Mitigation of dense gas releases in buildings: use of simple models

D.M. Deaves [*], S. Gilham, H. Spencer

WS Atkins Consultants, Woodcote Grove, Ashley Road, Epsom, Surrey KT18 5BW UK

Abstract

When an accidental release of a hazardous material is considered within a safety case or risk assessment, its off-site effects are generally assessed by calculating the dispersion of vapour from the site. Although most installations handling flammables will be in the open air, many types of plant, particularly those handling toxics, are enclosed, partly to provide some form of containment and hence to mitigate the effects of any release. When such a release occurs within a building, the gas or vapour will undergo some mixing before emerging from any openings. The degree of mixing will depend upon the building geometry and the nature of the ventilation, which in turn may be modified by the leak. This situation is considered in this paper, with specific application to calculating the rate of release of a dense vapour from a building. All the calculations presented are based upon simple zone modelling, such that the region occupied by the vapour is assumed to be well mixed, and, in the isothermal case, either its concentration or its depth increases as it is fed by the gas leak. Transfer of air or gas/air mixture through the building openings is estimated by use of standard ventilation calculation methods. For the non-isothermal case, a preliminary model is presented in which it is assumed that there is complete mixing throughout the building and no wind-driven ventilation effects. A moderate release of chlorine is used as an example, and results are shown of the effects of various ventilation possibilities on the release rate to the atmosphere. In addition, comparisons are given between model results and experimental data, demonstrating the level of confidence which can be placed in the models, and also identifying areas where there is scope for further improvement. © 2000 Elsevier Science B.V. All rights reserved.

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[*] Corresponding author. Tel.: +44-1372-726140; fax: +44-1372-740055; e-mail: dmdeaves@wsatkins.co.uk

1. Introduction

In many industrial installations, it is possible for toxic or flammable materials to be released accidentally as vapour or as rapidly vaporising liquid within buildings. The impact on the surrounding population of such a release can then be assessed by undertaking gas dispersion calculations using a suitable source term. Determination of the source term is frequently undertaken either by ignoring the building, or by assuming complete mixing and unmodified natural ventilation within the building. In order to improve such source term estimates, research has been undertaken into this problem, using both advanced CFD techniques [1] and simpler 'zone' type models.

This paper assesses the application of zone modelling to the problem of the leakage of accidentally released gas from a building. The most relevant existing available methodologies have been assessed in relation to typical industrial accident problems, and further specific development undertaken in order to extend their range of application.

After a review of the physical processes to be modelled, brief outlines are given of the modelling for both isothermal and non-isothermal cases. Some validation of the models is given, comparing predictions with measurements from specially commissioned tests which were designed to simulate some of the important features of typical industrial releases. Finally, the use of such models in risk assessments is discussed, and recommendations given for their most effective use.

2. Physical processes

The situation considered is an accidental release of a toxic material as a result of a flange, pipework or storage tank failure. This generally results in either a vapour release (from the tank vapour space or vapour pipework) or a flashing liquid release. In contrast to flammable materials, where rapid dilution to below the LFL is desirable, the principal need for toxic releases is to contain the release. For this reason, many toxic materials are stored and processed within relatively well sealed buildings which can temporarily contain the release and thus mitigate its effect. Additionally, the work described here has focused on materials which form denser-than-air vapours such as ammonia and chlorine. A typical example would be the chlorination room of a water treatment works.

In general, the degree of mitigation provided by the containment building, and thus the rate at which the toxic material is released to atmosphere, is determined by the ventilation characteristics of the building and the details of the release. For relatively well sealed buildings, the extent of mixing is principally driven by the release characteristics, the release momentum and its geometry determining the extent of the mixing. The location and flow characteristics of any adventitious openings in the building then determine the transient release from the building. In these circumstances, the mixing and release from the building is driven by the source itself and its complex fluid dynamic and thermodynamic behaviour. For the industrial situation, there is an additional complication in that the buildings in which a release is likely to occur are large and have complex geometries, typically including storage tanks, bunds and extensive pipework runs.

For all but the most severe accidental releases, where all containment is lost, the geometrical scales of the release are likely to be small compared with those of the building. The release typically lasts of order tens of minutes, and is characterised by a two-phase flashing high speed liquid jet, which through impingement can also result in the formation of an evaporating pool, although some releases may be of vapour only. Both the mixing induced by the release and its thermodynamic behaviour are important in determining the building release characteristics. This range of physical processes, geometrical scale and time scales presents a number of significant modelling challenges: resolution of flow features which range from the details of the release through to the flow within the room; a range of turbulence levels which can potentially vary from high Reynolds number flows (in the jet) to low Reynolds number or transitional flow; geometrical features which vary in scale from room scale to the scale of the pipework; transient dense gas build-up with potential for significant stratification; two-phase flow and heat transfer.

In principle, all these features can be incorporated within CFD modelling, albeit with varying levels of confidence. The CFD modelling approach has been considered, and results of CFD application and sensitivity studies are presented by Gilham et al. [1]. The alternative is to make some gross simplifications and assumptions to enable zone models to be developed. This approach is taken in the modelling described here, which is in two separate parts, depending upon the nature of the release. For vapour releases, it is assumed that the system is isothermal and detailed modelling has been undertaken relating to the effects of opening size and location, wind driven ventilation, etc. For flashing liquid releases, thermodynamic effects are important, and temperature and pressure are included as calculated variables. However, the non-isothermal modelling only considers the case of a fully mixed flow at present. The various physical processes considered in each model are set out below.

3. Isothermal model

3.1. Assumptions

Gas is released at a steady rate into a volume of uniform horizontal cross-sectional area and fixed height. The building volume has openings, adventitious or otherwise, at a specified height above the floor, and at the base, whose areas are specified (either could be zero). The geometrical arrangement is shown in Fig. 1. In all the equations derived and calculations presented, it is assumed that the gas density is greater than that of air (e.g., chlorine); similar considerations apply to low density releases, but the method does require a non-zero density difference between gas and air.

It is assumed that there is no significant pressurisation of the building. In practice, although this restricts the model to relatively small releases, this is not considered to be a significant limitation, as larger releases would almost certainly be of flashing liquid. It should also be noted that large instantaneous releases could result in sufficient over-pres-
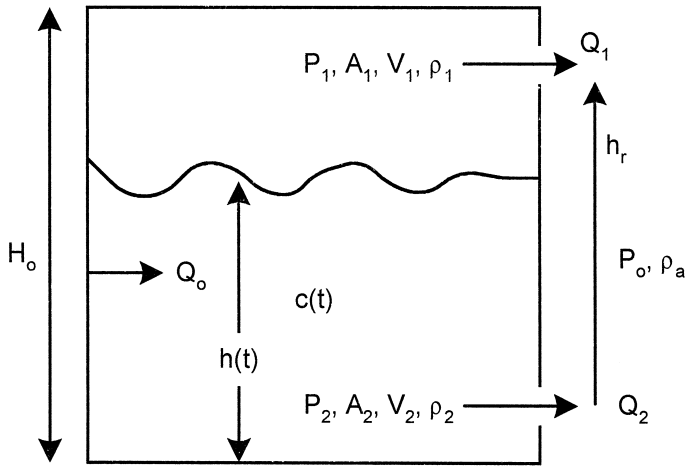
Fig. 1. Schematic diagram of model of isothermal release within a building.

surisation that the containment is compromised. The assumption of no pressurisation implies that there is a balance between the volumetric leak rate into the building and the net volumetric outflow from the building openings. Because of the isothermal assumption, any natural ventilation due to thermal buoyancy forces has been ignored. Such effects can be shown to be small compared with the likely magnitude of wind driven ventilation or even gravity-driven flows set up by the dense gas release.

The model allows for two separate well-mixed zones within the building, whose depths may vary with time, one of which contains vapour while the other does not. This allows the modelling of cases where the momentum of the leak may be insufficient to induce significant mixing, resulting in a layer of high concentration whose depth steadily increases. Options are therefore provided so that various degrees of mixing can be specified. This is slightly simplified compared with the model of Cleaver et al. [2], which includes a third zone which is a variable interface. The Cleaver model was concerned with internal gas build-up, and therefore did not include the effects of ventilation or of release from the building.

The natural ventilation of a building due to the ambient wind can be calculated from information given in BS 5925 [3]. This gives pressure coefficients on the faces of buildings for normal incidence, but does not cover oblique incidence. The ventilation rate is dominated by the location of the openings, with the most effective ventilation occurring when there are openings upwind and downwind. It is therefore assumed that openings are on these faces, and that the wind-driven ventilation rate is unaffected by whether these openings are at high or low level.

It is assumed that the two openings are on the upwind and downwind faces, respectively. However, due to the vapour density effects, the flow regime depends upon whether the low level opening is on the upwind or downwind face. The two possibilities are illustrated in Fig. 2. In the *enhanced* mode (Fig. 2a), the tendency of the dense gas to drive a flow through the lower opening is enhanced by the action of the wind,

a)   **Enhanced Mode**
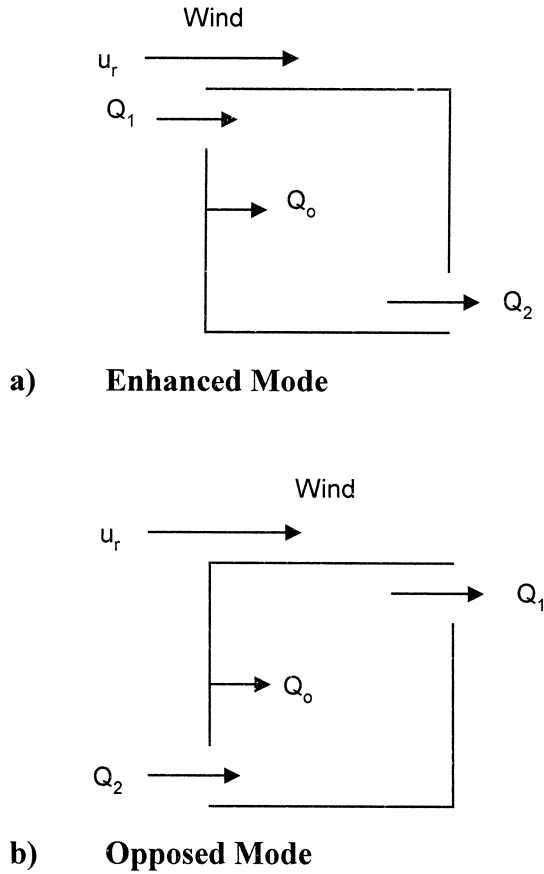

b)   **Opposed Mode**

Fig. 2. Combined effects of ventilation and dense gas release.

whereas it is *opposed* in Fig. 2b. In this latter case, it is possible that the gas build-up in the building is sufficient to prevent the ventilation wind flow entering the lower opening. It should be noted, however, that the model relates to mean air flow through openings. In practice, even when mean pressures are nominally equal across an opening, both diffusion and fluctuations due to turbulence in the atmosphere will result in some exchange between interior and exterior regions.

3.2. Flow regimes considered

The complexity of the equations, and of their solution technique, depends upon the number, locations and sizes of the openings and on the existence or otherwise of wind effects. Model equations for the following subset of possible conditions have been set out in Section 3.3.

3.2.1. Single opening, no wind

The volumetric inflow and outflow rates are equal. The emission from the building is then purely dependent upon the height of the opening and the mixing assumptions made within the building.

3.2.2. Multiple openings, no wind

Where there is more than one opening at the same horizontal level, the assumption of complete mixing in a horizontal plane implies that the flow patterns follow those for single openings, but with the efflux from each outlet distributed according to its area. If openings are at different levels, and the release is of a dense gas, a stratified layer begins to form in the lower part of the building, resulting in a hydrostatic driving pressure which would ensure that gas leaked preferentially from the lower opening. As the dense layer builds up in the base of the building, the total volume outflow from the lower opening increases. Since the flow is essentially incompressible, the net inflow and outflow must balance, suggesting that, at some point, the outflow from the lower opening may exceed the gas release rate and hence implying that the flow at the top opening is reversed. Finally, a steady state is reached in which a fixed layer depth and concentration results in a volume outflow at the lower opening which exceeds the gas release rate.

3.2.3. Multiple opening, wind driven ventilation

The ventilation rate is dominated by the location of the openings, with the most effective ventilation occurring when there are openings upwind and downwind. It is therefore assumed in this discussion that openings are on these faces, and that the initial wind-driven ventilation rate is unaffected by whether these openings are at high or low level. As noted above, the flow regime can be either enhanced or opposed, depending upon whether low level openings are on the leeward or windward face, respectively. This gives the potential for inflow or outflow at either opening, requiring different equations in each case.

3.2.4. Concentration decay

Once the leak has stopped, either through activation of a valve or depletion of the inventory, the flow pattern changes. In the cases considered here, there will be no external ventilation, and therefore a 'drainage' flow is set up, driven purely by the density difference remaining in the building. It is assumed that buoyancy driven ventilation is initially dominant and during this phase the gas layer height reduces while the concentration remains fixed.

3.2.5. Doorway flows

Where the opening has significant vertical extent, it is possible for a stratified internal gas layer to set up a 'doorway exchange' type of flow, independently of any wind effects or of any flow being driven by an internal release. The effects of such flows are likely to be greatest when there is little wind effect and there is no gas release. Thus, doorway flows would be of greatest application to the decay phase for a single distributed opening.

3.3. Model equations

The model which has been developed for isothermal releases is known as GRAB (Gas Release Attenuation by Buildings) and is based upon the equations described below.

3.3.1. Single opening, no wind

Inflow and outflow must balance, giving $Q_0 = Q_1$ or Q_2. The gas layer builds up from the floor, implying that, for a layer depth less than the height of the top opening, gas only leaves the room if the opening is at low level. In this case

$$Q_0 = Q_2 \qquad (3.1)$$

The build up of gas within the room is given by

$$A\frac{\mathrm{d}(hc)}{\mathrm{d}t} = Q_0 - Q_2 c(t) \qquad (3.2)$$

where h or c remains constant, depending on the mode of mixing assumed.

In this case, solutions are fairly trivial and can be obtained analytically. For example, with h fixed at the height of the building,

$$c = 1 - \mathrm{e}^{-t/t_0} \qquad (3.3)$$

where t_0 $(= V_0/Q_0)$ is the filling timescale of the release, $(V_0 =$ building volume$)$.

3.3.2. Multiple openings, no wind

Equations can be developed to cover the various stages of a transient in this case; those which follow deal with the initial gas-build-up stage prior to flow reversal at the top opening. After this, an indication is given of how the equations are modified to deal with the further build-up to the final steady state, with inflow at the top opening. It should be noted that effective opening areas A_1 and A_2 are used, incorporating any discharge coefficients.

The balance of inflow and outflow at any given time enables relationships to be determined between Q_2, c and h as a function of the parameters Q_0, A_1, A_2 and ρ_g, the density of the undiluted contaminant gas. The form of the equations depends upon whether Q_1 is positive or negative. For the case with outflow from both openings $(Q_1 > 0)$,

$$Q_1 = A_1 v_1$$
$$Q_2 = A_2 v_2$$
$$Q_0 = Q_1 + Q_2$$
$$P_1 - P_0 = \frac{1}{2}\rho_a v_1^2$$
$$P_2 - P_0 = \frac{1}{2}\rho_2 v_2^2$$

This gives

$$P_2 - P_1 = \frac{1}{2}\left(\rho_2 v_2^2 - \rho_a v_1^2\right) = \Delta P \qquad (3.4)$$

where ΔP is a function of the density difference between top and bottom;

$$\Delta P = (\rho_2 - \rho_a)gh = c(\rho_g - \rho_a)gh = c\Delta\rho gh \tag{3.5}$$

Manipulating these relationships, and setting $\rho' = \Delta\rho/\rho_a$ gives:

$$Q_2^2\left(\frac{1}{A_1^2} - \frac{1+c\rho'}{A_2^2}\right) - \frac{2Q_0Q_2}{A_1^2} + \frac{Q_0^2}{A_1^2} + 2c\rho'gh = 0 \tag{3.6}$$

Eq. (3.6) therefore provides a relationship between the three variables c, h and Q^* $(= Q_2/Q_0)$ which is generally valid in the region where $Q_0^* < Q^* < 1$. Setting $A^* = A_1^2/A_2^2$, the equation can be manipulated to give a quadratic equation for Q^*:

$$\alpha Q^{*2} + \beta Q^* + \gamma = 0 \tag{3.7}$$

where:

$$\alpha = A^*(c\rho'+1) - 1$$
$$\beta = 2$$
$$\gamma = -(1 + 2c\rho'X) \tag{3.8}$$

and

$$X = \frac{ghA_1^2}{Q_0^2} \tag{3.9}$$

It can be seen that, for fixed geometry (A_1, A^*) and release (Q_0, ρ'), the coefficients α, β and γ are functions of c and h. After flow reversal, there is outflow from the lower opening only. Q_1 is now an inflow, such that $Q_0 = Q_2 - Q_1$ and $\Delta P = 1/2(\rho_2 v_2^2 + \rho_a v_1^2)$. A similar manipulation to that given above gives Eq. (3.7) again, but this time with

$$\alpha = A^*(c\rho'+1) + 1$$
$$\beta = -2$$
$$\gamma = 1 - 2c\rho'X \tag{3.10}$$

Eqs. (3.7) through (3.10) apply at any time during the relevant parts of the transient. In order to obtain the time history of any gas build-up scenario, the appropriate relationships should be combined with Eq. (3.2).

3.3.3. Multiple openings, wind driven ventilation

For ventilation driven only by the wind, BS 5925 [3] gives:

$$Q_w = A_w u_r (\Delta c_p)^{1/2} \tag{3.11}$$

Δc_p = change in pressure coefficient across building

u_r = reference ambient windspeed (ms^{-1})

$$A_w = \frac{A_1}{\sqrt{1 + A^*}}$$

Δc_p is dependent upon the orientation of the building relative to the incident wind flow. A value of around 1 is appropriate for normal incidence, and the variation with angle is only slight. $\Delta c_p = 1$ has therefore been assumed in this model.

The wind driven ventilation will begin to dominate over the release effects when Q_w exceeds Q_0. For a release rate of 1 m³ s⁻¹ (3 kg s⁻¹ for chlorine), it can be shown that, for a very 'tight' building ($A_1 = 0.1$ m²), a strong wind (> 14 m s⁻¹) is required before wind ventilation effects dominate, whereas the wind is likely to affect the gas build-up for $A_1 = 1$ m² for much of the time ($u > 1.4$ m s⁻¹). Hence wind effects dominate for most windspeeds when $Q_0 = 0.1$ m³ s⁻¹, even for a 'tight' building.

As noted above, the release from the building is either enhanced or opposed. In either case, Eq. (3.7) will still apply, but with γ modified as indicated below. The *enhanced* mode is complicated by the fact that the flow at the top opening can be reversed initially.

The *opposed* mode is also complicated, but this time by the fact that flow can now enter through the bottom opening. This is the case when a solution for Q^* cannot be found or if a negative Q^* is found. In either case, Q_2 is set to zero and the gas inside the building builds up until the hydrostatic pressure is sufficient to drive the flow out through the bottom opening against the wind, or until it emerges from the top opening. It can then be shown that:

$$\gamma = \pm 1 - 2c\rho' X \pm \frac{A_1^2}{Q_0^2} u_r^2 \tag{3.12}$$

where the first $\pm$ refers to after $(+)$ and before $(-)$ flow reversal, respectively, and the second $\pm$ refers to opposed $(+)$ or enhanced $(-)$ mode.

If, in the opposed mode, it is found that there is inflow through the bottom opening, the gas builds up as in the case of a building with only a high level opening. This continues until a positive value for Q^* can be found.

3.3.4. Concentration decay

The calculations presented above have been undertaken for the gas build-up phase, during which the release rate into the building Q_0, is constant. The calculation of the transient for the decay after the leak has stopped follows a similar methodology to that already presented, except that $Q_0 = 0$. The initial conditions for height and concentration are the conditions predicted within the build-up phase when the release ends.

The relevant equations are those for reversed flow, since during the decay phase there is inflow through the top opening to balance the outflow from the lower opening. It can be shown, after some manipulation that:

$$Q_2 = A_1 \sqrt{\frac{2c\rho' g(\pm u_r^2)}{A^*(c\rho' + 1) + 1}} \tag{3.13}$$

$$= 0 \text{ for } u_r^2 > 2c\rho' gh \text{ in the opposed mode}$$

.

$$\frac{d(hc)}{dt} = -\frac{cQ_2}{A_0}. \tag{3.14}$$

For $u_r = 0$, assuming c is constant, this can be solved analytically to give:

$$h = \left(\sqrt{h_r} - \frac{A_1}{2 A_0} \sqrt{\frac{2 c \rho' g}{A^* (c \rho' + 1) + 1}} (t - T_r) \right)^2 \tag{3.15}$$

where T_r is the time at which the decay phase starts (the release time) and h_r is the height of the gas layer at this time. This phase continues until the height reaches zero or wind driven ventilation takes over.

3.3.5. Doorway flows

For a doorway of height H and width w, Wilson and Kiel [4] give the following formula for the volumetric flow rate induced, Q:

$$Q = \frac{K}{3} w \left(g' H^3 \right)^{1/2}. \tag{3.16}$$

where: $g' = g \, \Delta \rho / \rho_a$; $\Delta \rho$ = density difference between inside and out; ρ_a = density of air; K = door orifice coefficient.

Similar formulae are given by Linden et al. [5] and BS 5925 [3]. However, in these cases, K is replaced by 0.25 and C_d, respectively, where C_d is a discharge coefficient (~ 0.61). On the basis of a series of experiments, Wilson and Kiel found that K varied with g', taking values between 0.4 and 0.6. For the purposes of this study, it was decided to take a constant value of $K = 0.4$.

It should be noted that the flow rate Q in Eq. (3.16) represents flow both into and out of the building. Thus, in the case of a dense gas release, Q m^3 s^{-1} of vapour/air mixture leaves the building from the lower half of the doorway and Q m^3 s^{-1} of fresh air enters through the upper half. Eq. (3.16) can be used directly in the decay phase, where relevant. During the gas build-up phase, it is theoretically possible for such an exchange flow to be set up above the escaping gas/air mixture. This effect is modelled by matching the velocity of the exchange flow with that of the direct outflow beneath it.

3.4. Solution technique

Several of the equations identified above have simple analytical solutions. These can in principle be applied sequentially through the various stages of a transient, although it is necessary to keep track of the depth and concentration of the vapour/air layer, and the flow direction through the various orifices. In practice, solutions are obtained using standard Runge–Kutta integration techniques in the program GRAB (Gas Release Attenuation in Buildings), which incorporates the logic to ensure that the correct forms of the equation are used at each stage.

4. Non-isothermal model

4.1. Assumptions

The contents of the room are assumed to be fully mixed, implying that a one-dimensional model can be developed, as opposed to a set of spatial differential equations which would require computational fluid dynamics in order to find a solution. It is

assumed that the pressurised liquid material enters the room, which is initially at ambient pressure and temperature and is full of air, at a constant rate and at ambient temperature, and that the room has only one opening to the external environment.

Once the material has entered the room, a proportion flashes off immediately and, of that remaining, a further proportion vaporises at a rate which depends on the temperature of the room. When the material vaporises, the gas mixes completely with the contents of the room. The unvaporised, liquid, material forms an aerosol, which also mixes completely with the contents of the room. Pool formation and subsequent evaporation has not yet been incorporated into the model. After a proportion has flashed off, the heat of vaporisation of the remainder of the vaporising material is taken from the contents of the room, which uniformly reduces in temperature.

Heat transfer occurs from the walls, and varies as the room temperature and wall temperature vary. The temperature varies through the thickness of the walls, which have constant properties across their width. Ambient air outside the room heats the walls and the walls heat the contents of the room. The heat transfer coefficients at the wall internal faces are assumed to be due to natural convection. Additional heat transfer between the walls and the material droplets occurs when the temperature of the room reduces to the boiling point of the material.

The state of the room is assumed to pass through two phases. First, when the temperature is above the boiling point, all of the pollutant either flashes off immediately or vaporises soon after. The vaporising liquid mixes with the contents of the room and reduces the temperature, which falls until either a steady state is approached or the boiling point of the pollutant is reached. If the heat transfer from the walls is sufficiently large, a steady state temperature can be reached above the boiling point. Otherwise the temperature reaches the boiling point and the second phase of the calculation is reached. During this phase, the temperature remains at the boiling point of the pollutant but only a fraction of the liquid pollutant released into the room vaporises. It is assumed that the concentration of gaseous pollutant is sufficiently high that liquid does not evaporate to take the temperature below the boiling point — i.e. the liquid and vapour phases are in equilibrium.

Outflow from and inflow to the room are calculated from the pressure differences between inside and out. Hence, if the pressure inside the room is less than ambient, air enters through the opening, thereafter instantaneously and completely mixing with the contents of the room. Conversely, if the pressure inside the room is greater than ambient, gas/air/liquid mixture from the room leaves through the opening.

4.2. Model equations

The model which has been developed is referred to as GRAB-T (GRAB-Thermal effects). It consists of equations for the rates of change of four independent variables, temperature, T, density, ρ_t, and mass fraction of gaseous and liquid pollutant, c_g and c_ℓ and also an equation for the temperature profile through the wall. The equations for the rates of change of these independent variables are defined in terms of the independent variables and various other dependent variables, such as the pressure in the room, the flow rate through the opening and the evaporation rate of pollutant.

4.2.1. Flow in the room

The average molecular mass of the gaseous mixture in the room, m_{ga}, is given by:

$$m_{ga} = \frac{m_a m_g (1 - c_\ell) m_c}{m_g - m_a}. \tag{4.1}$$

where:

$$m_c = \frac{m_g - m_a}{m_g (1 - c_\ell) - c_g (m_g - m_a)}.$$

The average density of the gaseous mixture in the room, ρ_{ga}, is given by:

$$\rho_{ga} = \rho_c \, \rho_t (1 - c_\ell) \tag{4.2}$$

where:

$$\rho_c = \frac{\rho_\ell}{\rho_\ell - c_\ell \rho_t}.$$

The pressure in the room, P, is given by

$$P = \frac{\rho_{ga} R_0 T}{m_{ga}} \tag{4.3}$$

The flow rate through the opening, $\dot{m}_d$, is given by:

$$\dot{m}_d = \begin{cases} -\rho_0 C_d A_d \sqrt{\dfrac{2}{\rho_0}(P_a - P)} & \text{if } P_a > P \\[4mm] \rho_t C_d A_{d_t} \sqrt{\dfrac{2}{\rho_t}(P - P_a)} & \text{if } P > P_a \end{cases} \tag{4.4}$$

The other important dependent variable is the evaporation rate of pollutant $\dot{m}$. This is different for each phase. When the temperature is above the boiling point, $\dot{m}$ is given by

$$\dot{m} = \dot{m}_0 \tag{4.5}$$

When the temperature is at the boiling point and flow is inward, $\dot{m}$ is given by

$$\dot{m} = \frac{\left\{ \dot{m}_0 \left[F_f H + \dfrac{1}{2} v_0^2 + \dfrac{P}{P_\ell - c_\ell \rho_t} \right] - \dot{m}_d \left[c_{p,a}(T_a - T_b) + \dfrac{1}{2} v_d^2 + \dfrac{P}{\rho_t} \dfrac{1 + m_c c_g}{1 - c_\ell} \right] + q \right\}}{H + \dfrac{P}{\rho_t (1 - c_\ell)} \left(m_c (1 - c_g - c_\ell) - \dfrac{\rho_\ell - \rho_t}{\rho_\ell - c_\ell \rho_t} \right)}. \tag{4.6}$$

When the temperature is at the boiling point and flow is outward, $\dot{m}$ is given by

$$\dot{m} = \frac{\left\{ \dot{m}_0 \left[F_f H + \frac{1}{2} v_0^2 + \frac{P}{\rho_\ell - c_\ell \rho_t} \right] - \dot{m}_d \left[\frac{1}{2} v_d^2 + \frac{P}{\rho_t} \frac{\rho_\ell}{\rho_\ell - c_\ell \rho_t} \right] + q \right\}}{H + \frac{P}{\rho_t(1 - c_\ell)} \left(m_c(1 - c_g - c_\ell) - \frac{\rho_\ell - \rho_t}{\rho_\ell - c_\ell \rho_t} \right)}. \quad (4.7)$$

When the pressure difference between the room and the outside air is small, slightly different equations are used. The flow rate through the opening is given by:

$$\dot{m} = \dot{m}_0 - V_r \frac{\rho_t^2}{\rho_\ell} \left[m_c(1 - c_\ell) \frac{\mathrm{d}c_g}{\mathrm{d}t} - \frac{1 - c_\ell}{T} \frac{\mathrm{d}T}{\mathrm{d}t} + \left(\frac{\rho_t - \rho_{ga}}{\rho_\ell} + m_c c_g \right) \frac{\mathrm{d}c_\ell}{\mathrm{d}t} \right], \quad (4.8)$$

and the pressure in the room is given by:

$$P = \begin{cases} P_a - \dfrac{1}{2} \left(\dfrac{\rho_0 \dot{m}_d}{C_d A_d} \right)^2 & \text{for } \dot{m}_d < 0 \\[4mm] P_a + \dfrac{1}{2} \left(\dfrac{\rho_t \dot{m}_d}{C_d A_d} \right)^2 & \text{for } \dot{m}_d > 0 \end{cases}. \quad (4.9)$$

Next the relations for the rates of changes of the dependent variables are defined. The rate of change of density, ρ_t, is given by

$$\frac{\mathrm{d}\rho_t}{\mathrm{d}t} = \frac{1}{V_r} (\dot{m}_0 - \dot{m}_d). \quad (4.10)$$

The rate of change of mass fraction of gaseous pollutant in the room, c_g, is given by:

$$\frac{\mathrm{d}c_g}{\mathrm{d}t} = \begin{cases} \dfrac{1}{V_r \rho_t} \left\{ \dot{m} - c_g \dot{m}_0 + c_g \dot{m}_d \right\} & \text{if } \dot{m}_d < 0 \\[4mm] \dfrac{1}{V_r \rho_t} \left(\dot{m} - c_g \dot{m}_0 \right) & \text{if } \dot{m}_d > 0 \end{cases} \quad (4.11)$$

The rate of change of mass fraction of liquid pollutant, c_ℓ, is given by:

$$\frac{\mathrm{d}c_\ell}{\mathrm{d}t} = \begin{cases} \dfrac{1}{V_r \rho_t} \left\{ \dot{m}_0(1 - c_\ell) - \dot{m} + c_\ell \dot{m}_d \right\} & \text{if } \dot{m}_d < 0 \\[4mm] \dfrac{1}{V_r \rho_t} \left(\dot{m}_0(1 - c_\ell) - \dot{m} \right) & \text{if } \dot{m}_d > 0 \end{cases} \quad (4.12)$$

When the temperature, T, is at the boiling point, the rate of change of temperature is zero.

When the temperature is above the boiling point and flow is inward, the rate of change of T is given by:

$$\frac{dT}{dt} = \frac{T}{V_r\left(\rho_t c_p T - P\right)}$$

$$\times \left\{ \begin{array}{l} \dot{m}_0\left[\dfrac{P}{\rho_t}\left(1 - m_c\left(1 - c_g\right)\right) - c_p\left(T - T_b\right) - \left(1 - F_f\right)H + \dfrac{1}{2}v_0^2\right] \\[2mm] -\dot{m}_d\left[\dfrac{P}{\rho_t}\left(1 + m_c c_g\right) - c_p\left(T - T_b\right) + c_{p,a}\left(T_a - T_b\right) + \dfrac{1}{2}v_d^2\right] + q \end{array} \right\}$$

$$(4.13)$$

and when flow is outward, T is given by:

$$\frac{dT}{dt} = \frac{T}{V_r\left(\rho_t c_p T - P\right)} \left\{ \begin{array}{l} \dot{m}_0\left[\dfrac{P}{\rho_t}\left(1 - m_c\left(1 - c_g\right)\right) - \left(1 - F_f\right)H + \dfrac{1}{2}v_0^2\right] \\[2mm] -\dot{m}_d\left[\dfrac{P}{\rho_t} + \dfrac{1}{2}v_d^2\right] + q \end{array} \right\}$$

$$(4.14)$$

where c_p is the overall heat capacity of the room contents, given by:

$$c_p = \left(1 - c_g - c_\ell\right)c_{p,a} + c_g c_{p,g} + c_\ell c_{p,\ell} \qquad (4.15)$$

4.2.2. Temperature profile through the walls

The temperature at the inner surface of the walls is required in order to calculate the heat transfer rate to the room, q. Therefore, the transient temperature profile through the wall is found from the solution of the one dimensional heat equation. The boundary conditions on either side of the wall are defined using different heat transfer coefficients between the wall and the ambient air, and between the wall and the room. These are currently based upon natural convection flows, but it is intended to review this assumption in the future development, particularly in the light of the results of the validation studies presented in Section 5.

4.3. Solution technique

A set of four coupled first order linear ordinary differential equations are produced as a result of the above modelling. Since no analytical solutions are available, they are solved numerically using Runge–Kutta techniques. In this case, appropriate logic is also incorporated to determine whether the temperature is at or above the liquid boiling point, and therefore to invoke the relevant equations.

5. Model validation

The review of Hall et al. [6] identified a number of data sets relating to ventilation flows, most of which only considered the flow patterns and air quality within the rooms. The review also identified a different type of experiment, which was primarily designed to allow the rate of gas build-up within an enclosure to be determined. This included internal gas build-up studies by Cleaver et al. [2]. Gilham et al. [7] considered these data in more detail and concluded that the data available did not adequately cover the conditions which may be of interest for QRA studies, and hence for typical GRAB or GRAB-T applications. A series of tests was therefore commissioned by HSE using the experimental facilities at Silsoe. These have been presented by Gilham et al. [8], and provide some useful information for at least a partial validation of GRAB.

In addition, one third scale model tests were undertaken by the Health and Safety Laboratory, in order to represent typical chlorine releases into a chlorination room. These involved a release of Freon-22 into the room, which had openings which were representative of a real chlorine site. In view of the thermal properties of the Freon-22, the tests were not isothermal, and temperature measurements were taken as well as the concentration measurements. Full details of the experiments and of the data have been given by Bettis and Allen [9]. Although these were undertaken primarily for CFD validation [1], the results are used here to assess the performance of GRAB.

5.1. Comparison for isothermal model, GRAB

A series of gas build-up tests has been conducted at Silsoe Research Institute [8], primarily to provide validation for CFD modelling. Six tests were undertaken in which CO_2 was released into a 2.44 m cubical enclosure at two release rates (0.6 and 0.95 m^3 min^{-1}) and with three different opening configurations (top, bottom or both). In the context of the simple model developed here, the results with two openings are of greatest interest, i.e., Runs 4 (0.6 m^3 min^{-1}) and 7 (0.95 m^3 min^{-1}). For these runs, it appeared that a fairly well-mixed layer was formed covering roughly the lower 2/3 of the building height, being slightly greater for the higher release rate. It was therefore considered appropriate to use the fixed layer depths of 1.4 m (Run 4) and 1.5 m (Run 7) in the simple modelling.

The CO_2 was released via a flexible bag which acted as an intermediate containment. This allowed its temperature to equalise with the ambient temperature, and enabled it to be released at a higher rate than would have been possible purely from the supply cylinder. Although this system worked reasonably well, it did result in some leakage of air into the CO_2 supply, giving initial release concentrations of 70% for Run 4 and 80% for Run 7. The variation of concentration with time for these runs is shown in Figs. 3 and 4, respectively, in which the GRAB results are normalised by the release concentration.

When considering these plots, it should be noted that the simple model results are based on the assumption of a uniform concentration throughout the mixed layer. The results will also depend upon the layer depth which has been used, and would, for example, be closer to the experimental data for Run 4 if a slightly lower depth
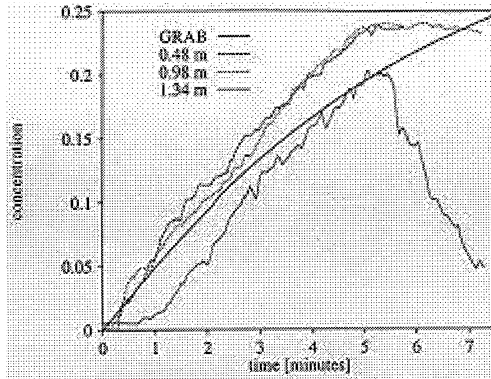
Fig. 3. Comparison of GRAB results with measurements for Silsoe Run 4 (the heights are those of the measurement locations).

(< 1.4 m) was used. With these reservations, it can be seen that there is reasonable agreement between model and experiments, although model constants can clearly be adjusted to achieve a 'good fit'.

The openings in the experiment were designed primarily to ensure that there was no significant pressure build-up within the enclosure. Their area, 0.01 m^3, was therefore sufficiently small that they did not have a large effect on the gas build-up. The comparisons given in Figs. 3 and 4 can therefore hardly be considered to be a detailed validation of the methodology developed in the preceding sections. In practice, these results have been most useful in demonstrating the existence of a well-mixed layer whose depth is less than the complete building height.

Results from GRAB were also compared with Trial 4 of the HSL tests, a high release rate jet of freon into a room which represented a typical chlorine room at 1:3 scale (see Fig. 5). Gas samplers at different heights throughout the room showed that the freon is well mixed, so the complete mixing assumption was used. The only exit from the room is a pair of ducts which open into the room near the floor and combine into one duct
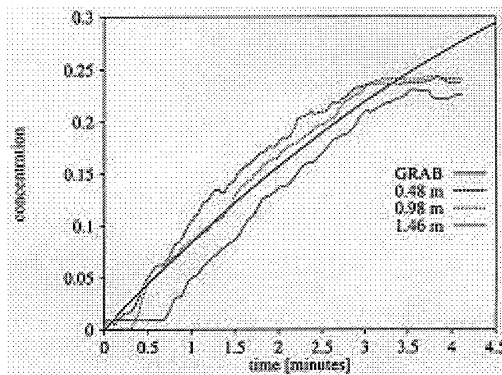

Fig. 4. Comparison of GRAB results with measurements for Silsoe Run 7 (the heights are those of the measurement locations).
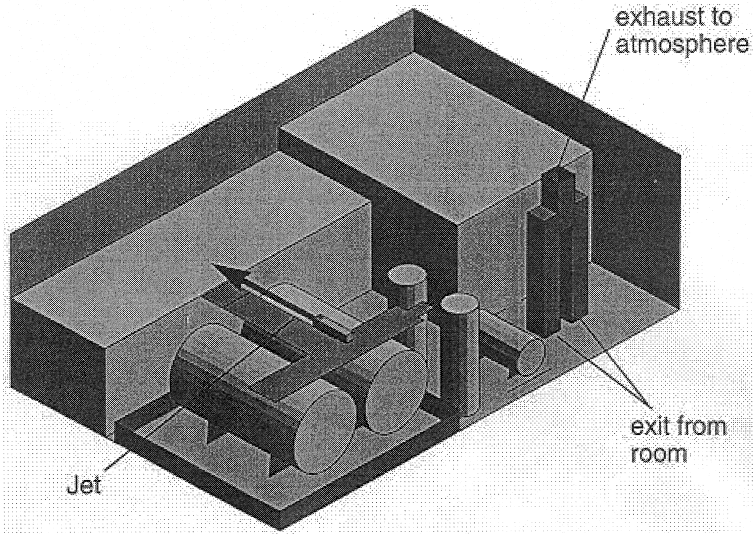
Fig. 5. Room geometry for HSL Trial 4.

before exhausting the gas through the ceiling. Therefore, the opening through which the gas leaves the room is not distributed in height and is at a low level. GRAB is applied in this case, using a fixed layer depth equal to the room height (~ 2.4 m).

A comparison between the concentrations calculated by GRAB and the concentrations measured at the room exit is shown in Fig. 6. The concentration gradient (dc/dt)
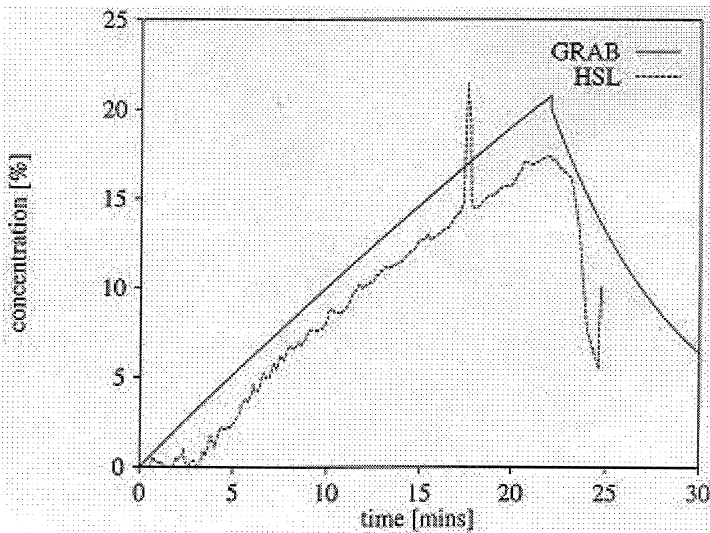

Fig. 6. Comparison of GRAB results with measurements from HSL Trial 4 made in the room outflow.

compares well, showing that the complete mixing assumption is appropriate for this case. However, there is a delay before the concentration starts to increase in the trial results. This is due to the initial drop in temperature as the freon vaporises, which reduces the volume of the contents of the room and therefore delays outflow from the room; in Trial 4, outflow is delayed by about 3 min.

5.2. Comparisons for temperature-dependent model, GRAB-T

Comparisons of the current model predictions have been made with the results of HSL Trial 4, for which time dependent measurements of temperature and concentration are available. Comparisons are made with the measurements of temperature and volumetric concentration in the exhaust.

The test room has a height of 2.4 m, a wall total surface area of 123 m^2 and a volume of 52.7 m^3. Since GRAB-T requires the height, breadth and width of a simple, rectangular room, an equivalent width and breadth are chosen to give the correct surface area and volume. The walls are predominantly made of 15 mm thick medium density fibreboard, and appropriate thermal properties are used. The jet velocity at the point where the flash fraction has just flashed off is assumed to be the local speed of sound through dry air at the boiling temperature, and the measured flow rate of 0.032 kg s^{-1} was used.

Four GRAB-T calculations were performed, with different heat transfer coefficients, and the results are compared with temperature measurements made in the exhaust during Trial 4 in Fig. 7. It was found that using the natural convection heat transfer coefficient
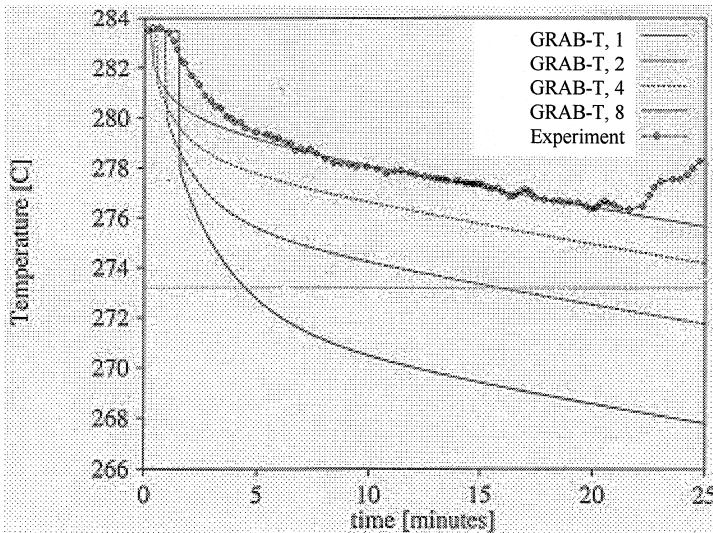

Fig. 7. Average temperature profile for Trial 4.

under-estimates the heat transfer from the walls hence giving under-predictions of temperature (see curve GRAB-T, 1 on Fig. 7). This probably indicates that forced rather than free convection heat transfer coefficients should be used, but may also be as a result of the impingement of the jet on the wall. Such effects cannot be included in such a simple, one dimensional model; to predict this behaviour, detailed information about the geometry of the room and position of the release are required, then computational fluid dynamics is required in order to solve the system taking into account this information. Multipliers on the heat transfer coefficient of 2, 4 and 8 are therefore used, and the results of these calculations are also shown in Fig. 7. This shows that the heat transfer coefficient has to be multiplied by a factor of 8 to achieve agreement between the measurements in the exhaust and the predictions. This would raise the heat transfer coefficient from 2 to 16 W m^{-2} K, which is consistent with the difference between natural to forced convection.

A comparison between the volumetric concentration calculated by GRAB-T and measurements made in the exhaust during Trial 4 is shown in Fig. 8. This shows that, between 2 and 3 min after the beginning of the release, the concentration calculated by GRAB-T is significantly too high. After this time, the agreement is better, but the measurements always lag slightly behind the predictions. This is due to the long exhaust region in the test room, resulting in a time delay before the conditions in the room reach the sampler in the exhaust.

Fig. 9 shows the mass flow rate of mixture passing through the opening. Initially, air enters the room due to the negative pressure in the room caused by the drop in temperature and therefore density. When the temperature in the room levels out due to heat transfer from the walls, vapour/air mixture begins to flow from the opening. This
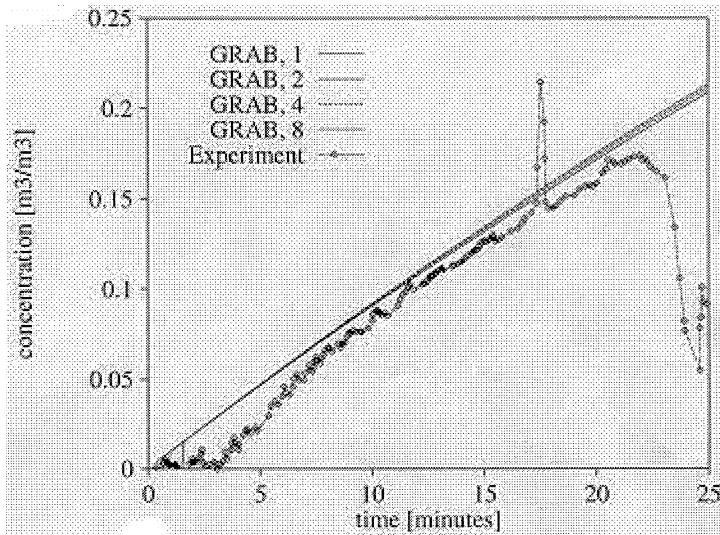

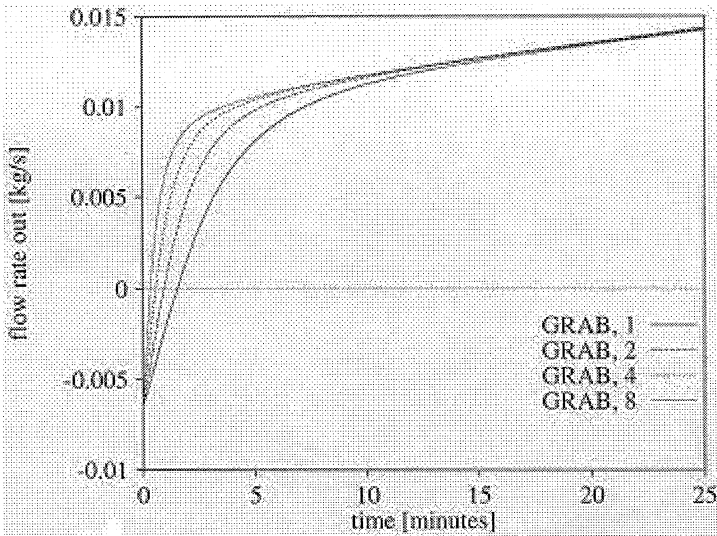Fig. 8. Average volumetric concentration profile for Trial 4.

Fig. 9. Flow through the opening calculated by 'GRABT' for Trail 4.

initial inflow due to cooling is an important feature of the flow which can be modelled using GRAB-T, but clearly cannot be predicted by the isothermal model GRAB.

6. Inclusion of building buffer effects in risk assessment

6.1. Base case assessment

In order to determine the sensitivity of QRA to the inclusion of building buffer effects, it was first necessary to define and assess the risks associated with a particular base case risk assessment. The incorporation of building buffer effects for those scenarios which dominate the risk then allowed the sensitivity of the overall results to the inclusion of such effects to be determined.

The example chosen as the base case was a toxic gas risk assessment for a bulk chlorine storage site, as such sites are relatively common in the UK and can lead to significant risks to off-site populations at some distance from the plant. A particular water treatment works site was chosen, comprising the following main items of equipment which represent major hazards:

- two bulk chlorine storage vessels (storing chlorine under pressure at ambient temperature)
- a chlorine road tanker off-loading bay
- various sections of 25 mm diameter liquid chlorine pipework

Loss of containment failures involving any of these items of equipment could lead to the formation and downwind dispersion of a toxic gas cloud.

The chlorine is stored in the central portion of a large 'U' shaped building of overall length 120 m. The room itself is around $20 \text{ m} \times 10 \text{ m} \times 8 \text{ m}$ high, and is fairly

uncongested but irregularly shaped. It contains $2 \times 30t$ chlorine tanks, set in a bunded area, and a ventilation extract system which can be used to clear small releases of chlorine. It is in fact the room which was modelled in the HSL tests described in Section 5 (Bettis and Allen [9]), and therefore its shape is represented by Fig. 5.

The release scenarios which were considered all occur in the vicinity of the chlorine bulk storage area. This area consists of the two cylindrical chlorine storage tanks surrounded by a 0.88 m high bund wall, designed to contain any chlorine spillage. The tanks are arranged horizontally and are surmounted by a walkway, and chlorine pipework runs between this walkway and the adjacent wall. Also present in the room are two vertical scrubber units, which stand adjacent to the chlorine storage area, and a large horizontal pressure relief vessel.

The room can be ventilated through two fans located in the ceiling of the room and by a large vertical extractor duct. The extractor duct, which is located near one of the corners, bifurcates 4.75 m above the ground, before terminating in two rectangular openings at about 0.6 m above the floor, each of which has an area of 1.03 m². The roof fans each have an area of 0.51 m². Although there are also three doorways leading into the chlorine room, a survey of the site indicated that these are likely to be well sealed when closed.

The set of representative scenarios (from Carter et al. [10]) corresponding to a typical small chlorine installation, such as that being considered, has been used, and it was only when the potential importance of building buffer effects was considered that actual building dimensions from the site were used.

Each of the 40 events in Carter et al. were considered in 4 representative weather conditions, namely D2.4, D4.3, D6.7 and F2.4, where the letter corresponds to the Pasquill stability category (D for neutral and F for stable), and the numbers correspond to the wind speed in m s⁻¹. The percentage frequencies of these four weather conditions were taken to be 17%, 20%, 45% and 18%, respectively, based on the average data over 20 years from a nearby meteorological station. For ease of application, a uniform wind rose has been assumed, and the risk results presented are therefore a function only of distance, and not of direction. The dispersion of chlorine vapour clouds has been assessed using the models in HGSYSTEM [11]. Continuous releases have been modelled using the HEGADAS-S code, and instantaneous releases have been modelled using HEGABOX followed by HEGADAS-T.

The risk calculations involve a summation of the risks from each event in each of the representative weather conditions. The risks have been calculated for a typical residential population, with standard assumptions used for the indoor/outdoor population split. The risks to persons indoors were based on a calculation of the time varying concentration inside the building, using an air exchange rate of 2 air changes per hour (ach) for all conditions except D6.7, where the higher wind speed implies a higher air exchange rate of 3 ach. The persons indoors were assumed to remain indoors for 10 min after the cloud has passed before evacuating to fresh air, but in no case did evacuation take place until at least 30 min had elapsed from the start of the release.

The risk calculated in this study was the risk of people receiving a dangerous dose (or worse) of chlorine, where the dangerous dose for chlorine is defined, as a function of concentration and time, as 108,000 ppm² min. The possibility of escape from the cloud

was modelled by assuming that, at concentrations between 300 and 500 ppm, there was a 20% chance of escape for persons outdoors, and that below 300 ppm there was an 80% chance of successful escape.

6.2. Consideration of transient releases

In all cases where there was a building buffer effect, the emission rate from the building followed a transient, non-steady, curve. For some cases, where there was a delay between the commencement of the release and the start of the outflow from the building, the representation of this transient as a steady state may not be particularly realistic. In order to determine the effects of treating a transient as a steady state, the output of certain GRAB results has been used within both HEGADAS-S (steady state) and HEGADAS-T (transient).

The configuration which has been used in GRAB was that of a single high level opening, with mixing up to the level of the release (6 m above the floor) to a concentration of c_m, such that there was, in each case, approximately 10 min delay. This gave a c_m value of 0.5 for the 3.6 kg s^{-1} release, and pro-rata for the other releases. Fig. 10 shows the predictions of concentration against downwind distance for a 3.6 kg s^{-1} chlorine release in D2.4 weather conditions using the following 6 alternative modelling approaches:

(a) A 20-min release at 3.6 kg s^{-1} using the steady state HEGADAS-S dispersion model (no building buffer effect).

(b) A 20-min release at 3.6 kg s^{-1} using the transient HEGADAS-T dispersion model (no building buffer effect).

(c) A 30-min release at 0.71 kg s^{-1} using the steady state HEGADAS-S dispersion model (using the average release rate calculated by GRAB).

(d) A 30-min release at 0.71 kg s^{-1} using the transient HEGADAS-T dispersion model (again using the average release rate calculated by GRAB)

(e) A time varying release rate using the transient dispersion model HEGADAS-T (using the time dependent release rate predicted by GRAB)

(f) An 8.8 min release at 2.5 kg s^{-1} using the steady state HEGADAS-S dispersion model (based on maximum release rate from GRAB).

The results for cases (a) and (b) are fairly similar, showing that for a 20 min continuous release it is not necessary to undertake a transient dispersion model. Cases (c) and (d) for the 30 min release are also similar to each other, but predict much lower risks than without the building effects.

In principle, the best way to model building buffer effects would be to calculate the time varying release rate using GRAB and use this in a transient dispersion model such as HEGADAS-T. This gives case (e), which shows that the release may lead to significant underestimates of the risk, whilst failing to allow for building buffer effects may give gross overestimates. However, in view of the practical difficulties associated with the use of transient dispersion in models (such as HEGADAS-T), it is worth considering whether any simplified approaches could lead to similar results. The method recommended here is to use a steady state dispersion model (such as HEGADAS-S) with the release rate set to the maximum release rate calculated by GRAB (2.5 kg s^{-1} in
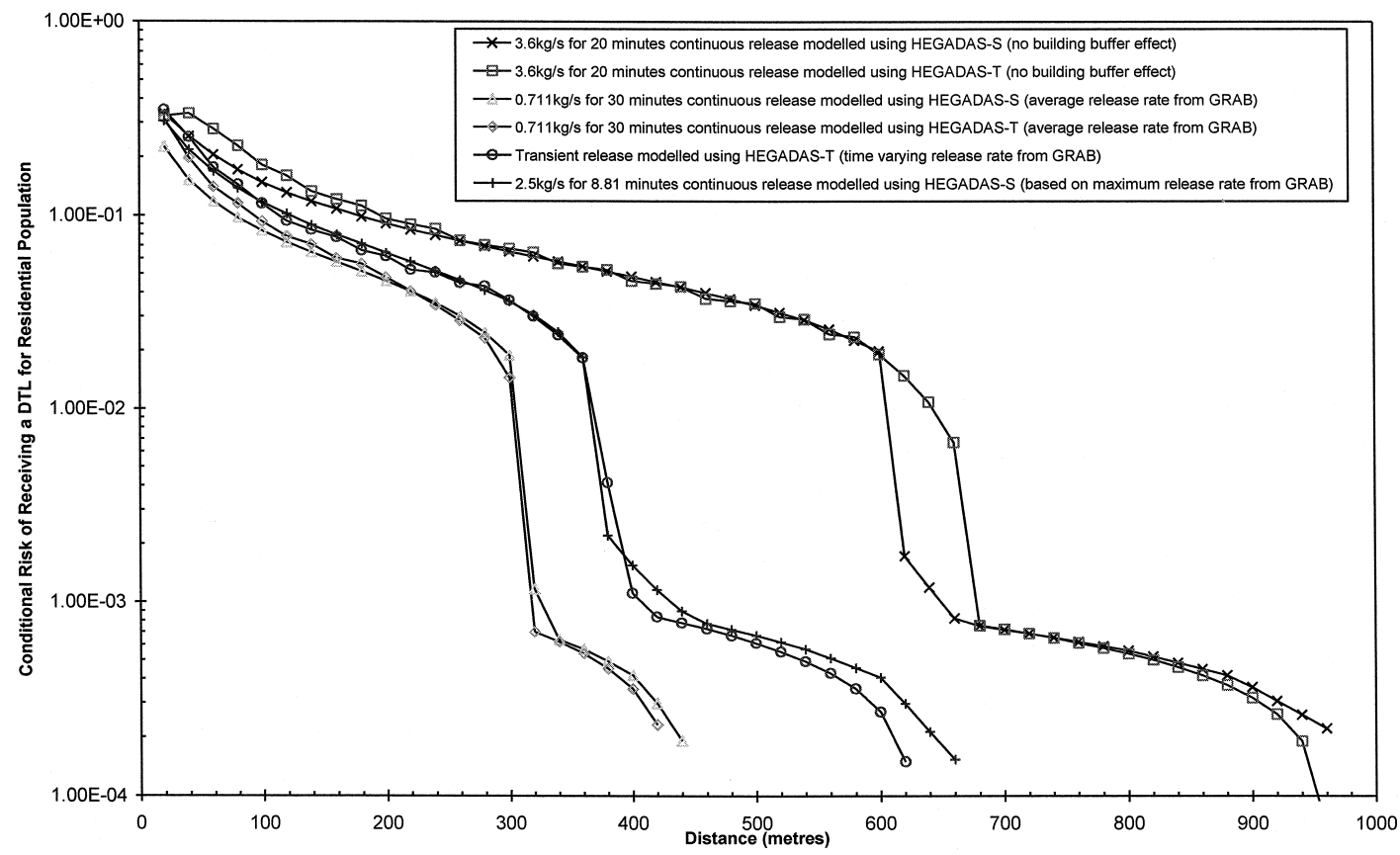
Fig. 10. Comparison of the conditional risks for a 3.6 kg s^{-1} chlorine release in D2.4 weather conditions using various methods.

The chart legend reads:

- 3.6kg/s for 20 minutes continuous release modelled using HEGADAS-S (no building buffer effect)
- 3.6kg/s for 20 minutes continuous release modelled using HEGADAS-T (no building buffer effect)
- 0.711kg/s for 30 minutes continuous release modelled using HEGADAS-S (average release rate from GRAB)
- 0.711kg/s for 30 minutes continuous release modelled using HEGADAS-T (average release rate from GRAB)
- Transient release modelled using HEGADAS-T (time varying release rate from GRAB)
- 2.5kg/s for 8.81 minutes continuous release modelled using HEGADAS-S (based on maximum release rate from GRAB)

The vertical axis is labelled "Conditional Risk of Receiving a DTL for Residential Population" and the horizontal axis is labelled "Distance (metres)".
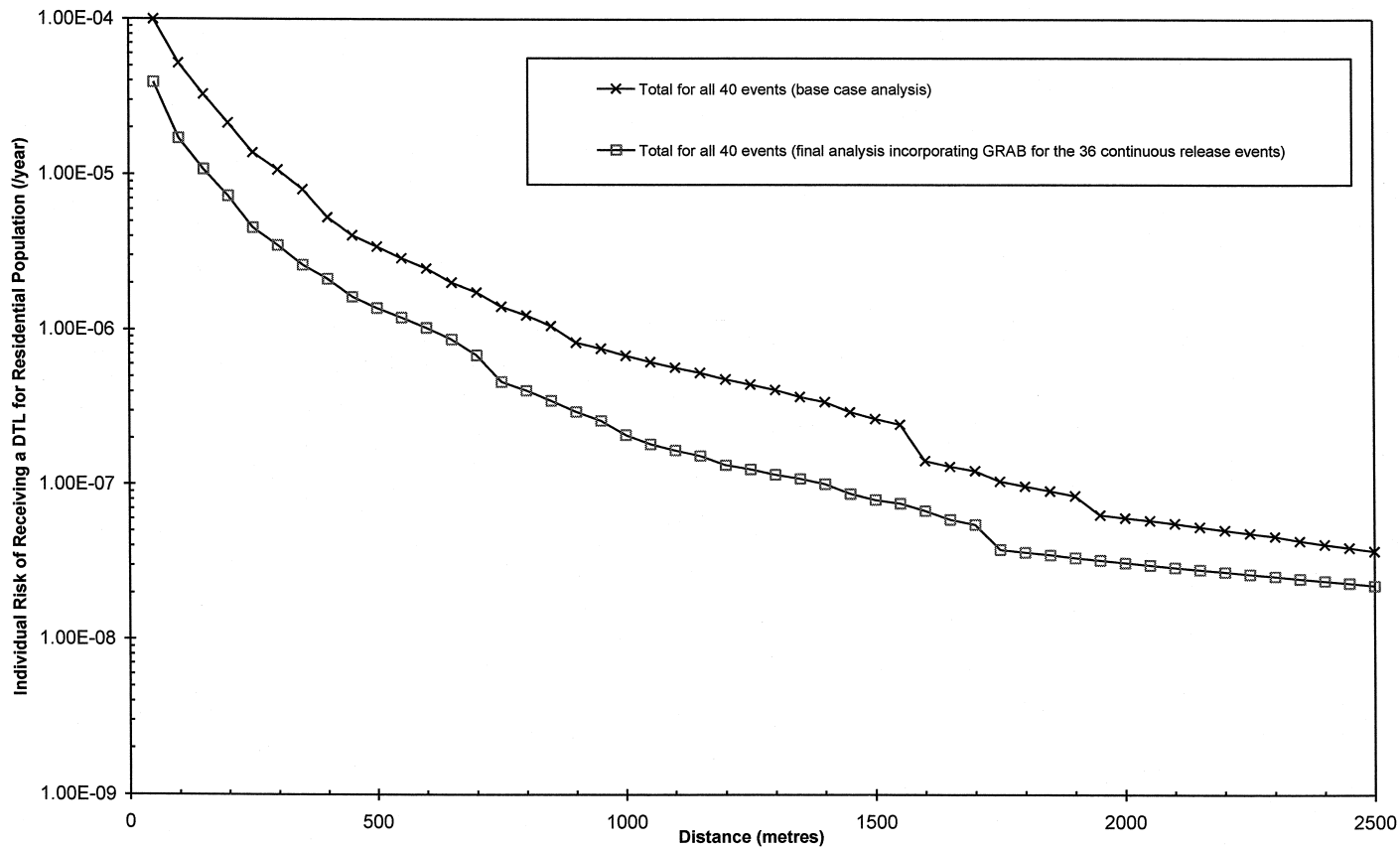
Fig. 11. Comparison of the overall results for the base case and final analyses, showing the effect of incorporating building buffer effects using GRAB.

this example). The effective release duration is then defined as the total quantity of chlorine released from the building, predicted by GRAB (1320 kg), divided by the maximum release rate, which gives an effective release duration of 8.8 min in this example.

Comparison of cases (e) and (f) in Fig. 10 shows that this simple approach gives very good agreement with the much more complex modelling of the full transient.

6.3. Revised QRA including building effects

The results from the simple modelling have demonstrated that building buffer effects can provide significant reduction in effective emission rates. They have also shown that these emission rates can be strongly dependent upon the opening configuration. In principle, each QRA should include a consideration of the likely openings, and apply GRAB or GRAB-T modelling accordingly. However, for the purposes of this study, it was considered appropriate to use relatively extreme modelling. The most extreme modelling would give no outflow over the period of interest, which would clearly give zero risk. An alternative is to take cases which give a reasonable delay before any emission occurs from the building, as in the cases considered above.

The methodology advocated above was applied to all the *continuous* releases considered to obtain in each case the peak release rate from the building and an effective release duration (equivalent to approach (f) above). Fig. 11 shows a comparison of the results of this final revised risk assessment with the results from the original base case analysis. This shows that the inclusion of the building buffer effect has reduced the overall risk by a factor of 2 to 4, depending on distance, with a correspondingly significant reduction in the distance to specific risk levels. For example, the distance to the 3×10^{-7} year^{-1} risk contour is reduced from 1450 m to 900 m, implying that the area of the consultation zone would be reduced by nearly a factor of 3.

7. Discussion

The modelling currently has significant limitations, and GRAB-T is due to undergo further development to increase its range of applicability. However, it has been shown that the simple modelling tools can be useful in certain circumstances. In this respect, the following points are noted below.

· GRAB appears to be able to predict *release rates* adequately where there are openings at more than one level, and the released vapour is reasonably well mixed.

· Neither GRAB nor GRAB-T is currently able to model the case with only one opening, where the initial part of the transient is dependent upon a fine balance between internal and external pressures.

· It appears from the CFD results [1] of the cases studied that good mixing is likely to be obtained for many practical cases of two phase releases. This implies that the current limitation of GRAB-T to fully mixed cases may not be a major disadvantage, although there may be some cases, such as an evaporating pool or an impinging jet, to which GRAB-T could not be so confidently applied.

· GRAB-T is currently limited to single openings with no wind-driven ventilation, and this should be rectified to render it more useful.

The risks associated with a toxic release generally depend on both the concentration and the duration of exposure. Releases from buildings tend to result in lower emission rates, but the release may continue for a longer period. These combined effects generally lead to a reduction in risk. Releases from buildings are also likely to be diluted, with time-varying dilution rates, and may emerge from openings at more than one level. Currently QRA methodologies are not likely to include this level of detail.

Although most accidental releases are normally modelled as steady continuous releases for a finite duration, releases from buildings tend to vary significantly with time. For example, the time delay that may occur after the leak commences indoors, before it starts to be released to atmosphere, may sometimes be important, particularly where mitigatory actions can be implemented within a few minutes. These transient features can either be modelled explicitly using time dependent (transient) dispersion models, or else a suitable approximation must be made, where the time varying release is considered equivalent to a continuous release for a specified duration.

It is concluded is that the most appropriate approximation that is generally applicable is to calculate the peak release rate from the building (Q_p), using a model such as GRAB, and then calculate an effective release duration, based on either:

(a) the total mass released inside the building divided by Q_p; or

(b) the total mass released from the building in the first 30 min (calculated by GRAB) divided by Q_p (periods other than 30 min may sometimes be more appropriate).

The first of these options is likely to be the most conservative, and hence appropriate for safety cases. However, it has been shown that the risks calculated using a continuous dispersion model with a release rate Q_p and an effective release duration as calculated by (b) above will generally lead to broadly similar risks to those calculated using the time dependent release rate and a transient dispersion model. This leads to a significant reduction in the effort required for the dispersion modelling part of a typical QRA.

However, in cases where there is a need for the analysis to be as accurate as possible, it is recommended that the full time dependent release rate from GRAB should be used with a transient dispersion model.

8. Conclusions

Two separate zone models have been developed to allow the predictions of emission rates from buildings into which hazardous materials have been released. GRAB is an isothermal model, and is therefore applicable primarily to pure vapour releases. It allows various opening configurations, mixing assumptions, wind ventilation conditions, etc. GRAB-T includes temperature dependence, and hence can be applied to flashing releases, but is currently restricted to a single opening and complete mixing throughout the whole room.

Validation has been presented of the results of these models compared with test measurements. This showed reasonable agreement, but has highlighted some deficiencies of the thermodynamics and heat transfer modelling in GRAB-T. It is intended to undertake further development to improve these areas of modelling.

It has finally been shown how zone models can be used to incorporate building buffer effects into risk assessments. Significant reduction in risk can be demonstrated, but care should be taken to ensure that GRAB (or GRAB-T) output results are used appropriately and conservatively. Recommendations have therefore been given on how this can best be undertaken.

Notation

Isothermal model

Q_0	gas release rate (m^3 s^{-1})
Q_1	rate of emission from top vent (m^3 s^{-1})
Q_2	rate of emission from bottom vent (m^3 s^{-1})
h	height of mixed layer (m)
c	concentration of mixed layer (m^3 m^{-3})
A_1	effective area of top vent (m^2)
A_2	effective area of bottom vent (m^2)
v_1	velocity through top vent (m s^{-1})
v_2	velocity through bottom vent (m s^{-1})
P_1	pressure at top vent (Pa)
P_2	pressure at bottom vent (Pa)
P_0	pressure external to building (Pa)
ρ_a	ambient air density (kg m^{-3})
ρ_2	density of mixture at lower outlet (kg m^{-3})
A	building horizontal cross-sectional area (m^2)
V_0	building volume (m^3)
t_0	filling timescale(s)
ΔP	pressure differences (Pa)
$\Delta \rho$	density difference (kg m^{-3})
g	gravity (m s^{-2})
ρ^1	reduced density difference
Q^*, Q_0^*	normalised flow rates
A^*	(ratio of opening areas)^2
α, β, γ, X	coefficients in Eq. (3.7)
Δc_p	difference in pressure coefficients
u_r	wind speed (m s^{-1})
A_w	effective opening area (m^2)
h_r	gas layer height (m) — Eq. (3.15)
T_r	decay start time (s)
Q	doorway flow rate (m^3 s^{-1})
w	doorway width (m)
H	doorway height (m)
g^1	reduced gravity (m s^{-2})
K	door orifice coefficient

Non-isothermal model

A_d	area of opening (m^2)
c_1	liquid pollutant mass fraction
c_g	gaseous pollutant mass fraction
c_p	specific heat of room contents at constant pressure ($J\ kg^{-1}$)
$c_{p,a}$	specific heat of ambient air at constant pressure ($J\ kg^{-1}$)
$c_{p,g}$	specific heat of gaseous pollutant at constant pressure ($J\ kg^{-1}$)
$c_{p,l}$	specific heat of liquid pollutant at constant pressure ($J\ kg^{-1}$)
C_d	discharge coefficient of opening
F_f	flash fraction
H	heat of vaporisation of pollutant ($J\ kg^{-1}$)
m_a	ambient air molecular mass ($g\ mol^{-1}$)
m_g	pollutant gas molecular mass ($g\ mol^{-1}$)
m_{ga}	average molecular mass of pollutant gas/air mixture ($g\ mol^{-1}$)
$\dot{m}_0$	release rate of liquid pollutant ($kg\ s^{-1}$)
$\dot{m}_d$	flow rate through opening ($kg\ s^{-1}$)
P	pressure ($N\ m^{-2}$)
P_a	ambient pressure ($N\ m^{-2}$)
q	heat transfer rate to room (W)
R	universal gas constant ($J\ mol^{-1}\ K^{-1}$)
t	time (s)
T	temperature (K)
T_a	ambient temperature (K)
T_b	boiling point of liquid pollutant (K)
V_r	volume of room (m^3)
v_d	discharge velocity ($m\ s^{-1}$)
v_0	release velocity of two phase jet ($m\ s^{-1}$)
ρ_{ga}	average density of pollutant gas/air mixture ($kg\ m^{-3}$)
ρ_0	density of initial conditions and of ambient air ($kg\ m^{-3}$)
ρ_1	density of liquid pollutant ($kg\ m^{-3}$)
ρ_t	total density of air/pollutant mixture ($kg\ m^{-3}$)

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