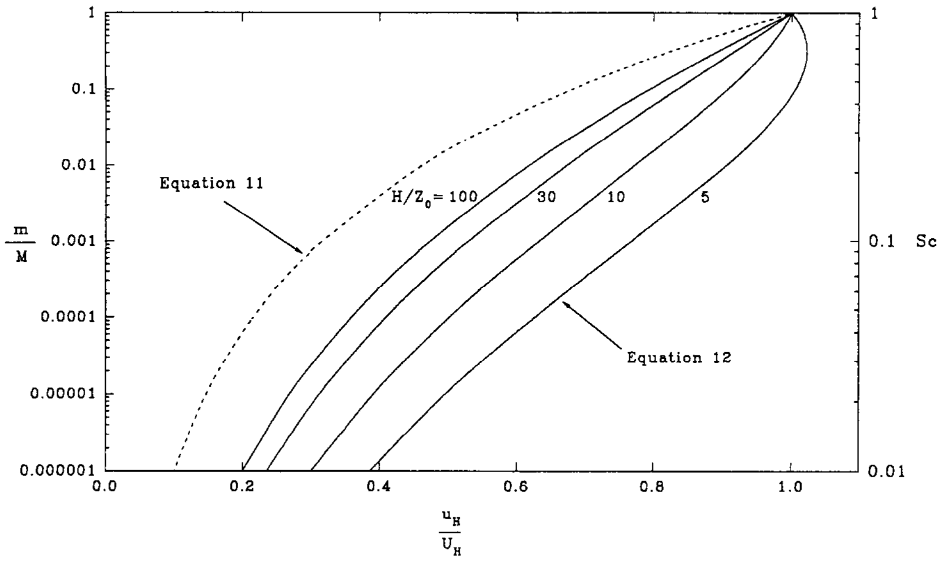

Fig. 3. Scaling relationships between mass and velocity ratios for model to full scales, for different surface roughnesses.

It must be noted that a single experiment on a reduced scale actually corresponds to a range of potential full-scale releases for a variety of matching release masses and windspeeds, depending upon the assumed scale. Fig. 3 shows this as a plot of the model to full-scale mass and velocity ratios, m/M and u_H/U_H for various values of H/Z_0, derived from Eq. (12). As in Fig. 2, the simple square root relationship for u_h/U_H is also shown for comparative purposes. Since m/M varies with the cube of the scale, the right hand axis of Fig. 3 also shows the related scale for a given value of m/M. Fig. 3 contains all the basic scaling parameters. It can therefore be used either to determine the range of full release masses and windspeeds corresponding to a particular model test or to determine the range of model experiments that will correspond to a particular full-scale release.

3.4. Time scales

The scaling parameter to be satisfied is the dimensionless time,

$$\frac{UT}{L}, \tag{13}$$

which must have the same values at full and model scales, so that,

$$\frac{UT}{L} = \frac{ut}{l}. \tag{14}$$

The time t, T, may be, for example, the time of passage of the gas cloud or its release time, t_r, T_r.

Since,

$$\frac{l}{L} = S_c \text{ and } \frac{u}{U} = S_c^{0.5}, \tag{15}$$

then,

$$\frac{t}{T} = \frac{U}{u} \cdot \frac{l}{L} = S_c^{0.5}. \tag{16}$$

Thus a scaled release of finite duration should have the release time appropriately reduced. Considering again the example of a 1/10 scale model, time scales in the dispersing plume, including the release time, will be reduced to about one third of full scale.

3.5. Scaling continuous releases

The scaling parameter for a continuous release at a volume rate q, Q, is the dimensionless release rate,

$$\frac{Q}{UL^2}, \tag{17}$$

which must have similar values at model and full scale. Thus,

$$\frac{q}{Q} = \frac{u}{U}\left(\frac{l}{L}\right)^2 = S_c^{2.5}. \tag{18}$$

For our example of a one tenth scale model, the release rate can thus be reduced to about one three hundredth of the full-scale value.

This scaling is not fundamentally different to the scaling of a time-dependent release considered earlier. If the release rate, Q, is regarded as a time-dependent release for which the release time, T, is so large as to be indistinguishable from a continuous release, then,

$$Q = \frac{V}{T}, \tag{19}$$

and for a scaled release,

$$\frac{\left(\frac{v}{t}\right)}{\left(\frac{V}{T}\right)} = \frac{v}{V} \cdot \frac{T}{t} = S_c^{2.5}, \tag{20}$$

the same result as for a continuous release in Eq. (18).

3.6. Scaling atmospheric stability

The discussion so far has considered only a neutrally stable atmosphere. However, a major concern in risk assessment, especially with heavy gas releases, is with stable stratification since it tends to produce the highest plume concentrations at the ground.

The discussion of atmospheric stability will therefore concentrate on stable stratification, though the principles are generally applicable to unstable stratification. Only the essential features of the problem for scaling purposes will be discussed here. More detailed explanations and definitions of the various stability parameters can be found in [11,10].

In the first instance, a simple way of considering the scaling of stratification is with the bulk Richardson number in the form of Eq. (10). The length scale for the bulk Richardson number becomes the height above the ground, the windspeed that at the same height and the density ratio $\Delta\rho/\rho$ relates to the difference in atmospheric density over this height. In principle, identical values of this atmospheric bulk Richardson number are required for the model as occur in the full scale. For the gas release, Section 3.3 notes that satisfying Eq. (8), for the gas/air density ratio, and Eq. (9), for the reference windspeed, automatically provides correct Richardson number scaling. Because the same material is released at model and full scale, the release gas/air density ratio remains the same in model and full scale and the windspeed must be reduced to satisfy Eq. (9). The same requirement then applies to the Richardson number for atmospheric stability. Since the scaled windspeed satisfies the need for the same full-scale/model gas release densities, it also implies a requirement for the same atmospheric density difference. However, in the model the atmospheric density difference applies over the reduced-scaled reference height. Thus in the model the required density gradient has to increase inversely as the scale.

The implication of this for scaling atmospheric stability is that a given level of stability, with its associated density gradient, will appear less severe in a model than in the full scale. That is, reduced-scale experiments will effectively tend towards neutral stability.

For meteorological purposes there are a number of classifications of atmospheric stability in use. Two of the most common are Pasquill's typing scheme and the Monin–Obukhov length scale, L_m. They can be related to one another and to various forms of Richardson's number; details can be found in [10,15]. Fig. 4, taken from [1] shows the relationship between Pasquill's stability categories and the Monin–Obukhov length scale, which is probably the most important parameter for present purposes. The Monin–Obukhov length scale has an unfortunate characteristic for scaling purposes in that it approaches infinity for neutral stratification and low values (positive and negative, respectively) for high levels of stability and instability. Because of this, in Fig. 4 the axis is $1/L_m$, whose value is zero for neutral stability. The abscissa is the aerodynamic roughness height, z_0, which also affects the Pasquill stability class. The curves on the figure show the divisions between the different Pasquill stability classes. For convenience, the figure has been annotated with values of the Monin–Obukhov length scale along two values of z_0, 3 cm and 30 cm (marked with broken lines), which correspond to the model and full-scale values of z_0 in the example which has been used throughout this paper. The annotations are at the boundaries between the Pasquill categories and at their nominal mid-range values. It can be seen in Fig. 4 that the Monin–Obukhov length scale varies between factors of two to five between one Pasquill stability category and the next, depending upon the surface roughness and whether the category is stable or unstable. For stable stratification there is typically a factor of five variation between

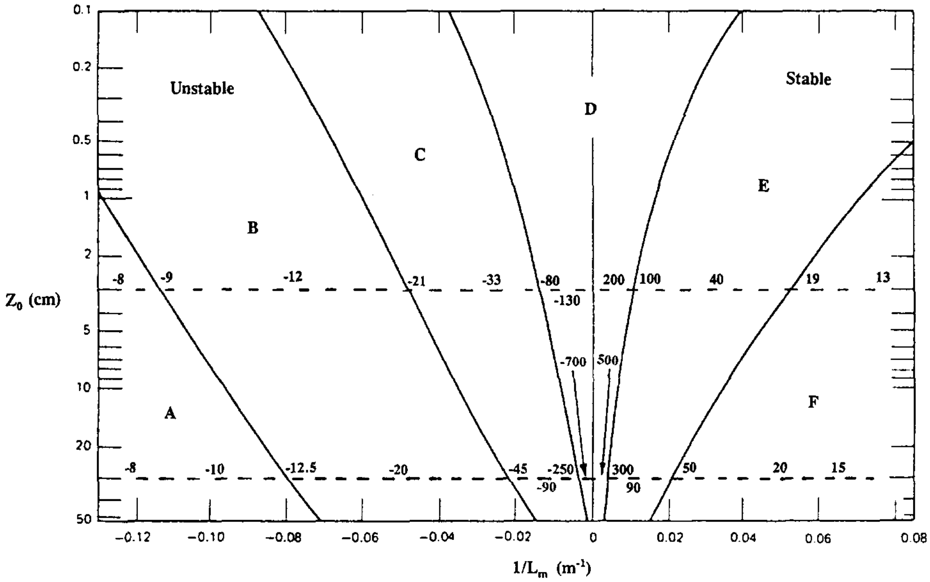

Fig. 4. Relationship Between Pasquill stability class and Monin-Obukhov length scale. From Golder ([1]). Annotated values are of the Monin-Obukhov length scale L_m at two values of z_0, 3 cm and 30 cm.

each Pasquill stability category at both the values of z_0 annotated. It can also be seen in the figure that there is a reduction in the Monin–Obukhov length scale between the two example surface roughnesses for the same nominal Pasquill stability class, by a factor of about 2.5 for this order of magnitude change in surface roughness.

For true meteorological scaling of stratification, the Monin–Obukhov length scale should simply scale linearly along with the other length scales of the experiment. Thus,

$$\frac{l_m}{L_m} = S_c. \tag{21}$$

A model therefore requires smaller values of the Monin–Obukhov length than its full-scale equivalent and a particular level of atmospheric stratification appears closer to neutral stability in a model than will the full scale. Considering again the example of a one-tenth scale model, Fig. 4 indicates that an order of magnitude reduction in the Monin–Obukhov length scale, in combination with the reduction in z_0 required over a model, is approximately equivalent to passing from one Pasquill stability category to the next. Thus a full-scale release in category E, for example, would need to be modelled at one tenth scale in category F to produce the equivalent atmospheric stratification.

The requirement for scaling the Monin–Obukhov length scale, together with the other scaling requirements, leads to two points of meteorological interest.

Firstly, the scaling of surface heat flux. From the definition of Monin–Obukhov length, we have,

$$\frac{l_m}{L_m} = S_c = \left(\frac{u_*}{U_*}\right)^3 \cdot \frac{H_f}{h_f}. \tag{22}$$

Where h_f, H_f, is the surface heat flux. Substituting for u_*/U_* $(=u_h/U_H$, Eq. (11)), gives,

$$\frac{h_f}{H_f} = S_c^{0.5}. \tag{23}$$

Thus, due to the requirement for a lower windspeed over the model to provide Froude number scaling for the gas release, the required value of the Monin–Obukhov length scale over the model can be obtained with a lower surface heat flux than in the full scale. In the example of a one tenth scale model, the surface heat flux need only be about one third of the full-scale value.

Secondly, the vertical temperature gradient, or rather the temperature difference $\Delta\theta$, $\Delta\Theta$ from the ground to the reference height h, H. In stably stratified flows the temperature gradient is normally given by,

$$\frac{\Delta\theta}{t_*} = \frac{1}{\kappa}\left(\ln\left(\frac{h}{z_0}\right) + 5\frac{h}{l_m}\right), \tag{24}$$

for the model and

$$\frac{\Delta\Theta}{T_*} = \frac{1}{\kappa}\left(\ln\left(\frac{H}{Z_0}\right) + 5\frac{H}{L_m}\right), \tag{25}$$

for the full scale, where,

$$T_* = -\frac{H_f}{c_p \rho_a U_*},\ t_* = -\frac{h_f}{c_p \rho_a u_*} \tag{26}$$

and c_p is the specific heat of air.

For a correctly scaled experiment, the equivalent ratios in the right hand sides of Eqs. (24) and (25) above are identical, so that,

$$\frac{\Delta\theta}{\Delta\Theta} = \frac{t_*}{T_*} = \frac{h_f}{H_f}\cdot\frac{U_*}{u_*} = S_c^{0.5}\cdot S_c^{-0.5} = 1. \tag{27}$$

Thus the required atmospheric temperature change, over the reference height, should be the same in full scale and in the model. This result is identical to that of the simple argument using Richardson's number discussed at the start of this section.

In practice atmospheric stability is a more complex matter than the simple approach presented here, which is intended only to give an indication of the way in which stability needs to be considered in a reduced-scale model in the atmosphere. In stable atmospheres it is common to find large variations in temperature gradient and the other stability parameters for the same nominal specific stability conditions. It is common, for example, to find significantly greater temperature gradients closer to the ground than are indicated by Eqs. (24) and (25). Also, at high stabilities (that is, low values of the Monin–Obukhov length scale) the atmosphere may laminarise completely, so that this sort of scaling loses its significance. In the present case it is the modified turbulence characteristics which are of prime concern since it is these that directly affect gas cloud dispersion. They are better measured directly and used to infer stability levels. Another useful approach is to measure the dispersion of a passive tracer just before an HF release to provide some indication of conventional dispersion rates, against which the HF dispersion rate can be compared and which can be used to assist estimating the nominal stability level.

3.7. Scaling atmospheric turbulence

In Section 3.2 the atmospheric boundary layer scaling was assumed to be controlled solely by z_0. In a dispersion model it is essential that both the turbulence intensities and eddy-scale distributions (that is, the turbulent frequency spectrum) are correctly scaled if the dispersion rates are to be correct. This section looks at the matter in a little more detail.

Turbulence intensities scale with U_*, the value of U'/U_* remaining approximately constant with height in the logarithmic part of the boundary layer. Since U_* is directly related to U and Z_0 (Eq. (1)), provided a model is set up with an appropriately scaled value of z_0, the dimensionless turbulence intensities, u'/u and U'/U, should be the same at the scaled height in the boundary layer as in the full scale. For example, Panofsky and Dutton [10] give formulae for the turbulence intensity in the neutrally stable atmosphere of the form,

$$\frac{U'}{U_*} = \frac{\kappa A}{\ln\left(\frac{H}{Z_0}\right)}, \tag{28}$$

where U' is the turbulence intensity and A is a constant (of value of about 2.5 for the longitudinal component, 2 for the lateral component and 1.3 for the vertical component). It can be seen from Eq. (28) that if the value of H/Z_0 is the same in model and full scale, which is presupposed here, then the dimensionless turbulence intensity, U'/U_*, remains the same at model and full scale at the relevant scaled heights.

The frequency spectrum also scales with height, so on this basis should be correctly scaled between model and full scale. As an example an atmospheric frequency spectrum for neutral stratification is shown in Fig. 5, using Kaimal's standard spectral data, taken from [5], plotted in the conventional fashion of $nS(n)/U_*^2$ against the dimensionless frequency, $N(=FZ/U)$. It shows the spectra of the three components of turbulence. The integral under each curve gives the overall turbulence intensity of that component, $(U'/U_*)^2$ etc. The vertical axis of the plot is scaled by U_*^2, so correctly scales between model and full scale. The dimensionless frequency, FZ/U, on the horizontal axis, where F is frequency with units of 1/time, is essentially a dimensionless time as considered in Section 3.4. Thus for a correctly scaled model we need,

$$\frac{fh}{u} = \frac{FH}{U}, \tag{29}$$

which rearranged gives,

$$\frac{F}{f} \cdot \frac{u}{U} \cdot \frac{H}{h} = S_c^{0.5} \cdot S_c^{0.5} \cdot \frac{1}{S_c} = 1. \tag{30}$$

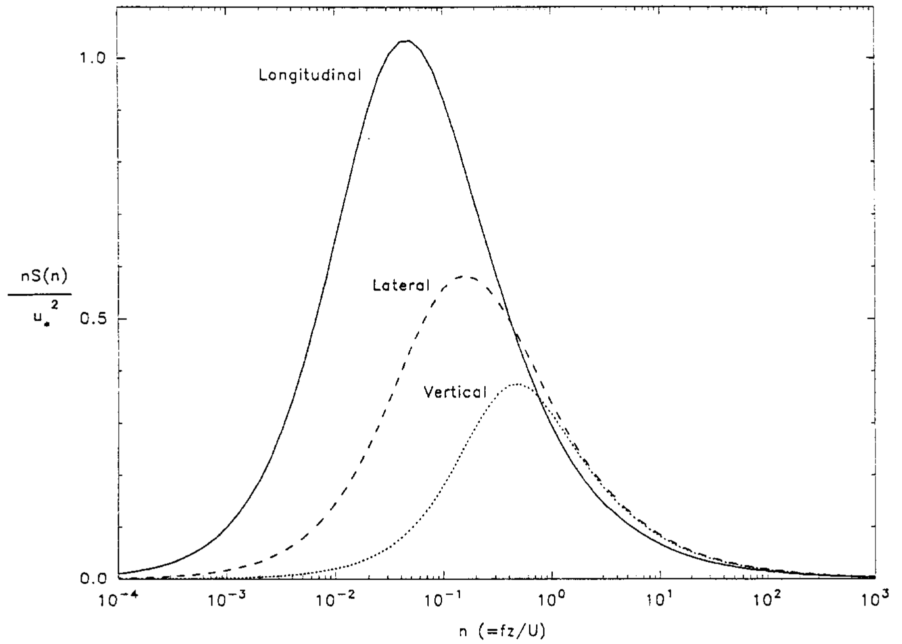

Fig. 5. Standard turbulent spectra for a neutrally stable atmosphere. Taken from Hall and Emmott ([5]), using Kaimal's standard spectral data.

Thus the turbulent eddy scales automatically adjust in size for the model as the scaled heights are reduced, as long as the other basic scaling requirements outlined earlier are observed. This argument is reasonably valid for the vertical component of turbulence, but less so for the longitudinal and lateral components. Here there are additional contributions to the turbulence components due to larger scale eddy motions generated by longer term variations in wind speed and direction. It can be difficult to separate these from the contributions of shear turbulence.

Similar arguments can be used to deal with turbulence scaling in stratified flows, using in addition the Monin–Obukhov length scale, L_m. However, as with the discussion on scaling stratified flows, there are additional complexities in the behaviour of spectra in stably stratified flows and these are not considered here.

3.8. Scaling discharged droplet size distribution and deposition

A critical feature of flashing releases is the presence of evaporating liquid droplets in the gas cloud, which result in its continued cooling. This section considers the scaling requirements for the fluid dynamic behaviour of discharged droplets, their falling speeds and inertial resistance to following the same dispersion patterns as the gas cloud. The problems of the chemical and thermodynamic equilibria of these droplets and their scaling are considered separately in Section 3.10.

Liquid droplets may form a high proportion of the discharged mass, up to about 80% of the total. A wide droplet size distribution can be expected, from droplets several millimetres in diameter (about the largest sustainable single droplet size) down to a fine aerosol at micrometre sizes. The droplet size distribution in a gas cloud will change continuously, due both to the loss of large droplets falling out of the cloud to the ground and to a general reduction in droplet size due to evaporation. The loss of large droplets falling out of the cloud depletes the cloud near the source and effectively reduces the source term. Small droplets (typically those below about 100 μm in diameter) are carried and dispersed by the cloud in the same way as the gas content. Droplets of intermediate size may be too small to deposit but have sufficient inertia to disperse at a lesser rate than the vapour in the cloud. In present numerical models droplets are divided between the two extreme regimes, accounting for the behaviour of the intermediate sizes introduces too great a complexity.

Because they are a critical feature of the cloud it is clearly necessary that the droplet behaviour should be either correctly scaled or should be shown to be independent of scale. Droplet behaviour in an airflow can be described (to first order at least) by two parameters, the falling speed in still air, v_f, V_f, and the droplet inertia. There are a number of ways of defining droplet inertia. The most convenient for present purposes is the stop distance, d, D, which indicates the length scales within which droplet inertial effects are apparent. For small droplets which fall within the Stokes (viscous) flow regime, the stop distance is defined by,

$$D = \frac{V_f U}{g}. \tag{31}$$

For large droplets, outside the Stokes flow regime, this simple relationship is lost and the stop distance diverts steadily further from Eq. (31). For the present discussion, the upper droplet diameter for this approximation can be taken to be about 50 μm, which is also the size limit of practical interest. The inertial behaviour of larger droplets will not be considered here.

On this basis, correct scaling of droplet behaviour can be obtained if,

$$\frac{v_f}{u_h} = \frac{V_f}{U_H} \text{ and } \frac{d}{l} = \frac{D}{L}. \tag{32}$$

The ratio v_f/u_h, V_f/U_H, is the angle of descent of the particle in the mean wind, which is thus required to remain the same. These scaling requirements give,

$$\frac{v_f}{V_f} = \frac{u_h}{U_H} = S_c^{0.5} \text{ and}$$

$$\frac{d}{D} = \frac{l}{L} = S_c. \tag{34}$$

Thus the particle falling speed must reduce with the square root of the scale, as does the reference windspeed, and the stop distance with the scale. If the scaling requirements for v_f and u_h are fed into the definition of stop distance, Eq. (31), we have,

$$\frac{d}{D} = \frac{v_f}{V_f} \cdot \frac{u_h}{U_H} = S_c^{0.5} \cdot S_c^{0.5} = S_c. \tag{35}$$

Thus in the Stokes flow regime, the stop distance is automatically scaled in the model if the falling speed is correctly scaled.

The ratio d/l, D/L, is, of course, the Stokes number of the flow and we are effectively requiring that its value remains the same between model and full scales. This is appropriate for correctly scaled particle behaviour.

This requirement can be relaxed if the Stokes number for the flow is small, less than 0.1 say. In this case droplet inertia becomes of steadily less importance to its dispersion pattern and the particle inertial behaviour starts to become independent of scale. The choice of reference length scale for the Stokes number is important in this case. If, as here, we are considering the behaviour of dispersing droplets, the appropriate length scale is that of the turbulence in the flow.

For the example of a model at one tenth scale, droplet falling speeds would have to reduce by about one third. In the Stokes flow regime (for small droplets) $v_f \propto d^2$. For larger droplets above about 50 μm, we have $v_f \propto d$ approximately. Thus, small droplet diameters would need to be about one half of full scale and large droplet diameters about one third. This correction for larger droplets is not strictly correct since stop distances are not properly defined by Eq. (31), but it is not proposed to consider this matter further here.In practice neither falling speed or stop distance are of much importance for the smaller droplets in the present case. A droplet of 50 μm diameter has a falling speed of about 7 cm s^{-1} and in a windspeed of 2 m s^{-1} has a stop distance of about 1.4 cm. Thus for droplet sizes below this upper bound, inertial scales are small compared with the scale of a dispersion experiment, which even at reduced scale will be of the order of metres. Also droplets will be dispersed rather than deposited if the falling speed is less than the typical turbulence velocities in the gas cloud. In a windspeed of 2 m s^{-1} with a vertical turbulent intensity of 15% (a typical value for a neutrally stable atmosphere) the turbulence velocities would be around 30 cm s^{-1}, easily sufficient to keep airborne most droplets up to 50 μm diameter.

In a practical experiment it would be more satisfactory to produce only small droplets if at all possible. Depositing large droplets deplete the source and unless the size distribution is known fairly precisely it is difficult to estimate the proportion of the source material remaining in the cloud. The main purpose of the experiment under consideration here is to examine the development of buoyancy in the gas cloud rather than the behaviour of the source. For this it is better to know the amount of material in the gas cloud precisely and that deposition losses will be minimal. From the considerations in the previous paragraph an upper size limit around 50 μm would be a reasonable value to aim for.

3.9. Scaling source momentum fluxes

A flashing release of gas, the subject of the present investigation, must discharge into the atmosphere with some degree of momentum. This must be correctly scaled along with the discharge buoyancy. The latter is automatically correctly scaled with the discharge parameters and windspeed scaling discussed previously. Discharge momentum flux is correctly scaled if the dimensionless discharge momentum flux parameter retains the same value at model and full scale. That is,

$$\frac{M_f}{U_H^2 L^2} = \frac{m_f}{u_h^2 l^2}. \tag{36}$$

Applying the scaling rules for L and U (Eqs. (6) and (11)) gives,

$$\frac{m_f}{M_f} = \left(\frac{u}{U}\frac{l}{L}\right)^2 = S_c^3. \tag{37}$$

The momentum flux m_f, M_f, is a total discharge momentum flux in whatever form the discharge takes and it is expected that this form will be similar between model and full scale. If, for example, the discharge is through an orifice of area a, (A), with velocity w, (W), then

$$M_f = W^2 A \frac{\rho_g}{\rho_a} \text{ and } m_f = w^2 a \frac{\rho_g}{\rho_a}. \tag{38}$$

Note that the discharge momentum flux used here is not a true momentum flux, it is given as a relative momentum flux with respect to air as this is a more convenient form for scaling purposes. Since the density of air is nominally 1.2 kg m^{-3}, the value of the discharge momentum flux is in fact little altered.

Since the density ratio ρ_g/ρ_a is fixed in the present model, in scaling the momentum flux it is the product $W^2 A$ which has to be scaled. Any combination of W and A which does this appropriately is acceptable, as long as the size of the discharge is small relative to the gas cloud that is produced.

In the case of discharge through an orifice, Eqs. (37) and (38) lead to,

$$\frac{m_f}{M_f} = \frac{w^2 a}{W^2 A} = S_c^3. \tag{39}$$

If the orifice areas are directly scaled, then

$$\frac{a}{A} = S_c^2, \text{so that } \frac{w}{W} = S_c^{0.5}. \tag{40}$$

Since the reference windspeed also scales as $S_c^{0.5}$, this simply means that

$$\frac{w}{u_h} = \frac{W}{U_H}. \tag{41}$$

That is, discharge velocities are then scaled in proportion to the reference windspeed.

If it is necessary to scale a flashing release at specific temperatures and pressures in order to obtain the correct thermodynamic and chemical behaviour, which is an important feature of the present work, then in practice we can expect similar discharge velocities at model and full scale ($w = W$) if the discharge pressure is sufficient to produce a choked flow. In this case, for discharge through an orifice, in order to obtain the correct discharge momentum, we must have,

$$\frac{a}{A} = S_c^3. \tag{42}$$

Thus the area of the orifice must reduce below scale in the model to compensate for the proportionately higher discharge velocity. In the case of a one tenth scale model, the orifice diameter must be about one thirtieth of full scale rather than one tenth. This argument is strictly only valid for inviscid flows. In practice the effects of Reynolds number on nozzle boundary layers would affect the flow rate at different scales. However, with the relatively modest scales considered here, such effects should be second order.

3.10. Chemical, thermodynamic and aerosol equilibria

The present interest is in a dispersing gas cloud in which there is chemical reaction (oligomerization), a thermodynamic process (cooling due to droplet evaporation and heating due to HF/water vapour interaction) and a droplet/vapour equilibrium which controls the rate of evaporation of droplets in the cloud. The rates at which these processes occur as the gas cloud disperses and entrains air are important as they directly affect the local buoyancy of the cloud. In a reduced-scale model the time scales alter in proportion to $S_c^{0.5}$ and it is clearly desirable that the local chemical and thermodynamic equilibria in the dispersing plume should not be affected by these reduced time scales. This requires either that the time scales of the various equilibria should reduce in proportion to $S_c^{0.5}$ or that they should be so short in comparison with their rate of change in the dispersing cloud that there is more or less instantaneous adjustment to local conditions. The former seems a little unlikely, but the latter is a practical possibility.

This latter assumption, of instantaneous local adjustment, is known as the homogeneous equilibrium assumption and is an important feature of most numerical models of this type of dispersion. Because of its importance it has become the subject of fairly detailed attention and its application to ammonia clouds has been investigated by Kukkonen et al. [6] and by Nikmo et al. [9]. It is also discussed in [14]. These papers consider the thermodynamic equilibria in dispersing ammonia clouds and provide a comparison with a numerical model using the homogenous equilibrium assumption and a true equilibrium. They do not give response times for the thermodynamic equilibria directly since they calculate these during the passage of a dispersing gas cloud, but the examples considered show that the homogeneous equilibrium assumption seems to hold fairly well at full scales. For the equilibrium between evaporating droplets and the surrounding air, Kukkonen et al. ([6]) comment that the assumption holds well for droplet sizes below 200 μm in diameter, which would cover almost all of the airborne aerosol.

In a reduced-scale model the factor acting against the homogeneous equilibrium assumption is the reduced time scales of the dispersing cloud. However, by the standards of equilibrium response calculations the differences between model and full-scale times are not great. In the earlier example of a one tenth scale model the time scales are reduced by about a factor of three. The variation in time scales in full-scale releases over the range of windspeeds and release rates of practical interest is far greater than this. The factors acting in its favour are the reduced physical scale of the model, which reduces the distances over which the equilibrium must be sustained (between an evaporating droplet and the vapour concentration in the surrounding air, for example) and the reduced droplet size distribution which Section 3.8 indicates is required in a model. Smaller droplets will respond more rapidly to changes in the equilibrium state.

There seems a good probability that the homogeneous equilibrium assumption will hold in a reduced-scale model. However, the matter cannot be fully resolved here and would merit some further attention.

3.11. Gas cloud lift-off

An important feature of a hydrogen fluoride release is the development of buoyancy in the gas cloud and the possibility of this buoyancy being sufficient to lift the gas cloud largely clear of the ground. This 'lift-off' phenomenon must be correctly scaled. The question of the lift-off of buoyant plumes is of more general interest, in fire plumes for example, and has been the subject of previous attention. A lift-off criterion was first proposed by Briggs [16] in an unpublished note, and has been the subject of small-scale wind tunnel experiments in [7,2,3].

Briggs proposed a lift-off criterion, L_p, of the form,

$$L_p = \frac{gH}{U_*^2}\frac{\Delta\rho}{\rho}, \tag{43}$$

where H in this case was described as 'the thickness of the plume', that is a length scale indicating the depth of the plume. Briggs suggested a (revised) value of L_p of 29, based on Meroney's experiments. Hall et al. ([2]) applied Briggs' criteria to the rise of plumes from the surface of a building (a model of a release from a nuclear reactor building) but suggested a modified version of it which incorporated the buoyancy flux in the plume. The dimensionless buoyancy flux parameter has the form,

$$\frac{F}{U_*^3 L}, \tag{44}$$

where L is a suitable length scale and the buoyancy flux F is defined as,

$$F = g\frac{\Delta\rho}{\rho}\frac{Q}{\pi}. \tag{45}$$

This has the advantage that F can be expressed directly in terms of a heat release. Hall et al. ([2]) were concerned with building interactions, so took Briggs' H as the building height, H. It was then assumed that, for a building of width B,

$$H = \frac{Q}{UB}, \tag{46}$$

on which basis Eqs. (43) and (44) become equivalent to one another. Hall et al. ([2]) also found that on this basis their experiments largely confirmed Briggs' lift-off criterion and his estimate of its value. In a scaled experiment, as considered here, the choice of a value of H can be arbitrary as it simply becomes a scaling factor for the size of the plume.

For the present scaling exercise, comparison of Eq. (10), defining the Richardson number, and Eq. (43) shows that Briggs' criterion is simply a form of Richardson's number. The dimensionless buoyancy flux used by Hall et al. ([2]) is a combination of the Richardson number and the dimensionless release rate, Eq. (17), multiplied together.

It has been noted earlier that both the Richardson number and the dimensionless release rate are correctly scaled if the earlier scaling requirements are satisfied. It follows from this that the 'lift-off' characteristics of the gas cloud should also be correctly scaled.

4. Discussion and conclusions

Table 1 gives a summary of the main scaling requirements and other results from the discussion of Section 3.

The requirements for the particular example of a one tenth scale model which has been used throughout this paper are outlined below:

- The released mass of gas reduces to one thousandth of full scale, that is kilogrammes of released gas are equivalent to tonnes.
- The windspeed at the fixed full-scale reference height has to reduce to about half of the full scale.
- All length scales, including the required surface roughness, are reduced by one tenth. This also includes the hazard boundaries of the dispersing plume.
- Time scales (including release times) are reduced by about one third.
- Continuous release rates are reduced by about one three hundredth.
- Atmospheric stability shifts by about one Pasquill stability class towards neutral.
- Atmospheric turbulence, and thus the plume dispersion rates, should scale if the other basic scaling parameters are achieved.

Table 1
Summary of scaling factors required for model for a scale S_c ($S_c = 0.1$ for a scale of 1/10)

Parameter	Scaling Factor
Characteristic length scale, L	$V^{1/3}$
Discharged gas quantity, m/M, v/V	S_c^3
All length scales, l/L, h/H, z/Z, z_0/Z_0 etc.	S_c
Windspeed, u/U, at scaled reference height h, H	$S_c^{0.5}$
Friction velocity, u_*/U_*	$S_c^{0.5}$
Time scales, t/T	$S_c^{0.5}$
Continuous releases, q/Q	$S_c^{2.5}$
Atmospheric stability:	
Monin-Obukhov length scale, l_m/L_m	S_c
Surface heat flux, h_f/H_f	$S_c^{0.5}$
Vertical temperature gradient, $\Delta\theta/\Delta\Theta$	1
Droplet falling speed, v_f/V_f	$S_c^{0.5}$
Droplet stop distance, d/D	S_c
Droplet diameter, d, (in the viscous flow regime)	$S_c^{0.25}$
Source discharge momentum, m_f/M_f	S_c^3
Discharge through an orifice:	
Orifice opening area, a/A	S_c^2
and discharge velocity, w/W	$S_c^{0.5}$
Or if $w = W$ (choked jet), a/A	S_c^3

- Scaled small discharged droplet diameters need to reduce by about half, but this is probably not a significant requirement for small airborne droplets below about 50 μm in diameter as their inertial scales and falling speeds are relatively small.
- Chemical, thermal and aerosol equilibria within the cloud should be retained, provided that the homogeneous equilibrium assumption holds.
- The momentum flux in the source discharge needs to be reduced by one thousandth. If the discharge is from an orifice whose size is correctly scaled, then the discharge velocity needs to be reduced in proportion to the scale reference windspeed, that is by about one third. If the discharge is a flashing release through a choked orifice, the discharge velocity remains fixed and the orifice diameter must reduce to about one thirtieth of full scale.
- Gas cloud buoyancy and lift-off behaviour will scale correctly if the other basic scaling parameters are satisfied.

The main conclusion from the present study is that, within some constraints, it is practicable to produce a small-scale model in the atmosphere of a larger scale flashing release of a toxic gas. All the major parameters of a model can be scaled suitably according to a set of simple rules. In particular, the meteorological parameters, windspeed, surface roughness etc., will all correctly scale.

Because the released mass of gas reduces with the cube of the assumed scale, there is a considerable reduction of the released mass at even quite modest scales. With the example of a scale of one tenth outlined above, kilogrammes of material released in a model are equivalent to tonnes of material released at full scale. Similarly the hazard boundaries for the experiment are reduced with the scale. Thus a correctly scaled experiment offers considerable attractions in both cost and safety considerations. It also greatly eases the problems of finding suitable experimental sites, which can be of much smaller extent while still containing the hazard boundaries for the release.

The main constraints on a model of this sort in the atmosphere are a lower limit to the windspeed that can be practicably modelled and a reduction in the apparent degree of atmospheric stability experienced by a model. This is due to the need for Froude number scaling of heavy gas clouds, which requires reduced windspeeds at reduced scales and enhanced atmospheric density gradients to generate equivalent levels of atmospheric stability. However, these limitations still leave a useful range of experimental conditions that can be used.

The present paper has dealt only briefly with a number of matters which would merit further consideration. The four most important are, firstly, the scaling of chemical, thermal and aerosol equilibria in the model. It has been assumed that the homogeneous equilibrium assumption holds, that is the rates of approach to equilibrium are fast compared with plume dispersion rates. This assumption is quite plausible but ought to be considered in more detail. Secondly, the behaviour of droplets in the plume, especially where there is a droplet size distribution including larger size droplets with significant falling speeds or stop distances. Thirdly, the scaling of atmospheric stability and the possibilities of obtaining the high stability levels needed to model stability at reduced scale. Finally, there is the behaviour of buoyant gas clouds lifting off the ground. This feature is fundamental to the present study and the mitigation to hazard boundaries that it might permit. Though it has been the subject of previous experiments (as outlined earlier) it is still not a very well understood phenomenon and its sensitivity to the governing parameters is not well defined.

Though the direct concern of the present work is a small-scale field release of hydrogen fluoride at the ground, the scaling principles described are generally valid for a reduced-scale field release of any material, heavier or lighter than air. Thus, for example, they could be applied equally well to a small-scale model of a fire plume (though not directly to a fire itself) or to a passive release of a heavy gas.

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