Atmospheric Dispersion Modelling
Liaison Committee

Annual Report 2004/2005

INCLUDING

Review of guidelines for atmospheric dispersion modelling

Calculation of air concentration indoors

AND

Dispersion following explosions
In 1977 a meeting of representatives of government departments, utilities and research organisations was held to discuss methods of calculation of atmospheric dispersion for radioactive releases. Those present agreed on the need for a review of recent developments in atmospheric dispersion modelling, and a Working Group was formed. Those present at the meeting formed an informal Steering Committee, that subsequently became the UK Atmospheric Dispersion Modelling Liaison Committee. That Committee operated for a number of years. Members of the Working Group worked voluntarily and produced a series of reports. A workshop on dispersion at low wind speeds was also held, but its proceedings were never published.

The Committee has been reorganised and has adopted terms of reference. The organisations represented on the Committee, and the terms of reference adopted, are given in this report. The organisations represented on the Committee pay a small annual subscription. The money thus raised is used to fund reviews on topics agreed by the Committee, and to support in part its secretariat, provided by NRPB. The new arrangements came into place for the start of the 1995/96 financial year. This report describes the tenth year in which the Committee has operated under the new arrangements, and during which it placed three contracts. These covered a review of the guidelines for atmospheric dispersion modelling prepared by the Royal Meteorological Society, the calculation of air concentration indoors and a review of atmospheric dispersion modelling for releases following explosions. The technical specifications for the contracts are given in this report, and the contract reports are attached as annexes to this report. The Committee funded 21 studies in previous years; they are described in its earlier annual reports.

The Committee intends to place further contracts in future years and would like to hear from those interested in tendering for such contracts. They should contact the Secretary:

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The organisations on the committee during the year covered by this report were:

Amersham plc
Atomic Weapons Establishment, Aldermaston
British Nuclear Fuels plc
BNFL Magnox Generation
Defence Science and Technology Laboratory
Department for Environment Food and Rural Affairs (DEFRA)
Environment and Heritage Service, Northern Ireland
Environment Agency
Food Standards Agency
Health and Safety Executive
Methodology and Standards Development Unit, Hazardous Installations Directorate
Nuclear Installations Inspectorate
Health Protection Agency
Meteorological Office
National Nuclear Corporation
National Radiological Protection Board
Nuclear Department, HMS Sultan
Rolls Royce Naval Marine
Scottish Environment Protection Agency
Shell Global Solutions
Westlakes Research Institute

The Chairman and Secretary are provided by NRPB.
2 TERMS OF REFERENCE

The terms of reference of the committee are:

Areas of technical interest

1. ADMLC's main aim is to review current understanding of atmospheric dispersion and related phenomena for application primarily in authorization or licensing of discharges to atmosphere resulting from industrial, commercial or institutional sites. ADMLC is primarily concerned with dispersion from a particular regulated site or from discrete sources, and will not normally consider work in the following areas: traffic pollution, acid rain and ozone.
2. ADMLC is concerned both with releases under controlled conditions occurring at a constant rate over long periods, and with releases over shorter periods such as accidents or controlled situations where the release rate varies.
3. ADMLC is concerned with modelling dispersion at all scales, including on-site and within buildings.

Organisations and outputs

4. The Committee shall consist of representatives of Government Departments, Government Agencies and organisations with an interest in modelling dispersion of material for the situations identified above. Each organisation represented on the Committee shall pay an annual membership fee.
5. ADMLC believes that it can be most effective by limiting its membership to about 25 organisations. New organisations will only be admitted to membership of ADMLC if the majority of existing members agree to their membership.
6. ADMLC aims to review, collate, interpret and encourage research into applied dispersion modelling problems. It does not endorse particular brands or suppliers of commercial models. However, it is concerned to ensure that users for industrial applications are aware of what is available, how it can be applied to particular problems and of the uncertainties in the results.
7. The Committee will commission work on selected topics. These should be selected following discussion and provisional agreement at meetings of the Committee, followed by confirmation after the meeting. It will produce reports describing current knowledge on the topics. These may be reports from contractors chosen by the committee or may be based on the outcome of conferences or workshops organised on behalf of the committee. The money raised from membership fees will be used to fund contractors, organise workshops and report on their outcome, and any other matters which the Committee may decide.
3 WORK FUNDED DURING THE YEAR

3.1 Review of dispersion modelling guidelines

Discussion in ADMLC identified lack of appropriate guidance/training in Atmospheric Dispersion Modelling as a root cause of inadequacy in some applications of atmospheric dispersion models. ADMLC considers that publication of up to date guidance on Dispersion Modelling may be one way to facilitate possible improvement in applications although this cannot be a replacement for proper training.

The work will include

1. Specify the scope and content of the guidelines.
   Draw up a contents list for the revised guidelines. This will be section headings plus a short paragraph on what each section will contain.

2. Obtain comments on the document from step 1.
   Consult relevant organisations (e.g. ADMLC, DMUG, IAQM, RMS) to gain endorsement for and improve upon the proposed scope and content of the guidelines. This will seek comments from the organisations represented on those "committees", rather than the views of the "committees" themselves. The document will also be placed on the ADMLC web site (with links from IAQM, NSCA web sites?), so that comments can be obtained from other people.

3. Produce a draft of the final guidelines
   Establish a "Working Group" to review the comments, and produce the first draft of the final guidance.

4. Obtain comments on this draft as in step 2.
   Collate the comments received.

5. Prepare the final version of the guidelines
   The "Working Group" reviews the comments from step 4, and prepares the final version of the document.

6. Publish the final guidelines
   The report on this work is published as ADMLC/2004/1.
### 3.2 Air Concentration in Buildings from Sources Outdoors

Previous studies undertaken for ADMLC have examined concentrations outdoors from sources outdoors. The Committee is now interested in models for calculating concentrations inside a building from material in a cloud outside the building, or of reviewing published information on the ratio of indoor and outdoor concentrations. A simple model for this (see page 96 of [http://www.admlc.org.uk/ar96-97(new).htm](http://www.admlc.org.uk/ar96-97(new).htm)), leads to the conclusion that the concentration inside buildings is about half or less of that outside buildings. Some reviews suggest that indoor and outdoor concentrations are similar.

The committee is interested in work on the following aspects of the problem:

- **a** Modelling the air concentration indoors from a short release, including the time variation of the indoor concentration as it builds up and then reduces. This should also provide typical values for the parameters of the model reflecting UK building types.
- **b** The comparative indoor concentrations of aerosols (particularly PM$_{10}$ and PM$_{2.5}$) and reactive and inert gaseous pollutants.
- **c** The effect of atmospheric conditions on the concentrations indoors.
- **d** The equilibrium ratio of indoor and outdoor concentration for materials which are present in outdoor air at a reasonably constant rate over an extended period of time.

The report on this work is published as ADMLC/2004/2

### 3.3 Aspects of Dispersion following an Explosive Release

ADMLC is interested in reviewing models for predicting the dispersion of toxic and flammable gases and particulates following explosive releases and very short duration catastrophic events.

The main aim is to produce an overview of current knowledge describing the distribution of material that is produced immediately after the explosion, and how the size and distribution of material within that plume might depend on the characteristics of the event. Thus the emphasis is on providing a source term for use with a standard dispersion model. The review needs to identify what appropriate processes need to be considered when modelling the subsequent dispersion, but not to explore that dispersion in depth.

The scope of the review could include:

- **e** high explosive combined with radioactive material, as in terrorist events,
- **f** high explosive combined with toxic material as in terrorist events.
- **g** releases from terrorist attacks on bulk shipments, (e.g. LNG)
- **h** releases from terrorist attacks on road/train shipments of toxics
releases from catastrophic failure of pressurised storage vessels
releases involving fast chemical reactions such as the sudden addition of water to a spill of a water reactive material generating a toxic vapour.

The review should cover the following aspects of the problem:

a) The size and height of the initial plume produced by the explosion, as functions of the explosive yield, including penetration of the boundary layer.

b) The distribution of material within the plume formed immediately after the explosive release, and the size distribution of aerosols, as a function of explosive yield.

c) The most appropriate way of describing the processes immediately after the initiating event including the dispersion and deposition of the resulting plume, and a review of models for such calculations. This could include consideration of the buoyancy of the initial cloud and the deposition of large particles released, together with any other features that are relevant.

d) Comments on the extent to which the subsequent dispersion could be predicted using simple Gaussian plume models, or how such models could be extended for this application.

The report on this work is published as ADMLC/2004/3
Indoor concentrations in buildings from sources outdoors

J.T. Milner, C. Dimitroulopoulou, H.M. ApSimon

ABSTRACT

This study reviews current knowledge on indoor air pollutant concentrations from sources outdoors, drawing on research from the UK and worldwide as well as including work undertaken by the authors. Particular emphasis is given to the current modelling tools available for simulation of indoor concentrations due to both short bursts and more prolonged releases of conventional air pollutants and radioactive or toxic contaminants. The first part of the report focuses on the factors that influence indoor air pollution concentrations and the ways in which outdoor air impacts on indoor air, including the influence of atmospheric conditions. The principles of the two main model types for the simulation of indoor air pollutant concentrations from outdoor sources (mass-balance models and computational fluid dynamical models) are then discussed in detail along with examples of both types of models and their relative advantages and limitations. The contrasting applications of the model types have also been compared using two example illustrations with specific models, including some examination of their validation. In the next section of the report, simultaneous indoor and outdoor measurements reported in the literature for different building types have been reviewed for both conventional air pollutants (carbon monoxide, particulate matter and nitrogen dioxide) and radioactive contaminants. Finally, based on the findings of the work, practical guidance and best-practise recommendations are provided for situations that have different characteristics and modelling requirements. The situation in which pollution sources are close to the building has been identified as being in particular need of more research, since most current models cannot adequately account for a spatially non-uniform concentration over the building envelope.

This study was funded by the UK Atmospheric Dispersion Modelling Liaison Committee.

The views expressed in this report are those of the authors, and do not necessarily represent the views of ADMLC or of any of the organisations represented on it.

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EXECUTIVE SUMMARY

There is growing concern over the penetration into indoor environments of both conventional outdoor air pollutants and radioactive or other toxic releases. Short bursts of contamination, whether due to rush-hour emissions or toxic incidents, are of particular concern due to the high indoor concentrations that may result thereafter and the potential for controlling them.

In the absence of internal sources, indoor air pollutant concentrations depend mainly on dispersion processes around the building, the ventilation and airtightness of the building, and the physical and chemical properties of the pollutant. Indoor concentrations may also be highly influenced by the prevailing atmospheric conditions, although currently very little research has been conducted into the effects of specific meteorological variables on indoor concentrations. This work is vital to enable accurate parameterisation of models.

The strongest penetration of pollutants into buildings occurs at areas of both high pressure and high contamination concentration. Urban landscapes will influence both pressure and concentration on the building, potentially leading to extremely complex patterns of both. Variations in the concentration on the building façades will decrease as the distance from the source increases. Where sources are close to buildings, wind tunnel models and complex computational fluid dynamical (CFD) models (with great uncertainty) are available to predict concentration and pressure patterns on the building envelope, although more work is needed to study dispersion at fine spatial and temporal scales, especially in urban areas.

This report reviews models that have been developed to predict indoor air pollutant concentrations from outdoor sources. Such modelling tools enable the model user to quantify relationships between concentrations and important variables, extrapolate from just a few measurements to a large sample, quantify the relative contributions of different pollution sources, estimate indoor concentrations in situations in which measurements are unavailable, and determine the ventilation and indoor air quality of a building before it has been constructed. Of the models that have been developed, the most widely used are mass-balance models, which constitute the majority of current modelling work, and CFD techniques.

Mass-balance models are used to simulate average indoor air pollutant concentrations as a function of outdoor concentrations, building and pollutant characteristics and indoor sources. These models consider transport of air pollutants between outdoors and indoors (as a simple parameterisation of the fluxes), as well as between indoor compartments in the buildings, and are widely used due to the simplicity of the mathematics involved. There are three forms of mass-balance technique: statistical regression models, microenvironmental models and multizone models.
In cases where only long-term trends are required, the simplest screening method for calculating indoor concentrations from outdoor sources is the indoor/outdoor (I/O) ratio found by statistical regression of experimental data. Indicative I/O ratios for different pollutants are presented in this report. The method is fast and straightforward and often the only option if little is known about the building of interest. However, such a method cannot differentiate between indoor and outdoor sources and is unsuitable for modelling a short burst of contamination.

Microenvironmental mass-balance models are used to predict average concentrations in one or two indoor microenvironments or compartments within a building. These models calculate indoor concentrations that may be well compared to experimental data and may be easily linked to exposure models. One significant recent improvement has been the development of probabilistic models to predict frequency distributions of concentrations, for example representing conditions typical for UK housing.

Multizone mass-balance models provide some improvement over microenvironmental models when studying more complicated buildings (e.g. buildings with many rooms or large indoor spaces). Currently, there are no probabilistic models of this type. The model user must decide whether a microenvironmental or multizone model is appropriate depending on the available information, such as the building geometry and whether air exchange rates are known in advance.

The major limitation of mass-balance modelling approaches is the assumption of a spatially uniform concentration in the envelope surrounding the building, although mass-balance models can account for temporal variations in outdoor concentrations.

More complex CFD models are capable of representing spatially non-uniform external concentrations. However, CFD models are still used only as research tools due to their highly complex nature and many CFD models may only represent steady-state conditions. Most research using CFD methods has, thus far, concentrated predominantly on either outdoor or indoor airflows and contaminant transport, and little has been done to link the two areas of research. It appears that the research community is moving towards CFD models that use large-eddy simulation (LES) methods to simulate turbulence, although a great deal more validation of the method is still needed.

There has recently been research conducted into exploiting the benefits (and overcoming the weaknesses) of different modelling approaches using combination modelling. In some cases, CFD models have been used to simulate the concentration and pressure fields around a building, with the results then being used as input to a multizone mass-balance model for the analysis of indoor air quality.

The models that are currently available are adequate for risk assessment in situations in which pollution sources are far enough away to assume a uniform concentration over the building. However, there is currently a gap in knowledge
relating to situations in which sources are close to the building and a uniform concentration may not be assumed. Thus, the key conclusion of this report is that the models that are currently available to simulate indoor concentrations from sources outdoors do not satisfactorily account for spatially non-uniform concentration and pressure fields in the building envelope. In addition, very few simultaneous measurements of concentration and pressure around buildings have been made. As such, more research is needed to study variations in concentration and pressure over buildings in different situations and environmental conditions and also to link this to internal circulation and air quality. Ideally, a project combining fieldwork, wind tunnel modelling and numerical modelling is required.
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APPENDIX A 68
# LIST OF SYMBOLS

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<table>
<thead>
<tr>
<th>Symbol</th>
<th>Parameter (units)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C$</td>
<td>Concentration (e.g. mg m$^{-3}$)</td>
</tr>
<tr>
<td>$Q$</td>
<td>Emission rate/source strength (e.g. kg s$^{-1}$)</td>
</tr>
<tr>
<td>$\bar{u}$</td>
<td>Mean wind speed at plume height (m s$^{-1}$)</td>
</tr>
<tr>
<td>$\sigma_y$</td>
<td>Standard deviation of concentration in the y-direction</td>
</tr>
<tr>
<td>$\sigma_z$</td>
<td>Standard deviation of concentration in the z-direction</td>
</tr>
<tr>
<td>$H$</td>
<td>Release height (m)</td>
</tr>
<tr>
<td>$ACH$</td>
<td>Air exchange rate/air changes per hour (h$^{-1}$)</td>
</tr>
<tr>
<td>$Q_V$</td>
<td>Volumetric airflow rate/ventilation rate (e.g. m$^3$ s$^{-1}$)</td>
</tr>
<tr>
<td>$V$</td>
<td>Interior volume (m$^3$)</td>
</tr>
<tr>
<td>$P$</td>
<td>Penetration factor (range 0 – 1)</td>
</tr>
<tr>
<td>$K$</td>
<td>Loss rate (e.g. min$^{-1}$ or h$^{-1}$)</td>
</tr>
<tr>
<td>$v_d$</td>
<td>Deposition velocity (m s$^{-1}$)</td>
</tr>
<tr>
<td>$A$</td>
<td>Interior surface area (m$^2$)</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Radioactive decay constant (s$^{-1}$)</td>
</tr>
<tr>
<td>$T_{1/2}$</td>
<td>Radioactive half-life (e.g. years)</td>
</tr>
</tbody>
</table>

Where equations used in individual models have been reproduced, the authors’ original notation has been used.
1 INTRODUCTION

1.1 Outdoor and indoor sources of air pollution

It is well known that in the developed world people spend between 85% and 90% of their time indoors (UK Parliament House of Commons Environment Committee, 1991). In the event of an incident involving a toxic or radioactive release, it is important to determine the extent to which this penetrates indoors and the resulting exposure in different circumstances. There is also a growing concern over the penetration into the indoor environment of conventional air pollutants generated outdoors, since they may cause adverse effects on human health and influence people’s comfort, well-being and productivity. This report will draw on related research and experience.

Road transport has been identified as probably the largest local pollution source in urban areas (QUARG, 1993; UK Department of the Environment, 1996). This is especially important since vehicle emissions may concentrate within the urban canopy leading to undesirable levels of pollutants in buildings near busy roads, particularly during peak traffic times. Other significant sources of air pollution include local and regional industrial pollution (for example, from industrial plant, boiler flues, incinerators, combined heat and power (CHP) plant and ventilation discharges) and also pollution from construction and demolition activities. A comprehensive review of air pollution in urban areas may be found in Kukadia et al. (1999) and Limb (1999).

Both incidents releasing toxic gases as well as conventional traffic and industrial activity can generate temporal peaks in outdoor air concentrations. Short bursts of air pollution, resulting either from rush hour traffic emissions or toxic incidents, are of particular concern due to the high indoor levels that may arise thereafter. It is, thus, essential to understand the mechanisms and factors that influence indoor/outdoor relationships of air pollutants.

Outdoor air penetrates into the indoor environment as a result of various factors (discussed in section 1.2). In the absence of indoor sources, indoor pollutant concentrations are generally lower than outdoors due to attenuation by buildings. However, in the presence of indoor sources (such as fuel combustion, cooking and smoking activity, consumer products and building materials), indoor air pollutant concentrations may well exceed the local outdoor levels (Berry et al., 1996; IEH, 1996). Recently, it has been recognised by the UK Department of Health (COMEAP, 2004) that the concentrations of certain air pollutants found in some UK houses exceed those demonstrated by epidemiological studies and may be associated with adverse effects on human health. Therefore, effective strategies to reduce human exposure to air pollution should consider the contribution from both outdoor and indoor environments and their sources (Dimitroulopoulou et al., 2001a).
1.2 Impact of outdoor air on indoor air

In the absence of indoor sources, pollutant levels within a building, resulting from outdoor sources, depend on:

a. dispersion processes around the building;
b. the ventilation of the building;
c. the airtightness of the building; and
d. the physical and chemical properties of the pollutants (deposition, resuspension, chemical reactions).

Other environmental parameters, such as temperature, relative humidity and concentrations of other indoor pollutants, also play important roles in influencing indoor pollution concentrations in indirect ways. A brief discussion of the main factors affecting indoor air pollutant concentrations and their representation in models is presented in the following sections. Although indoor sources (especially cooking and smoking activity) should be taken into account in modelling studies, these are out of the scope of this report.

1.2.1 Dispersion processes around buildings

Pollutant dispersion processes in urban areas from various sources are complex and are affected by many factors. As discussed in Kukadia and Hall (2004), the factors that determine the concentrations of contaminants and pressure distributions on the façade of a building include:

a. the type, concentration, position and distance of pollutant sources within the urban area;
b. the size, shape and orientation of individual buildings;
c. the distribution of buildings in relation to each other;
d. the surrounding topography; and
e. meteorological conditions including wind speed, wind direction, thermal stratification, heat island effects and prevailing weather patterns. The effects of meteorological conditions on indoor levels of pollutants and indoor/outdoor (I/O) ratios will be discussed further in section 1.2.3.

Outdoor air pollutant concentrations are strongly affected by the atmospheric conditions at the time. The prevailing meteorological conditions will affect the time taken for a pollutant to travel from its source to a building, especially for a far-off release. This will determine whether or not a uniform concentration may be assumed in the building envelope. For example, see Figure 1.
Figure 1. Pollution dispersion from a release (at point marked 'x') showing concentrations in the building envelope for a far-off release (top) and a close release (bottom).

Figure 1 shows a simple representation of the difference between a far-off and close release of a contaminant. For the far-off release, the concentration in the envelope surrounding the building may be assumed to be relatively constant. The meteorological conditions will play an important role in determining the direction in which the plume of pollution moves and the time taken for pollution to reach the building. For the close release, the outdoor concentration close to the building may not be assumed to be constant. More detailed information on the differences between sources at different ranges can be found later in this section.

Complex urban landscapes can cause additional effects depending upon the meteorological conditions. Disturbed wind flows in urban areas generate spatially variable concentration patterns that are sensitive to the source position and meteorological parameters, especially the wind direction (Hall et al., 1996). The street canyon effect for wind flows approximately perpendicular to the street-axis, whereby a vortex forms causing the wind direction at street-level to be opposite that above roof-level, can also greatly influence the outdoor concentration distribution around a building. This effect is shown in Figure 2.
Figure 2. Vortex formation in a street canyon resulting in higher pollutant concentrations on the upwind (leeward) side. For an open road (i.e. with no buildings) concentrations would be higher on the downwind (windward) side.

Advection caused by the vortex results in higher concentrations on the upwind (leeward) side of the canyon than on the downwind (windward) side. As a rule of thumb, the concentration at street-level is often a factor of approximately two greater on the upwind side. The concentration then decreases approximately exponentially with height above the ground on the leeward side. However, research has shown that a vortex may not form for wind speeds below 2 m s\(^{-1}\), though this remains the source of some debate (Caton et al., 2003). A vortex may also be formed within a street canyon due to thermal heating causing convection currents.

The contributions from different sources to the exposure of buildings in urban areas have been reviewed by Hall et al. (1997, 2003). According to this work, sources of pollutants in urban areas may be classified into three main distance regimes and have different impacts on the exposure of the building, as follows:

a. 'Short-range' sources (up to 500 m from the location of interest). These include very localised pollutant sources, such as from nearby vehicle exhausts, combustion appliances, standby generators, process plant and ventilation discharges, as well as from construction and demolition activities. Concentrations are usually high at short ranges and show high levels of temporal and spatial variability. They are also sensitive to source position, wind speed and direction. Concentrations from these sources may vary considerably over a building’s surface and fluctuate over short time periods down to seconds (for example, due to the passage of individual vehicles in streets). This has been demonstrated,
for example, in wind tunnel studies by Mfula et al. (2003, 2004a, 2004b) who found that sources closest to a building resulted in the highest variations in concentration over its surface. Buildings located close to busy roads may experience lower concentrations of traffic-related pollutants on the back façade than on the roadside one, since flow over a building creates a positive pressure zone on the windward side and negative zones on the lateral and leeward sides. Concentrations at building façades also generally decrease with height above the ground if the source of pollution is road traffic (Chang et al., 2003);

b. ‘Intermediate–range’ sources (between 500 m and 10 km from the location of interest). In this case, the sources may be the same as those listed above. However, at these ranges, there is more vertical mixing and lateral spreading of the dispersing plume. As a result, concentration fluctuations are reduced and the pollutants tend to envelop the building in relatively uniform concentrations. They show time variations over scales of minutes and hours (for example, reaching a peak during rush hour traffic);

c. ‘Long-range’ sources (distances > 10 km from the location of interest). Pollutants from these sources disperse well above the urban canopy and spread laterally over large areas. Therefore, pollutant concentrations on the building will tend to vary less sharply over time as plumes fluctuate towards and away from the location of concern (variations of the order of hours or even days).

The divisions between these three regimes are not sharply defined and the proportionate contributions of the three components to the total exposure of a building can vary considerably in different circumstances and for different pollutants. Clearly, the concentration distribution in the envelope surrounding a given building will usually be due to a combination of different sources at different upwind distances and the contributions of these individual sources may not easily be distinguished unless they have significantly different characteristics (Hall et al., 1996).

According to Kukadia et al. (1999), the penetration of pollutants into buildings occurs at points of both high pressure and high contaminant concentration. Thus, in order to predict the ingress of pollution into a building, one must first know whether a plume impinges on the building and then obtain the pressure and concentration patterns on the building envelope, whether by measurement or modelling (Hall et al., 2002). Relatively few simultaneous measurements of pressure and concentration distributions on buildings are available (for an example, see Kukadia et al., 1998). In urban areas, both parameters are affected by the urban array of buildings and the occupational density of that array. Based on field and wind tunnel data, Kukadia et al. (1999) concluded that both pressure distributions on buildings and concentration distributions from upwind sources rapidly become more evenly distributed over the building envelope as the urban occupational density increases. In other work, Hall et al. (2002) demonstrated that the size of the area surrounding a building within
which sources may contaminate that building increases with increasing occupational density.

The pattern of the pressure and pollutant concentrations on a building can become extremely complicated, particularly in urban areas and for short-range sources. Since the exposure of a particular site to pollutants can vary considerably, such potential variability needs to be considered carefully when designing buildings in urban areas for good air quality (Kukadia et al., 2000). There is currently little available information on where regions of high pressure and high concentration combine to produce areas of ‘high risk’ for ingress of pollution (Mfula et al., 2003). However, Hall et al. (1999b, 2000) identified parts of buildings where ventilation inlets should be positioned to minimise ingress and Hall et al. (2002) produced general guidelines indicating the probability of a building surface being exposed to high concentrations from local traffic sources and the resulting probability of the ingress of pollutants.

Further reviews of the topics covered in this section can be found in Hall et al. (1997) on dispersion at different spatial and temporal scales, Britter and Hanna (2003) on flow and dispersion in urban areas and Kukadia and Hall (2004) on the impact of building dimensions and form on concentrations and dispersion of pollutants.

1.2.2 Calculating concentrations on building façades

As discussed in section 1.2.1, the variation of the outdoor concentration over a building may be of great importance in determining the indoor concentration, especially for sources close to building when a spatially uniform outdoor concentration may not be assumed. There are currently several methods available for predicting pollutant concentrations at or close to the façades of buildings, although these are rarely used with consideration to indoor concentrations.

Gaussian plume methods model the release of pollution from a point source with empirical correlations for the growth with distance of the plume dimensions. The concentration, $C$, at a given point in space due to emissions from a continuous source is modelled as a continuous series of overlapping ‘puffs’ of pollution:

$$C(x, y, z) = \frac{Q}{2\pi \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right)$$

(see table on page ix)

The plume equation may be adapted to predict concentrations at a building depending on the location of the source. For example, for sources upwind of the building, the plume impinging on the building increases the rate of spreading of the plume, thus decreasing the concentration (Wilson and Britter, 1982). In the lee of the building, a recirculation zone may entrain or capture pollutants.
In urban areas, simple Gaussian dispersion theory does not generally apply due to the combined influences of complex dispersion around buildings, low wind speeds and street-level emissions from vehicles. In such situations, regulatory modelling programmes, such as the Operational Street Pollution Model (OSPM) (Berkowicz et al., 1997) and the more comprehensive Atmospheric Dispersion Modelling System (ADMS) (CERC, 2004), have been used increasingly in recent years. These semi-empirical models, which also include versions of plume models, allow the user to predict outdoor pollution concentrations for different road geometries and under different meteorological conditions. However, the locations at which the models can make predictions are generally fairly limited and, as a result, such programmes cannot be used to make predictions over the entire building façade.

Some complex dispersion patterns are not well represented by simple regulatory models. Physical (i.e. wind tunnel) models or numerical computational fluid dynamical (CFD) models, which both explicitly represent individual buildings, are more suited to modelling such effects. These models allow the detailed concentration and pressure fields over the entire building to be modelled and can also account for the effects of surrounding topography. Established CFD codes for industrial applications include STAR-CD, PHOENICS, FLOW3D and FLUENT. However, wind tunnel and CFD models are not appropriate for regulatory purposes and CFD, in particular, requires greater validation. For more details on CFD (including the limitations of the method), see section 3 on its application to indoor environments.

Although models are available to predict outdoor concentrations around buildings, a great deal more work is still needed to understand dispersion at fine spatial and temporal scales, particularly in urban areas. The DAPPLE project (Arnold et al., 2004), involving groups at six UK universities, is attempting to address some of these issues using field work and physical, analytical and numerical modelling with an aim to produce best practise guidelines that may be used to enhance regulatory modelling. The models described briefly in this section are summarised in greater detail by Vardoulakis (2002) and Colvile et al. (1999).

1.2.3 Effect of meteorological conditions

Atmospheric conditions greatly affect many of the factors that influence indoor concentrations and, hence, also affect indoor concentrations. First, meteorological conditions will affect dispersion and dilution of pollutants and, hence, concentrations outside a building. Second, human behaviour and air exchange rates (which will be discussed in greater detail in section 1.2.4) vary with meteorological factors. A literature review has been undertaken of observed indoor/outdoor (I/O) ratios (see section 5) and their dependence on atmospheric conditions will now be described. However, very little research has been conducted on this topic and more work is required in order to correctly parameterise models in different environmental conditions.
1.2.3.1 **Effect on I/O ratios**

Changes in atmospheric stability can affect the build up of pollutants outdoors and, consequently, I/O ratios. Stable conditions, resulting in limited dispersion, may cause pollutants to linger within the urban canopy and conditions in the canopy may also become decoupled from the conditions above roof-level, trapping pollution below. Chaloulakou *et al.* (2003) observed that peaks in CO concentrations occurred at times of the day when the meteorological conditions favoured high concentrations, for example, during the morning when there are often lower wind speeds and inversion conditions. Stabilising conditions at night may also lead to concentration peaks, though smaller in size. Ní Riain *et al.* (2003), based on the results of their study, state that although both the indoor and outdoor concentrations may be lower, I/O ratios at night may be greater than during the day due to retention of indoor pollution caused by lower wind speeds and lower air exchange rates.

1.2.3.2 **Effect on human behaviour and ventilation**

Atmospheric conditions may affect indoor concentrations in indirect ways, such as via their influence on human activity. One simple reason why I/O ratios and indoor concentrations of outdoor pollution may be lower in winter is that windows and doors are more likely to be closed, leading to lower air exchange rates (Man and Yeung, 1999). Conversely, as air exchange rates increase during the summer, pollutants enter at a greater rate (Dimitroulopoulou *et al.*, 2001a). Dimitroulopoulou *et al.* (2005) found that homes where windows were open for most or all of the time had significantly higher ventilation rates. As such, indoor concentrations have been shown to be greatly and quickly influenced by the opening and closing of windows (Sowa, 1998). Kirchner *et al.* (2002) found that, for slightly opened windows, there was a delay between outdoor and indoor peaks, while for large opened windows indoor and outdoor concentrations were similar.

1.2.3.3 **Effects of specific meteorological variables**

Several experimental and modelling studies have found meteorological conditions to be the major factor affecting I/O ratios and second only to outdoor concentration in terms of the effect on indoor levels (e.g. Drakou *et al.*, 1998; Chaloulakou *et al.*, 2003). Whilst meteorological factors (such as wind conditions, temperature, pressure, rainfall, relative humidity and solar irradiation) may vary continuously in the outdoor environment, indoor conditions will remain relatively constant. This produces natural fluctuations in the rate at which outdoor pollution is transported indoors. Knowledge of the effects of different environmental conditions will improve the accuracy and applicability of model predictions and, in turn, aid population exposure estimates. However,
little has so far been done to study indoor air quality with respect to atmospheric conditions, although a limited database of work does exist.

\textit{a. Wind}

The wind may influence indoor concentrations since infiltration is driven by pressure gradients that are affected by both wind direction and speed. Also, as discussed, the local wind conditions will influence outdoor concentrations and dispersion around the building envelope. Therefore, the influence of wind is highly complex. For example, while a high wind speed will enhance dispersion and decrease outdoor concentrations, it will also lead to increased penetration of this low concentration into buildings. The prevailing wind direction will also determine the origin of transported pollution. For example, in wind tunnel studies using a regular array of buildings, Hall \textit{et al.} (2000) found that the extent of a line source contributing to the exposure of a test building increased when the wind direction was skewed across the array. In addition, Mfula \textit{et al.} (2004a) demonstrated that the shape of the region of influence of a given source can also be affected by wind direction.

Only a few experimental studies have considered the effect of wind on indoor pollutant concentrations. Chaloulakou \textit{et al.} (2003) looked at the effect of the prevailing wind direction and speed on indoor transport of CO. The results showed an inverse relationship between wind speed and indoor concentrations for any wind direction, since low wind speeds favour accumulation of pollutants and are related to stable atmospheric conditions. Regression of the data showed that wind speed was the strongest predictor of indoor levels, after the outdoor concentration. In another study, Ní Riain \textit{et al.} (2003) found that correlation of indoor and outdoor levels of particulate matter and CO at a building situated on a busy road in London was improved when the data were sorted by wind speed and direction. The monitored building had a less heavily-trafficked road to its rear. I/O ratios were found to be at a minimum when the front of the building (i.e. the side facing the more polluted road) was leeward of the above-roof wind and at a maximum when the front was windward. The authors hypothesised that, under lee winds, the direction of the bulk airflow through the building would be from the rear to the front, due to pressure gradients. This would have the effect of diluting the air in the building with cleaner air from the quieter road, as shown in Figure 3.
When the front of the building was windward (i.e. if the wind direction was from left to right in Figure 3), the reverse would occur and polluted air from the busy road would be drawn into the building. The study concluded that I/O ratios are biased by the prevailing wind conditions, since the ratios depend on the frequency of occurrence of each wind direction. Thus, the results also demonstrated how significantly I/O ratios can be affected by the duration of monitoring and the integration period used. Not all studies on the effects of wind on indoor air quality have reached the same conclusions however. For example, initial analysis conducted by Kukadia et al. (1997) showed no simple relationship between wind (speed and direction) and either external or internal CO, while Chan (2002) found only a very low correlation between wind speed and indoor concentrations of NOX and particulate matter.

\[\text{b. Temperature}\]

Although wind appears to have the most significant and consistent effect on indoor concentrations, other natural factors may also affect I/O ratios, such as the temperature difference driving convective flow. Theoretically, a higher outdoor temperature will cause air to be forced into a building, while a higher indoor temperature will force air out of the building. This is supported by Chan (2002) who found that, generally, I/O ratios increased with increasing outdoor temperature. This increase in I/O equated to approximately 0.07 and 0.08 per °C for particulate matter and NOX, respectively. Temperature may also affect indoor concentrations in other ways, such as if the air flow stream is warmer than the building causing fine particles to deposit on the colder surfaces due to the thermopheresis effect (Chao and Tung, 2001).


**c. Pressure**

An increase in outdoor pressure should theoretically increase the pressure gradient between outdoors and indoors and, thus, increase the transport of pollution into buildings. However, Chan (2002) observed only a weak correlation between pressure and indoor concentrations, indicating that pressure has little effect. In the study, pressure gradients between indoors and outdoors were normally found to be close to zero, resulting in no additional effects due to pressure.

**d. Humidity and rainfall**

Chan (2002) found a strong correlation between outdoor humidity and rainfall and indoor concentrations, with I/O ratios generally increasing with increasing humidity, since increased outdoor humidity may wash out or absorb pollutants and lower the outdoor concentration. The study found that, in general, outdoor particulate concentrations were lower on rainy days. However, NOx levels remained similar or only slightly lower, suggesting that particulate matter is more readily washed out than gaseous pollutants. As a result of the lowered outdoor concentration, less pollution may be transported indoors. In this case, the indoor concentration will become dominated by indoor sources and the I/O ratio may increase (Chan, 2002).

**e. Solar irradiation**

Solar radiation is expected to affect indoor pollutant levels since it affects atmospheric stability. For example, increased solar irradiation will result in unstable conditions that will increase dispersion and mixing and, hence, decrease outdoor concentrations. Clearly, the effects of solar radiation will be closely connected to the effects of temperature (see b on page 11). However, an increase in solar irradiation also leads to further effects, such as increases in the rates of photochemical reactions. Chan (2002) found that I/O ratios generally increased with increasing solar irradiation, although with a weaker correlation than for temperature.

**1.2.4 Ventilation**

**1.2.4.1 (Intentional) Ventilation**

Ventilation is the means by which ‘stale’ indoor air is removed or diluted by ‘fresh’ outdoor air intentionally introduced and circulated throughout the building (Liddament, 1996). The air exchange rate, measured in air changes per hour (ACH), represents a measure of the building ventilation. It is defined as the volume of indoor air replaced by outside air per unit time and can also be
regarded as the efficiency of the air mass exchange (Chang et al., 2003). $ACH$ is given by the expression:

$$ACH = \frac{Q}{V}$$  

(see table on page ix)

Examples of measured air exchange rates may be found in the Appendix.

Indoor levels of pollutants from outdoor concentrations can be predicted if the air exchange rate is known. In theory, indoor concentrations will gradually increase with air exchange rate, if the concentration outdoors is higher than indoors. When the air exchange rate approaches a certain limit, effectively there will be no difference between indoor and outdoor pollutant levels. However, in reality the indoor concentration will not necessarily increase in proportion to the air exchange rate due to indoor sources, reactions and deposition.

Ventilation is essential for the health and comfort of building occupants. A wide variety of ventilation strategies is available to meet general ventilation needs. In an urban environment, choice and layout may be affected by local air pollution concentrations. A summary of ventilation strategies is given below.

\textit{a. Natural ventilation}

Natural ventilation is the intentional and, ideally, controlled provision of outdoor air into a space through openings such as windows, stacks and vents. Natural ventilation should not be confused with \textit{infiltration}, which is unintentional and uncontrolled. Natural ventilation is created by pressure differences between the inside and outside of the building, which are induced by wind and temperature differences. The relative importance of these driving forces depends on a number of factors. These include the height of the building, internal resistance to airflow, location and flow resistance characteristics of the building openings, the local terrain and the immediate shielding surrounding the building (Limb, 1996). The theoretical principles of natural ventilation have been extensively covered (e.g. BRE, 1978; Liddament, 1996; Limb, 1996; BRE, 1999). The main drawback of natural ventilation is the lack of control, which may result in inadequate ventilation, followed by periods of over ventilation and excessive energy waste (Liddament, 1996).

Dimitroulopoulou et al. (2005), in a study of ventilation rates and indoor air quality in 37 occupied homes in England over a two-year period, found that homes where windows were open (for most or all of the time) had significantly higher ventilation rates, both in winter and summer. The use of trickle vents was another factor that was found to affect ventilation rates. Trickle vents are small openings at the top of the window frame, which are required by Building Regulations to provide a minimum supply of fresh air for occupants and disperse residual water vapour. In the study by Dimitroulopoulou et al. (2005), most occupants were not aware of the trickle vent usage and the vents were fully closed in 1/3 of the homes. However, homes where trickle vents were used for most or all of the time had significantly higher ventilation than other homes in
summer. Also, homes with the lowest ventilation rates in winter had the trickle vents fully closed.

**b. Mechanical ventilation**

Mechanical ventilation is defined as the movement of air through a building using fan power; filtration and heating of air may also take place. The CIBSE Guide B2 (CIBSE, 2001b) provides comprehensive guidance on the requirements for the application of ventilation and air-conditioning to a range of different types of buildings. The guide refers to ventilation requirements to maintain indoor air quality in order to:

a. support human respiration;
b. remove body odour;
c. remove tobacco smoke;
d. remove emissions from building materials and furnishings (e.g. VOCs);
e. prevent radon gas entering a space via foundations and air intakes;
f. support safe and efficient operation of combustion appliances; and
g. allow smoke clearance in the event of fire.

Good external air quality is an essential requirement for effective ventilation: the ventilation air must be ‘fresh’, i.e. free from air pollutants. The quality of ventilation air is affected by several factors, as follows (Liddament, 1999):

a. the outdoor air quality;
b. the proximity of the air intake to a pollution source;
c. the application of filtration; and
d. the cleanliness of the ventilation system.

Mechanical ventilation and air-conditioning systems are often preferred to natural ventilation to ‘clean’ the incoming air for buildings in urban areas. However, studies (e.g. Kukadia *et al.*, 1996) have shown that these may not necessarily be any better in providing cleaner air than, for example, naturally ventilated buildings. What is important is a ventilation strategy that considers the local pollution sources (e.g. traffic, discharges from heating plant, building exhausts), the sizes and shapes of surrounding buildings and the local wind speed and direction.

**c. Filtration**

Filtration, fitted as standard in mechanical ventilation systems, is the means by which particulate matter and, sometimes, gaseous pollutants may be removed from the air by passing the contaminated air through a medium (Liddament, 1996). Filtration systems are selective and are only effective at dealing with the pollutants they are designed for. According to Fisk *et al.* (2002), relatively large decreases (e.g. 80%) in indoor concentrations of Environmental Tobacco Smoke (ETS) and outdoor fine particles can be achieved with practical filter efficiencies.
and flow rates. If it is necessary to remove gaseous pollutants, then activated adsorption filters are required. This is an exceptionally demanding and costly process.

In modelling studies of naturally ventilated buildings, the filtration characteristics of a building are often represented by using a penetration factor, \( P \), which characterises the ability of a pollutant to penetrate the building envelope. By definition, \( P \) must be between 0 and 1, where 1 represents no filtration by the building. It is widely believed that in naturally ventilated buildings, the building fabric presents no barrier to particulate matter (Thatcher and Layton, 1995). Dimitroulopoulou et al., (2001) assumed that if \( P=1 \) for particles, then gases penetrate equally efficiently and, hence, \( P=1 \) for gases as well. Further examples of studies to determine penetration factors in naturally ventilated buildings are provided in the Appendix.

d. Position of air intakes

Great interest has been taken in the placement of ventilation intakes to avoid ingestion of excessively high levels from very localised sources of pollution (e.g. UK Department of the Environment, 1995; Ajiboye et al., 1997; CIBSE, 1997; CIBSE, 1999; Liddament, 1999; Kukadia et al., 2000; CIBSE, 2001a). Review on the placement of ventilation inlets for minimising ingress of pollutants is given in Kukadia and Dimitroulopoulou (2002) and Hall and Kukadia (2004) and can be summarised as follows:

a. Place intakes away from the direct impact of short-range pollution sources (e.g. parking areas, welding areas, loading bays, adjacent building exhausts).

b. If intakes are located higher up a tall building, then contamination from, for example, exhaust stacks and boiler flues needs to be avoided. The possibility of drawing combustion products into buildings at high level has been shown to occur in mechanically ventilated buildings (Kukadia et al., 1996). In addition, tall buildings may carry pollutant sources from the ground up to their maximum heights on their lee sides (Littlefair et al., 2000).

c. In areas of high traffic, roof mounted intakes are recommended as a more robust design option than wall mounted intakes (CIBSE, 1999). Hall et al. (2003) conclude that air intakes for buildings positioned directly adjacent to urban roads should be located at high level to minimise the ingress of traffic pollutant.

d. At rush hour peaks, temporarily reducing the flow of external air or closing ventilation intakes may be an option (Kraenzmer, 1996, Ajiboye et al., 1997, Fletcher 1999). During periods of up to an hour the fresh air reservoir within the building may be used to meet needs (Liddament 2000).

e. Pollutants accumulate in street canyons and courtyards, especially during the daytime period, and do not disperse very readily (Hall et al., 1999a). Natural ventilation of buildings in such areas should be avoided.
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and another strategy needs to be used (Santamouris et al., 1998; Hall et al., 1999a).

f. When a site experiences one principal wind direction, it is advised that exhaust vents are located downwind of inlets in that direction (CIBSE, 1999). However, it is important not to generalise since, under certain circumstances, pollution may be drawn up the downwind side of a building resulting in increased concentrations above ground level on that side (see point b on the previous page).

g. Regions of high pressure differences combined with high external pollutant concentrations will give regions of high probable ingress of contaminants and, hence, lead to greater internal pollutant concentrations. These areas, therefore, need to be avoided when siting air inlets for all types of ventilation systems (Hall et al., 1999b).

1.2.4.2 Infiltration (airtightness)

A large proportion of air penetration into buildings is due to air leakage or infiltration. This is the uncontrolled flow of air through unintentional cracks and gaps in the building envelope. The corresponding loss of air from an indoor environment is called exfiltration (Liddament, 1996).

There are many benefits in reducing air infiltration in buildings: comfort of occupants, energy savings, reduced size of plant, avoidance of fabric degradation and the reduction of outdoor pollution entering the building. If the building structure is airtight, ventilation can occur through intentionally provided openings only. This permits more accurate design solutions and prevents air infiltration from interfering with ventilation performance. The philosophy is to ‘build tight and ventilate right’ (Liddament, 1996).

The largest database of air leakage rates in the UK is that by BRE and covers 471 dwellings (Stephen, 2000). The recent BRE study in 37 occupied homes built after 1995 improves understanding of the relationships between airtightness and ventilation (Dimitroulopoulou et al., 2005).

1.2.5 Deposition

Deposition on internal surfaces is a major mechanism for the removal of air pollutants in the indoor environment, resulting in lower concentrations than those outside. Particle deposition indoors has received an increasing attention, given the adverse effects that particulate matter causes on human health. The research is mainly related to deposition in experimental chambers, test houses, or real dwellings (e.g. Nazaroff and Cass, 1989; Byrne et al., 1995; Fogh et al., 1997; Thatcher et al., 2002; Chao et al., 2003). The available experimental results have been often reviewed (e.g. Wallace, 1996; Lai, 2002).
Studies in real dwellings usually refer to the loss rate of a pollutant. The loss rate, $K$, is proportional to the surface area available for deposition and is calculated as:

$$K = v_d \frac{A}{V}$$

(see table on page ix)

For pollutants with a large diffusive component, such as reactive gases, the surface area represents the total area and incorporates both wall and floor areas (Karlsson, 1994; Yamanaka, 1984; Grontoft and Raychaudhuri, 2004). The same stands for smaller particles. However, for gravitationally-dominated species, such as large particles, the surface area refers mainly to the lower horizontal area. The PTEAM study in the USA (Özkaynak et al., 1996) is the largest study of residences that estimated loss rates for PM$_{2.5}$ and PM$_{10}$.

Deposition velocities of particles depend on many factors such as the size, shape and density of a particle, the nature of the surface and whether the particles are affected by the air exchange rate (Wallace, 1996). For high air exchange rates, deposition will be small compared to other components in the transport process and may often be neglected (Chao and Tung, 2001). Deposition may also be affected by whether or not the particles or internal surfaces are electrically charged. This is of particular importance for the deposition of radionuclides. One major difference between conventional pollutants and radioactive contaminants is that deposited air pollutants may be ignored once deposited whereas nuclear substances will be potentially harmful and, hence, must still be considered. Thus, the half-life of the radioactive material is important (Andersson et al., 2004).

The indoor pollutant concentration may be reduced by deposition and may be increased by resuspension of deposited material. The amount of resuspended matter per unit time will be proportional to the mass loading of the surface (Lange, 1995). The potential for resuspension is traditionally explained as the potential for aerodynamic forces to exceed the forces holding the particle to the surface (Andersson et al., 2004). Clearly resuspension is highly influenced by human activities, such as cleaning. In modelling studies, resuspension from indoor surfaces is often ignored, especially for very high ventilation rates and for smaller particles; however it does need to be considered for larger particles. Typical values of deposition velocities, loss rates and resuspension rates are provided in the Appendix.

### 1.2.6 Indoor chemical reactions and nuclear decay

Indoor chemical reactions may play an important role in indoor concentrations of certain pollutants, such as NO$_2$. Chemical reactions can occur in the indoor air or on fixed surfaces to produce secondary pollutant products (Weschler et al., 1992). For instance, it is possible that ozone and oxides of nitrogen react with VOCs with unsaturated bonds to produce chemically reactive and irritating VOC species. Recent literature has investigated indoor chemistry and the possible
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effects on materials and occupants (e.g. Weschler and Shields, 1997; Weschler and Shields, 1999).

The existence or not of these reactions depends on factors such as the nature and reactivity of the pollutants and materials involved, the temperature and relative humidity, and the degree of air movement (Drakou et al., 1998). Weschler and Shields (2000) used a compartment mass-balance model to simulate reactions among indoor pollutants and the role of ventilation on these. Their results suggested that adequate ventilation is necessary not only to remove pollutants from indoor sources but also to limit reactions among indoor pollutants. For reactions occurring at rates comparable to the ventilation rate, decreasing the ventilation rate increases the concentrations of reaction products, which are often more irritating than their precursors (Nazaroff and Cass, 1986; Weschler and Shields, 2000).

The rate of decay of radionuclides is usually represented using the radioactive decay constant, $\lambda$, or the half-life, $T_{1/2}$, of the material. This is only of importance for short-lived isotopes since for those with half-lives greater than one day the ventilation rate will dominate (Lange, 1995). The half-lives of most radionuclides are well known and may be easily incorporated into models.

1.3 Need for modelling indoor concentrations

Wind tunnel measurements provide quantitative data on outdoor pollution distributions on building surfaces and enable effective siting of intakes and exhausts. Monitoring work in environmental chambers and buildings can provide valuable information on indoor pollution levels and characterise indoor sources. However, monitoring work may be difficult, costly and time consuming in terms of manpower and laboratory support. Furthermore, the results may only be valid for the specific conditions in which the experiment was carried out. So, monitoring studies report a wide range of indoor concentrations and, hence, I/O ratios due to the complexity of indoor-outdoor transport, indoor sources and the wide range of variable parameters that may have an effect.

On the other hand, modelling studies may:

a. quantify the relationships between air pollutant concentrations and important variables;

b. allow extrapolation from relatively few measurements to a large sample;

c. allow the relative contributions of different sources (e.g. indoor sources and outdoor penetration) to be assessed;

d. estimate indoor levels in situations where measurements are unavailable; and

e. determine the ventilation and indoor air quality of a building before it has been constructed.

It has been emphasised that modelling methods are vital for the development of regulation strategies since they may assess the benefits of being indoors in the
event of a chemical release with toxic effect and may easily and quickly allow for variations under different conditions to be estimated (Dimitroulopoulou et al., 2001b; Glytsos et al., 2004). However, in order to validate the results of any kind of modelling, monitoring work is required and should be carried out, where possible.

1.4 Types of models available

Several computer modelling techniques have been developed for indoor air quality studies. These include statistical regression analysis, mass-balance models, which constitute the majority of current modelling work, and computational fluid dynamics (CFD) techniques.

Mass-balance models take a macroscopic view by calculating average concentrations in different zones of a building. Usually indoor concentrations are modelled assuming well-mixed indoor environments. Mass-balance models may be split into regression models, microenvironmental models and multizone models. Microenvironmental models usually include a limited number of distinct building zones and are used to simulate physical processes of air pollutants and predict indoor air pollutant concentrations. This has been the most used approach to modelling thus far. Multizone models can have as many different zones as required and are mainly used for ventilation studies, by simulating airflows between zones.

CFD modelling takes a microscopic view by examining the detailed flow fields and concentration distributions within a room or between rooms. Although most whole-building analysis (mainly for ventilation purposes) currently relies on multizone modelling, the rapid development of computational speed and power over recent years has led to growing popularity of CFD methods. Each type of models has strengths and weaknesses and the choice of model must be determined by the requirements of the modelling work.

A detailed review of existing mass-balance and CFD models is given in sections 2 and 3, respectively.
Mass-balance models are used to simulate average indoor air pollutant concentrations as a function of outdoor concentrations, building and pollutant characteristics and indoor sources. These models consider transport of air pollutants between outdoors and indoors, as well as between indoor compartments in the buildings, and are widely used due to the simplicity of the mathematics involved. The strength of these models is the simulation of air pollutant concentrations that may be well compared with results from experimental measurements.

Mass-balance models are based on the following concept. The mass of pollutant in the room during a short time interval \( dt \), over which the parameters may be assumed to be constant, increases by an amount \( dm \), as a result of the penetration of outdoor air and indoor sources:

\[
\text{dm} = \text{inward mass flow} + \text{internal production} - \text{outward mass flow}
\]

Converting the pollutant mass to the concentration within the compartment, \( C \), at steady state this is usually written as an ordinary differential equation, such as:

\[
\frac{dC}{dt} = S - LC = 0
\]

where \( dC/dt \) is the rate of change of the indoor concentration, \( S \) is the sum of all sources and \( L \) is the sum of all sinks. The above equation may be analytically written including further parameters such as a loss rate (if the pollutant readily deposits), a decay rate (for radioactive contaminants), a filtration factor and a mixing factor.

The models may be divided into statistical regression models, microenvironmental models and multizone models. Examples of the models, their concepts and applications, and issues associated with their use will be discussed in detail in the following sections.

### 2.1 Statistical regression models

The simplest models available to predict indoor air pollutant concentrations from outdoor sources are statistical regression methods. These entirely empirical techniques are quick and easy to apply since they do not require complicated input parameters. Experimental data is used to estimate the associations between indoor and outdoor concentrations at equilibrium. Regression models are mass-balance models in steady-state form and hence cannot describe the time evolution of indoor concentrations. This makes regression models unsuitable for modelling short bursts of pollution.
An example of the use of regression modelling may be found in Kulkarni and Patil (2002) who demonstrated that, under certain assumptions, a mass-balance model such as that of Kulmala et al. (1999) (see section 2.2.1) reduces to:

\[ \bar{C}_{in} \approx k \bar{C}_{out} + \frac{1}{Q} S \]

where \( \bar{C}_{in} \) and \( \bar{C}_{out} \) are the time-integrated indoor and outdoor concentrations respectively, \( k \) is the penetration factor, \( Q \) is the airflow rate and \( \bar{S} \) is the average emission rate. This states that the average indoor concentration can be predicted by a simple linear function of the outdoor concentration where the slope \( k \) and intercept \( S/Q \) are characteristics of the particular building. Model validation showed that the model made very good predictions for homes with LPG stoves (measured against predicted \( R^2 = 0.98 \)) and satisfactory predictions for homes cooking using kerosene (\( R^2 = 0.64 \)), since for LPG there is a relatively greater contribution from outdoor sources and less from indoor sources.

Chao and Tung (2001) used a model based on average time-integrated indoor and outdoor particulate concentrations. In the absence of indoor activity or when the indoor contribution is significantly less than from the ambient air, the model states that:

\[ V \frac{dC_{in}}{dt} = PqkC_{out} - qkC_{in} - \sigma V_d C_{in} \]

where \( C_{in} \) is the indoor concentration, \( C_{out} \) is the outdoor concentration, \( V \) is volume of the room, \( P \) is the penetration factor, \( q \) is air flow rate, \( k \) is the room mixing factor, \( \sigma \) is indoor surface area and \( V_d \) is deposition velocity. Since the I/O ratio of particulate matter is strongly coupled with the air exchange rate and the decay parameter:

\[ \frac{\langle C_{in} \rangle}{\langle C_{out} \rangle} = 1 - Ae^{-\eta h} \]

where \( \langle C_{in} \rangle \) is the integrated average indoor concentration, \( \langle C_{out} \rangle \) is the integrated outdoor concentration, \( h = kq/V \) is the effective air exchange rate and \( A \) and \( \eta \) are parameters related to the transport process. In the above formula, \( Ae^{-\eta h} \) represents the extent to which the outdoor contaminant is attenuated by the building shell, \( A \) is an analogy to filter efficiency and \( \eta \) represents the ability of an air stream to transmit the contaminant. The model was found to have problems at high ventilation rates, possibly since it neglects re-suspension, which cannot be neglected at such rates. The modelled average I/O ratio agreed well with experimental data and it was found that the indoor concentration was almost identical to the outdoor concentration, if the exchange rate was greater than 4 h\(^{-1}\).

Ní Riain et al. (2003) used a time-averaged model followed by linear regression to estimate indoor particulate matter concentrations. In the model, which may also be applied to gases that have long lifetimes in the atmosphere (such as
CO), the time-averaged indoor concentration, $\bar{I}$, is related to the time-averaged outdoor concentration, $\bar{O}$, by:

$$\bar{I} = \frac{P \alpha \bar{O}}{\alpha + \lambda_d} + \frac{1}{V(\alpha + \lambda_d)} \bar{G}$$

where $P$ is the penetration factor, $\alpha$ is the air exchange rate, $\lambda_d$ is the rate at which particles deposit on indoor surfaces, $V$ is the indoor volume and $\bar{G}$ is the rate at which particles are generated or resuspended (Dockery and Spengler, 1981). For fine particles (i.e. less than 1 µm in diameter), the deposition rate is generally small compared to the ventilation rate and so:

$$\bar{I} = P \bar{O} + \frac{1}{Q} \bar{G}$$

where $Q = \alpha V$ is the volume flow rate. Thus, this relationship shows that the slope of linear regression of $\bar{I}$ against $\bar{O}$ results in the penetration factor and the intercept represents the resuspension or generation rate indoors. However, using this regression method to model indoor concentrations requires the assumption that $\lambda_d$, $P$ and $\alpha$ are constant over the averaging period and that the outdoor pollution is evenly distributed.

### 2.2 Microenvironmental models

These models are based on the concept of the microenvironment (ME). This is defined as a generic space with a homogeneous pollutant concentration in which people spend time (Duan, 1982). This has been the key concept in modelling of personal exposure and, as a result, microenvironmental models are often used together with exposure models.

A microenvironment may be a whole building, a section of a building (i.e. multiple rooms) or individual rooms. According to this definition, the air in a microenvironment is assumed to be instantaneously well-mixed (i.e. the pollutant concentration is the same everywhere). This assumption is only valid if the mixing in the indoor air occurs at a much greater rate than other factors affecting indoor air concentrations, such as air exchange and deposition (Kulmala et al., 1999). Microenvironmental models are used to predict average concentrations in one or two indoor compartments based on a simple parameterisation of the flow rates between them and between the compartments and the outdoor air. Examples of microenvironmental models are presented now.
2.2.1 Examples of microenvironmental models

Nazaroff and Cass (1986) developed an early multizone model based on a simple mass-balance approach:

\[ \frac{dC}{dt} = S - LC \]

where \( S \) is the sum of all sources (i.e. direct emissions, advective transport from outdoors, production by chemical reaction) and \( L \) is the sum of all sinks (i.e. homogeneous chemical reactions, transformation and removal processes on surfaces, transport from the chamber). For each chamber, air may enter directly from outside, from a mechanical ventilation system and from each of the other chambers (cross-ventilation) and may be removed to the outside, to the mechanical ventilation system and to each of the other chambers. The model gives predictions for many chemical species and can also be operated in a full-chemistry mode that can investigate all parameters affecting indoor air quality and study reactive pollutants that cannot be determined by more simple mass-balance models. Drakou et al. (1998) tested the model and found that the full-chemistry version is necessary when indoor sources are present.

Glytsos et al. (2004) developed a model based on a mass-balance equation in the same form as that of the model by Nazaroff and Cass (1986). The model is capable of taking into account complex chemical reactions, such as coagulation, nucleation and hygroscopic growth. The model was compared to a version of the Nazaroff and Cass (1986) model for Environmental Tobacco Smoke (ETS) in a two-zone building. Very good agreement between both models and experimental results regarding mass concentrations and particle size distributions was found (Glytsos et al., 2004).

Hayes (1989) developed a personal air quality model (PAQM), which estimated personal exposure of population groups moving among indoor and outdoor MEs. A mass-balance equation was used to calculate hourly indoor concentrations for a reactive pollutant in a single compartment, within which indoor air is recirculated and into which outdoor air is mixed by means of the building ventilation system, building air leakage and infiltration. Pollutants were also generated by indoor sources and removed by deposition. The single compartment model solves the following equation for a reactive pollutant:

\[ \frac{dC_i}{dt} = k a_M (C_o - C_i) + k a_F (E_F C_o - C_i) + k a_R (E_R - 1) C_i - k K \left( \frac{A}{V} \right) C_i + \frac{S}{V} \]

where \( C_i \) is the indoor concentration, \( C_o \) is the outdoor concentration, \( k \) is a room mixing factor, \( a_M \) is the infiltration rate, \( a_F \) is the outdoor make-up air flow rate, \( E_F \) is the efficiency of the make-up filter (the ability of the filter to remove pollution), \( a_R \) is the flow rate of recirculated air, \( E_R \) is the efficiency of the recirculation filter, \( S \) is an indoor source term, \( K \) is a pollutant reactivity factor, \( V \) is the room volume and \( A \) is the interior surface area. The first term represents infiltration, the second outdoor air, the third recirculating air, the fourth losses...
and the final term represents indoor sources. Koutrakis et al. (1992) used the mass-balance model developed by Hayes (1989) to analyse the data of the New York Study in 433 homes and estimate penetration factors, decay rates and PM$_{2.5}$ source strengths for cigarettes, wood burning stoves and kerosene heaters.

The study of Chaloulakou and Mavroidis (2002) also used the mass-balance formulation developed by Hayes (1989) to simulate indoor concentrations of CO in a public school building in Athens, Greece. In general, when the results were compared with experimental data, the model was found to perform reasonably well (predicted against measured $R^2 = 0.69$). However, the model performed poorly where rapid concentration changes were observed. The model utilizes both measured outdoor concentrations as well as predicted indoor concentrations from the previous time step and, hence, when the model has calculated the next concentration value, the prediction may be inaccurate for a short burst of pollution.

Lange (1995) simulated a short-term outdoor contaminant release increasing for 100 s, constant for 100 s and decreasing for 100 s using the following model:

$$\frac{dC_i(t)}{dt} + (\lambda_r + \lambda_d)C_i(t) = f\lambda_rC_o(t)$$

where $C_i(t)$ is the indoor concentration at time $t$, $C_o(t)$ is the outdoor concentration at time $t$, $\lambda$ is the air exchange rate, $\lambda_d$ is the deposition constant and $f$ is a filtration (penetration) factor. The study found a significant time delay from the start of the decline of the outdoor concentration until the indoor concentration was actually higher than that outdoors. Thus, the earliest time for advising the public to open doors and windows must be when the outdoor concentration approaches zero. Lange (1995) concludes that ventilation should be encouraged after the cloud has passed the inhabited area, especially if slow deposition gases are involved when the effect of ventilation will be greatest.

Kulmala et al. (1999) developed a dynamic model to account for the fact that, in principle, almost all variables associated with outdoor-to-indoor pollution transport are time-dependent. The time evolution of the particle or non-reactive gas concentration is given by:

$$\frac{dl}{dt} = l(O - I) - al + r_eB + Q$$

where $I$ is the indoor concentration, $O$ is the outdoor concentration, $B$ is the surface accumulation on indoor surfaces, $l$ is the air exchange rate, $s$ is a penetration coefficient, $a$ is the deposition rate, $Q$ is the production/sink rate of indoor sources/sinks and $r_e$ is the re-emission rate. The indoor air concentration is coupled with accumulation on indoor surfaces and the outdoor air concentration as follows:

$$\frac{dB}{dt} = (al - r_eB)\frac{V}{A}$$
\[ \frac{dO}{dt} = f(t, x_1, x_2, \ldots) \]

where \( V \) is the indoor volume, \( A \) is the indoor surface area and \( f \) is the functional outdoor concentration change, depending on time and other variables. Since this model allows one to take into account time-varying deposition and outdoor concentrations, it is particularly useful to predict the behaviour of indoor concentrations with respect to bursts of pollution, like chemical accidents and rush hour emissions. Kulmala et al. (1999) tested the model by altering the rate of ventilation, filtration and deposition. When periodic traffic behaviour and no indoor sources were introduced, it was found that the indoor concentrations followed those outdoors with some delay. Filtration was observed to lead to smaller penetration and, thus, smaller surface accumulation and lower indoor concentrations, while higher deposition rates caused higher accumulation and again lower indoor concentrations. Kulmala et al. (1999) concluded that it appears to be beneficial to use slower ventilation for the first hours following a burst of pollution and quicker ventilation at later times. This prevents contaminated air entering initially and removes any pollution from indoors in the longer term. Although the indoor pollution level was typically two orders of magnitude less than the original outdoor level, the model also suggested that there may exist a time shortly following a burst of pollution when the indoor concentration exceeds that outdoors. These findings are in agreement with the work of Lange (1995) described previously.

Fischer et al. (2002) used a 1st-order linear differential equation to model the transport of particles from outdoors to indoors that incorporates physical mechanisms for both time-dependent and size-dependent penetration and deposition:

\[
\frac{dC_{in,j}}{dt} = P_j(\Delta p, x)C_{out,j} - C_{in}(\beta_j(x) + \lambda) \]

where \( C_{in,j} \) is the indoor concentration of particles of size \( j \), \( C_{out} \) is the outdoor concentration, \( \lambda \) is the infiltration rate into the building, \( P_j(\Delta p, x) \) is the fraction of particles penetrating the building shell, \( \beta_j(x) \) is the deposition rate inside the building, \( \Delta p \) is the indoor-outdoor pressure difference and \( x \) represents other building factors, such as furnishings and indoor turbulent intensity. However, when the model was tested, the predicted I/O ratios were not consistent with measurement unless an unnaturally large deposition rate was assumed.

INTAIR (Dimitroulopoulou et al., 2001a), is a deterministic compartment model that allows indoor concentrations to be simulated into two separate microenvironments using the following mass-balance equation:

\[
\frac{dC_i}{dt} = -v_d(A_i/V_i)C_i + \lambda_r I C_o - \lambda_r C_i + \lambda_f (C_j - C_i) + \frac{Q_i}{V_i} \]

where \( C \) is the indoor concentration, \( C_o \) is the outdoor concentration, \( v_d \) is the deposition velocity, \( A \) is the surface area, \( V \) is the indoor volume, \( \lambda_r \) is the
indoor-outdoor air exchange rate, $\lambda_i$ is the air exchange rate between the indoor microenvironments, $f$ is a building filtration factor, $Q$ is the indoor emission rate and the subscripts $i$ and $j$ refer to the two individual microenvironments. INTAIR is linked to an exposure model and provides estimates of the contribution of indoor and outdoor sources on total exposure.

In Dimitroulopoulou et al. (2001a), the INTAIR model was parameterised to predict NO$_2$ concentrations in five different indoor microenvironments (residential and non residential). In another study, Dimitroulopoulou et al. (2001b) parameterised the INTAIR model to estimate PM$_{10}$ concentrations and to assess the contribution of smoking for typical homes in the UK. The microenvironmental models described so far in this report are deterministic in nature. The study of Dimitroulopoulou et al. (2001b) highlighted the need for more sophisticated probabilistic models.

The updated version of the deterministic INTAIR model is the INDAIR model (Ashmore et al., 2000; Dimitroulopoulou et al., submitted). In its probabilistic form, INDAIR simulates analytically (based on pollutant and building characteristics), the frequency distributions of indoor air pollutant concentrations in the three major rooms of the home (kitchen, lounge and bedroom); concentrations in four other non-residential microenvironments were simulated using I/O ratios. The model parameters and I/O ratios were defined in the INDAIR model as probability density functions to provide frequency distributions of air pollutant concentrations in different microenvironments. Model parameterisation was based on data (although limited) for the UK and the results were found to be consistent with measured microenvironmental concentrations in the UK. The model has also been linked with a time-activity based exposure model, EXPAIR. This version of INDAIR/EXPAIR modelling framework was designed to simulate indoor concentrations and personal exposures at specific locations, using an assumed and fixed activity pattern, in terms of smoking and cooking and was unable to accommodate time varying levels in outdoor concentrations caused by changes in traffic and meteorological conditions.

In the RUPERT project (Reducing Population Exposure from Road Transport) (Dimitroulopoulou et al., 2004; Ashmore et al., 2005), a more flexible version of the INDAIR model has now been designed and parameterised to address this shortfall. The new INDAIR-2 model predicts the frequency distribution of concentrations in each microenvironment as a function of the outdoor concentration and four regression coefficients. Two of these coefficients define the relationship between indoor and outdoor concentrations in the absence of any significant indoor source. The remaining two coefficients describe the incremental effect of various activities and sources, appropriate to each microenvironment, on the modelled concentrations. Each coefficient is defined as a probability density function, while the input outdoor concentrations are defined as log-normal distributions for each of four road categories. The INDAIR-2 code allows, if appropriate, for the values of these coefficients to be varied over the course of the day to reflect different levels of activity and emissions.
When dealing with a radioactive substance, additional factors must be used in models, such as in the mass-balance model for radon of Man and Yeung (1999):

\[
\frac{dC_i(t)}{dt} = J \frac{S}{V} + C_0 \lambda_v - C_i (\lambda + \lambda_v)
\]

where \( C_i(t) \) is the radon concentration in the room at time \( t \), \( J \) is the radon flux or area exhalation rate of concrete, \( S \) is the exhaling surface area, \( V \) is the room volume, \( C_0 \) is the concentration in outside air, \( \lambda_v \) is the ventilation rate and \( \lambda \) is the decay constant. The same model has also been employed in the work of Sahota et al. (2005).

### 2.3 Multizone models

Microenvironmental models assume the air within a building (or large parts of it) to be instantaneously well-mixed. However, the real airflow pattern within a building may be extremely complex and not adequately represented by a model with only a single compartment (or few compartments). Often some parts of a building, particularly basements or rooms with closed doors, exchange air only very slowly with other parts of the building and, thus, the actual mixing is far from instantaneous as assumed by microenvironmental models (Sinden, 1978). Therefore, real buildings are often more suitably represented as a large number of connected well-mixed chambers (Lorenzetti, 2002). This is the approach used in multizone modelling techniques, which are especially used to simulate ventilation rates.

Instead of a limited number of MEs, multizone models allow a set of compartments with certain flow rates between them. Each compartment has two vents: one representing the sum of all areas through which air vents inwards and one for air venting outwards. Air venting inwards has the properties of the outside air and air venting outwards has the properties of the room air (Colls, 2002). The flow rates into and out of a compartment must be equal and are again represented by ordinary differential equations.

Sinden (1978) provides a useful review of the mathematical theory of mass and pollutant transfer between chambers connected by a network of one-way passages. Whereas a microenvironmental model solves only a single differential equation, a multizone model solves a system of coupled mass-balance equations, where the number of equations is equal to the number of zones. In this network, zones represent areas in which uniform mixing may be assumed (either separate rooms or group of rooms) while connections simulate airflow paths between compartments (Sowa, 1998; Chang et al., 2003). It is also sometimes possible to break individual rooms up into smaller zones, since a large room in particular may be more satisfactorily represented in this way. This maintains the simplicity of the approach while capturing some of the heterogeneity in a large room (Sohn et al., 1999).
Although the equations that form the basis of both microenvironmental and multizone models are generally similar, there are significant differences between the two model types. First, in microenvironmental models, air exchange rates are specified in advance as model parameters, whereas multizone models allow the air exchange rates between zones to be predicted by the model. Additionally, there are differences in the uses of the models. Microenvironmental models are used more frequently for analysis of air quality, while multizone techniques are used predominantly to model building ventilation. However, some multizone models have been coupled with contaminant transport models (also based on mass-balance approaches) to predict air pollutant distributions within buildings using the modelled ventilation rates.

### 2.3.1 Examples of multizone models

Two of the most widely used multizone models are COMIS and CONTAM (Lorenzetti, 2002). Both models allow the user to assemble various sub-component models representing compartments and flow paths as required for a given building configuration. The programmes work by finding the pressures at points where the flow elements connect to each compartment (based on specified reference pressures), then by finding the flows in each path and, finally, by summing the flows in and out of each compartment. The solver then adjusts the reference pressures to achieve mass-balance. The flow results are then passed to a pollutant transport solver to calculate indoor concentrations (Lorenzetti, 2002).

Although COMIS (and, in fact, CONTAM) allows for only one type of well-mixed compartment, the model is capable of allowing several key components influencing air flow, such as cracks, fans and large openings. The user may define complex changes in indoor temperatures, fan operation, pollutant concentrations in zones, pollutant sources and sinks, opening of doors and windows and weather data (COMIS Multizone Air Flow Model website). CONTAM provides airflow models for infiltration, exfiltration and room-to-room flows driven by mechanical means, wind pressure and buoyancy (NIST Multizone Modeling website). The programme can also model the dispersal of contaminants transported by airflows, transformed by a variety of processes (including by chemical reactions, adsorption and desorption to building materials, filtration and deposition) and generated by a range of source mechanisms (NIST Multizone Modeling website).

The COwZ model (COMIS with sub-Zones) has been developed by the QUESTOR Centre at Queen’s University, Belfast. The programme is based on the COMIS multizone model but allows the user to divide individual rooms into smaller, discrete zones using a Cartesian grid (Stewart and Ren, 2004). The temperature and concentration within each sub-zone are then assumed to be represented by single values. The user may choose the appropriate size, shape and number of these sub-zones, although between 30 and 200 zones within a room is typical. The technique allows COwZ to more accurately predict mass transfer and
pollutant dispersion with respect to both time and space and is an intermediate step between multizone models and CFD (see section 3) (Stewart and Ren, 2004; QUESTOR Environmental Modelling Group website).

BREEZE, developed by BRE, is a suite of integrated models, including a multizone model and a pollutant transport model, capable of making air flow predictions over a range of environmental conditions (BRE, 1993). The model is also capable of calculating air exchange rates based on the specified scenario. Although BREEZE calculates steady-state airflow networks, it treats contaminants dynamically (i.e. a quasi-dynamic approach). BREEZE allows three types of contaminant sources: initial concentrations, feed rates (specified input rates which may vary with time) and adsorption (whereby adsorbents, such as carpets, may remove or release contaminants). Wind pressure, $P_w$, at an external opening is related to the wind speed, $V$, air density, $\rho_T$, and the wind pressure coefficient, $C_P$, as follows:

$$P_w = \frac{1}{2} \rho_T C_P V^2 d$$

where $d$ is $\pm 1$ depending on whether the previous node represents outside air or not. The pressure difference across an opening is calculated and the characteristic orifice equation for openings is then used to relate the pressure difference to the mass flow:

$$q = C_d A \rho \sigma \left( \frac{2|P|}{\rho} \right)^n$$

where $q$ is the mass flow, $C_d$ is the discharge coefficient, $A$ is the area of the opening, $\rho$ is the air density, $P$ is the pressure difference, $n$ is an exponent (in the range 0–1) and $\sigma$ is $\pm 1$. The program modifies this equation depending upon the type and size of the opening specified. Local flow approximations to account for the stack effect and turbulent diffusion are then applied. Multiple scenarios representing different environmental conditions may be simulated; for example winds may be attenuated for different wind speeds at different heights and multiple wind directions may be specified.

Sohn et al. (1999) used a multizone, mass conservation approach originally developed by Sinden (1978):

$$V_i \frac{\partial C_i}{\partial t} = S_i - C_i \sum_{j=0}^{n} f_{ij} + \sum_{j=0}^{n} C_{j} f_{ji}$$

for $i = 1, n$ and where $C_i$ is the concentration in zone $i$, $V_i$ is the volume of zone $i$, $S_i$ is the contaminant release rate in zone $i$, $f_{ij}$ is the air flow rate from zone $i$ to zone $j$ and $n$ is the number of zones. The study attempted to identify optimization methods for simultaneously estimating effective compartmental volumes and air exchange rates. Two optimization methods, steepest descent and simulated annealing, were tested and the results in a three-zone system
indicated that simulated annealing made better overall indoor air quality predictions.

Sowa (1998) discussed the addition of stochastic factors, such as fluctuations in weather conditions and changes in the outdoor pollution concentration, into a multizone model. According to this work, the simplest way of including stochastic factors in deterministic models is to replace constant values of input data with time series. Another method assumes that parameters may include a random component, such as:

\[ K_i = \bar{K}_i + K_i' \]

where \( K_i \) is the value of component \( K \) at point \( i \), \( \bar{K}_i \) is the mean value of \( K \) and \( K_i' \) is a random fluctuation on the mean. A third way to randomise processes in a deterministic model is by multiple generations of sets of possible input data and subsequently using a Monte Carlo simulation. Comparison of these methods for the situation of a two-compartment office using a version of the CONTAM model (CONTAM94) showed that the method of stochastic disturbance incorporation does not have an important influence on mean predicted concentrations but can result in major differences in the estimated distribution of concentrations.

### 2.4 Mass-balance model advantages and limitations

The types of mass-balance models described here are particularly useful to identify the key building factors that influence indoor concentrations of air pollutants. These models can also estimate the relative importance of different pollutant sources. Identification of emissions and building characteristics can assist in identifying homes where health risks are likely to be highest. In this way, mass-balance models, in conjunction with exposure models, can evaluate the potential benefits of measures to reduce indoor air pollutant levels and the implications of policy decisions on population exposure.

Mass-balance models also have some limitations. The major limitations are the assumption of a spatially uniform concentration outside the building and the internal well-mixed assumption. As discussed previously, the concentration in the envelope surrounding a building may be extremely variable, especially due to sources close to the building. Using a single value to represent the outdoor concentration at a given time may lead to serious inaccuracies in the results produced by mass-balance models. The use of internal well-mixed zones is only generally appropriate for average-sized residential buildings since intra-room mixing is usually orders of magnitude faster than inter-room exchange and physical walls act as partitions for each zone. However, in very large rooms with localized ventilation and/or source locations, a significant spatial concentration gradient may persist and a single well-mixed compartment may be inappropriate to represent a room, since it tends to underestimate concentrations close to the source (Sohn et al., 1999). Furthermore, in some cases, rooms, and particularly
large rooms, are not well-mixed over any length of time (Kulkarni and Patil, 2002; Gadgil et al., 2003).

The well-mixed assumption causes models (especially deterministic models) to lose some of the actual variability in indoor concentrations and, therefore, may not accurately represent the worst-case situation that may be important for a short burst of pollution. To account for these problems, the concept of a “mixing factor” (the fraction of ventilation air completely mixed in a room) or a “mixing time” (the earliest point following release after which the room concentration is essentially uniform) have been introduced into mass-balance equations (Gadgil et al., 2003). Examples of typical mixing times are provided in the Appendix. However, these approaches have been found to underpredict concentrations close to sources, for example near air inlets (Gadgil et al., 2003). Kulkarni and Patil, (2002) conclude that, usually, the way of using a mixing factor is erroneous.

Excluding stochastic parameterisation may lead to greater inaccuracy in the predictions of indoor air quality models. According to Chaloulakou and Mavroidis (2002), when there are large variations in the room-mixing factor, it is generally not appropriate to use mean parameter values since such a model would be unable to respond adequately to large outdoor peaks. The probabilistic nature of models such as by Ashmore et al. (2000) and Burke et al. (2001) allows estimation of the upper percentile of indoor concentrations, which is vital for effective risk assessment of indoor air. Simulation results are very sensitive to applied probabilistic methods, so care is always required.

Another issue is model parameterisation and the lack of data, which leads to many assumptions and simplifications. In the case of the UK, although the home environment has been quite well characterised, many of the physical features of non-residential MEs are still poorly understood and there is a lack of data to quantify the key model parameters (Ashmore et al., 2000; Dimitroulopoulou et al., 2001a).

The primary difficulty with multizone modelling is that the number, locations and sizes of well-mixed compartments must be known in detail beforehand (Sohn et al., 1999). This can be a considerable challenge where large rooms are involved and the defined sub-zones must adequately represent the heterogeneity of the room. Another issue is the modelling of all contaminant transport as instantaneous. This has the effect of overpredicting the speed at which pollutants spread through the building (Lorenzetti, 2002). It is often possible, however, to include pollutant transport delays (usually by the introduction of extra links in the network). The review of CONTAM and COMIS by Lorenzetti (2002) draws the conclusion that the programs may need to be modified or replaced for users wishing to apply them to certain types of problem, especially those with novel ventilation systems.
Mass-balance models cannot accurately account for non-uniform pollutant concentrations within rooms and in the envelope surrounding the building. As a result, CFD models that attempt to simulate actual air flows, mixing and, to some extent, contaminant distributions in and around buildings have been developed and used since the 1970s (e.g. Nielsen, 1973; Nielsen et al., 1978). CFD techniques are based on numerical solution of the Navier-Stokes equations, the fundamental equations governing the flow of fluids, and, in the case of pollutant transport studies, a transport equation for contaminant distributions (Emmerich and McGrattan, 1998; Nielsen, 2004). Whereas mass-balance models apply a macroscopic viewpoint, CFD examines the flow fields and pollutant concentration microscopically based on discretisation using a grid mesh. In the case of airflow within a room, the room is divided into grid points and the equations are solved numerically using an iterative procedure (Nielsen, 2004).

There are currently three CFD methods available: direct numerical solution (DNS), Reynolds-averaged Navier-Stokes (RANS) and large-eddy simulation (LES). DNS involves solving the governing equations directly with a grid fine enough to capture the smallest turbulent eddy (Emmerich and McGrattan, 1998). However, DNS cannot currently be used to study indoor airflows due to limitations of available computational memory and speed (Jiang and Chen, 2001). As such, other techniques have been used to model fine-scale turbulence.

RANS techniques constitute the most widely used CFD methods in most industrial applications (Jiang and Chen, 2001). In RANS, the Navier-Stokes equations are studied in time-averaged form and local turbulence is modelled with a turbulence model, the most common of which in engineering applications is the empirically-derived k-ε model, where k is the turbulent kinetic energy and ε is the dissipation rate of turbulent energy (Emmerich and McGrattan, 1998; Nielsen, 2004). The model, which decomposes the velocity into a mean and a fluctuating component, is robust and reliable but handles the physics in a simplistic manner. The k-ε model has been shown to give good predictions in many situations but, however, it may not be applied in all circumstances since too much information is filtered out in the averaging process (Davidson and Nielsen, 1996; Nielsen, 2004). As such, there are problems applying the k-ε model to room airflow, especially in rooms with unconventional geometries (Emmerich and McGrattan, 1998; Nielsen, 2004). RANS also calculates only mean flow parameters (equivalent to averaging a large number of identical simulations).

The types of flows for which RANS has been shown to be inadequate can often be more successfully modelled by LES (Davidson and Nielsen, 1996). The principle of LES is that, rather than time-averaging, the Navier-Stokes equations are filtered spatially to separate the large and small eddy motions, i.e. those
indoor concentrations in buildings from sources outdoors

above and below a specified filter width (Jiang and Chen, 2001; Chang et al., 2003). The large eddies are computed explicitly by solving the equations numerically while the small eddies are modelled with a subgrid-scale (SGS) turbulence model, usually the Smagorinski model (Zhang and Chen, 2000). Although LES requires more CPU time than RANS, the method results in a transient solution to the Navier-Stokes equations rather than a steady-state solution and is, hence, closer to the real-life situation (Emmerich and McGrattan, 1998). Since most of the turbulence is resolved, greater detail of information can be obtained compared with time-averaged methods (Davidson and Nielsen, 1996). Zhang and Chen (2000) state that ‘CFD with an LES model should be a next-generation tool to study indoor air flow, because the model is more universal, has fewer or no adjustable model coefficients, and can provide more flow information than other CFD models’.

3.1 Examples of CFD models

Commercially-available CFD packages, such as FLOVENT (see FLOMERICS Airflow Modeling website) and those available from ANSYS (see ANSYS website), have been used primarily for modelling airflows, ventilation and thermal comfort in indoor environments (for example, see Bojic et al., 2002 or Heiselberg et al., 2004) rather than pollutant transport. However, some researchers have attempted to model indoor pollution concentrations using CFD, although not often from outdoor sources.

Finlayson et al. (2004) used a commercially-available RANS code with a k-ε turbulence model to simulate dispersion in a large indoor space. The study found a good qualitative agreement between the model predictions and experimental data and concluded that the method results in acceptably good steady-state predictions (i.e. substantially better than a factor of 2) in the breathing plane. However, the problems associated with the application of RANS to indoor spaces were well illustrated by Gadgil et al. (2003) who again used a commercially-available RANS CFD code with a standard k-ε model. The study found that the method underestimates mixing times by an average of 30% compared to measurements and the authors suggested that this may be because the flow fields in the room used were not everywhere turbulent.

There are discrepancies in the literature relating to the use of LES methods for indoor airflow. Zhang and Chen (2000) state that ‘very few LES studies on indoor airflow have been reported’ in the literature and ‘the results in these studies do not agree very well with the experimental data’. On the other hand, Emmerich and McGrattan (1998) report on ‘recent studies that found LES results agree better with experimental results for situations examined’, indicating that ‘the research community is moving toward the application of LES methods’. This apparent disagreement is most likely due to the constant coefficient used in the Smagorinski SGS model, called the Smagorinski constant. The model requires that this constant be specified in advance (Jiang and Chen, 2001). However, this is not ideal since the Smagorinski constant is flow dependent and influences the
results greatly (Davidson and Nielsen, 1996; Zhang and Chen, 2000). Thus, the Smagorinski model may not be appropriate for indoor airflow studies.

Emmerich and McGrattan (1998) applied an LES method with the Smagorinski SGS model to predict flow for an isothermal, 3D room using the US National Institute of Standards and Technology (NIST) model, LES3D. It was found that the simulations capture the airflow pattern in the main portion of the room, although the model was found to predict poorly near the floor and ceiling.

As a consequence of such work, researchers have proposed dynamic subgrid-scale models (DSMs) to model the small eddies in LES methods. The study of Davidson and Nielsen (1996) tested a DSM proposed by Germano et al. (1991) in which the Smagorinski constant is computed by applying a second, coarser filter to the Navier-Stokes equations. The results obtained in a ventilated room with the DSM were in good agreement with experimental data. Zhang and Chen (2000) proposed a simple filtered dynamic subgrid-scale model (FDSM) for indoor airflows and found that the FDSM correctly predicted velocities and temperatures in a room but had more difficulty in calculating heat transfer near a wall and turbulence energy distribution. Jiang and Chen (2001) conducted a comparative study using both the Smagorinski model and a DSM to examine the accuracy of LES airflow simulation around a bluff body and in a room. It was found that the models computed mean air exchange rates at least 30% smaller than measured experimentally for single-sided ventilation. However, the DSM was found to perform better than the Smagorinski model, especially for the case of single-sided ventilation, which involves fully developed turbulence around the building, laminar flow inside and, thus, strong interactions between turbulent and laminar flow at openings (Jiang and Chen, 2001). Further research is still needed to assess whether DSMs can provide more realistic results than the Smagorinski model in LES methods.

3.2 CFD model advantages and limitations

CFD simulations are highly specific and, as such, the method is currently used primarily as a research tool with most work reported in the literature focussing only on indoor airflows rather than indoor air pollutant concentrations. Although the complexity of CFD models can be problematic, the technique allows the user to control far more parameters and variables. Another advantage is that CFD calculates a detailed, quantitative description of the situation and allows the user to visualise this as required (Gadgil et al., 2003). CFD may also be used to make predictions in occupied rooms (for example, to investigate the effects of furniture), unlike mass-balance models.

At present, CFD is still a research tool and most of the limitations of CFD models are due either to limitations relating to computational power or the level of expertise that is required (Maghrabi, 2004). Computational power has increased dramatically in recent years and is, hence, becoming less of an issue. However, accurate CFD predictions of room airflow remain a difficult proposition, requiring great experience and care (Gadgil et al., 2003). The geometries involved in
indoor air modelling can be extremely complex. This requires sufficient expertise to specify the detailed boundary conditions and appropriate grid system necessary for accurate results (Maghrabi, 2004). Good numerical predictions require a grid sufficiently refined that the solution does not depend on the grid used (Gadgil et al., 2003). Where a grid-independent solution is difficult, Nielsen (2004) recommends the use of CFD models of second-order or third-order accuracy where available. The order of accuracy indicates how fast the truncation error is reduced as the grid is refined. Even if these problems have been overcome, convergence of the solution makes CFD modelling difficult in buildings of more than two rooms (Chang et al., 2003). In addition, any errors present within CFD codes may be extremely difficult to discover (Maghrabi, 2004). Thus, thorough validation is of paramount importance. Sørensen and Nielsen (2003) provide a useful review of quality control as applied to CFD in indoor environments.

CFD methods for modelling indoor air pollution concentrations also fail to account for several key parameters that will affect the concentrations, most importantly deposition and chemical reactions. In theory, these factors could be incorporated into CFD codes but this is often not currently done in practise. Pollutants in CFD studies are generally modelled as passive tracer gases that do not influence the flow of air. This assumption is only appropriate for unreactive gases, such as CO, and fine particles.

The use of LES methods over RANS leads to more realistic transient solutions but also corresponds to an increased level of difficulty. Transient solutions will obviously require more time and computational power, as well as expertise (Maghrabi, 2004). Additionally, care must be taken to ensure that predictions of transient flows and pollutant dispersion remain independent of the time-step used (Gadgil et al., 2003). Thus, LES methods are often limited to problems requiring only fundamental understanding of the flow or for substantiating simpler models (Emmerich and McGrattan, 1998).

Most CFD studies of indoor airflow and pollutant transport have, thus far, concentrated only on the indoor environment and not on the transport of pollutants from outdoors to indoors. Jiang and Chen (2001) recommend that more work is needed in the area of combining indoor and outdoor CFD modelling since successful simulation of airflow around buildings helps provide the correct boundary conditions for studying the interiors of buildings.
4 MODEL ILLUSTRATIONS

This section presents two contrasting examples of models used to predict indoor concentrations from outdoor sources, highlighting the relative strengths and weaknesses of the different techniques. First, testing of the microenvironmental model INDAIR (Ashmore et al., 2005) is described for offices. Then, in section 4.2, an example of a current CFD research development is given.

4.1 Examples of simulations using INDAIR

The INDAIR model (see section 2.2.1) has been tested for particle concentrations using data from measurements carried out in office environments. Most of the available data are mean concentrations of $PM_{10}$ or $PM_{2.5}$ over periods of 12 or 24 hours and do not provide information on the short-term temporal variation in particle mass or number concentrations. Such data are important because they provide a sound basis for clearly identifying the different indoor sources and because good validation of INDAIR requires a test of its ability to simulate the dynamics of particle concentration changes.

For thorough model validation, simultaneous data on air exchange rates are also required. This limited the value of some available UK data. Therefore, model validation has focussed on datasets which have simultaneous indoor and outdoor concentrations and air exchange rates, including data from measurement campaigns within the INDAIR project (Hill et al., 2001).

The performance of the INDAIR model has been evaluated by comparison with office measurements of particles in Central London. Indoor and outdoor $PM_{10}$ concentrations were recorded by Mark (1999) in an attempt to investigate the penetration of outdoor traffic-related particles into buildings on one of the busiest roads in the UK (Marylebone Road). The offices were located in the University of Westminster and Westminster City Council buildings and were unoccupied over the sampling period.

In order to simulate these measurements, the input parameters for the room dimensions and the ventilation rates were taken from Mark (1999). For the loss rate of $PM_{10}$, a value of $0.65 \, h^{-1}$ was used. Although this value derives from the PTEAM study and is representative of the $PM_{10}$ loss rate in residences, it also yields good results in the case of office simulations.

Figure 4 illustrates the results for an office in the Westminster City Council building with the fan switched on. The results from the simulations with the INDAIR model compared well with the measurements. Some discrepancies derive from the fact that the ventilation rate was measured periodically and, hence, the same value is used in the simulation for a long period, which may not be representative for all of this period. This effect is even more intense in the simulation for a room in the University of Westminster. Figure 5(a) illustrates this when a mean value of $0.6 \, h^{-1}$ is used for the whole period, whereas Figure
5(b) gives a better picture, in some cases, when adjusted values in the range of 0.3 - 0.9 h\(^{-1}\) were used to fit the measurements.

**Figure 4.** Comparison of INDAIR modelling and Westminster City Council PM\(_{10}\) monitoring 5-7/08/1999; fan on, fixed 1.6 ACH (from Ashmore et al., 2000).
Figure 5(a). Comparison of INDAIR modelling and University of Westminster PM$_{10}$ monitoring 16-18/08/1999; fixed 0.6 ACH (from Ashmore et al., 2000).
INDOOR CONCENTRATIONS IN BUILDINGS FROM SOURCES OUTDOORS

4.2 Examples of simulations using FLUIDITY

Currently, there are no suitable models for predicting the concentration and pressure fields in the envelope surrounding a building that can be easily linked to operational models to predict indoor concentrations. At present, CFD and wind tunnel modelling are the most appropriate ways to achieve this. Therefore, this section illustrates a research development using CFD. It should be noted that the
work described here is in the early stages of development and is a long way from being applied to ‘real life’ situations.

FLUIDITY (Pain et al., 2001), developed at Imperial College London, is a general purpose CFD code which has been modified to allow large-eddy simulations to be performed. The code solves the fundamental flow equations on adaptive finite element meshes. This enables higher resolution to be obtained in areas where rapid changes in the flow field are observed and provides a temporal pattern of evolving eddy structures in the flow. This combination of LES and adaptive, unstructured meshes provides a powerful research tool.

The FLUIDITY code is currently being used to simulate airflow around and into a simple building that is represented by a three-dimensional hollow block. This technique allows for the simulation of a variable concentration over the building. Air is allowed to flow into and out of the building by a single ‘window’ in each of its four walls. Pollutant emissions are represented by volume sources that may be switched on and off as required. The flow variables (velocity, pressure and concentration) are then recorded at different locations within and around the building for time series analysis. Currently, only preliminary simulations have been conducted in order to gain an understanding of the flow fields and pollutant dispersion characteristics. Examples of the modelled flow fields are shown in Figures 6 to 9. Further information on the work can be found in Milner et al. (2005).

![Figure 6. Plan view in the x-y plane of FLUIDITY simulation of instantaneous velocity vectors around and inside the building at half the building height. The air is flowing from left to right.](image)
Figure 7. Side view in the x-z plane of FLUIDITY simulation of instantaneous velocity vectors around and inside the building in the centre of the building. The air is flowing from left to right.

Figure 8. Plan view in the x-y plane of FLUIDITY simulation of a uniform concentration ‘iso-surface’ showing pollution dispersing around the building and entering through a window.
Figure 9. Side view in the x-z plane of another FLUIDITY simulation showing the variation in outdoor pollutant concentration in a street canyon for wind flow perpendicular to the street (above-roof air flow from left to right). High concentrations are shown in orange and yellow while lower concentrations are shown in green and blue.

5 I/O EXPERIMENTAL MEASUREMENT

The relationship between the indoor (I) and outdoor (O) pollution level for a building at a given time is usually expressed in terms of the ratio of I to O. It is both technically difficult and expensive to measure indoor and outdoor concentrations simultaneously due to the equipment needed. Nevertheless, a relatively large database of work on I/O ratios does exist worldwide, although not for all indoor MEs. Unfortunately, there are difficulties in the application of this information to all cases due to differences in meteorology and ventilation rates around the world.

The I/O ratio gives an indication of the protective effect of a building for a given pollutant. As discussed in section 1.2.3, I/O ratios are affected by many factors. In fact, I/O ratios have been shown to vary greatly, even for an individual building (Chaloulakou et al., 2003). Fluctuations in the I/O ratio generally indicate either the presence of indoor sources or changes in the air exchange rate (Drakou et al., 1998). It should perhaps also be noted that external measurements at a single, fixed location may not be representative of the overall distribution of concentrations surrounding a building, as demonstrated by Kukadia et al. (1997). More on this issue can be found in section 1.2.1.
Differences in I/O ratios for a particular building will occur depending upon the type of pollutant. For example, transport into indoor environments of gaseous pollutants will clearly be easier than transport of particles. The I/O ratios of carbon monoxide, particulate matter, nitrogen dioxide and radioactive contaminants will now be discussed in more detail, as well as specific issues associated with each pollutant and examples of measured ratios taken from published studies.

5.1 Carbon monoxide (CO)

As a non-reactive pollutant, of which more than 85% in the atmosphere is traffic-related, indoor CO concentrations have been shown to closely follow outdoor levels, especially near busy roads (Chang et al., 2003). Theoretically, pollutants that are non-reactive with little or no filtration and negligible deposition, such as CO, should have an I/O ratio close to 1 in the absence of indoor sources. Neglecting indoor sources, the only occasion in which indoor concentrations of CO may become higher than outdoors is following a concentration peak, since the indoor gas is enclosed and, hence, has a longer residence time.

Indoor peak concentrations of CO have been measured to be slightly dampened and to lag behind outdoor peaks. Chaloulakou et al. (2003) measured indoor and outdoor CO levels in Athens, Greece and found a clear positive relationship between the concentrations, with outdoor levels generally higher than those indoors. As expected, due to attenuation by the building, the variation of indoor concentrations was smaller and more gradual than that outdoors. In a study in Birmingham, Kukadia and Palmer (1998) found both a naturally ventilated and a mechanically ventilated office building provided greater attenuation of peak CO concentrations than of mean concentrations. Morawska et al. (2001) suggested that, under low ventilation conditions, indoor concentrations are not immediately affected by outdoor concentration changes and that the effect of outdoor air on indoor concentrations could be delayed and inversely proportional to air exchange rates. This assertion is supported by Kirchner et al., (2002) who found that correlation between indoor and outdoor levels was much higher when a time lag was applied. Chaloulakou et al., (2003) found this delay to be between 30 and 40 minutes. Kirchner et al., (2002) found that season and ventilation rate had little effect on the transfer of CO from outdoors to indoors. A summary of CO I/O ratios reported in the literature is presented in Table 1, below.
Table 1. Summary of carbon monoxide I/O ratios reported in literature.

<table>
<thead>
<tr>
<th>Study</th>
<th>Location</th>
<th>Building type</th>
<th>Mean I/O ratio</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chaloulakou and Mavroidis (2002)</td>
<td>Athens, Greece</td>
<td>School</td>
<td>0.55</td>
<td>Summer weekdays</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.71</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.68</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.72</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.82</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.74</td>
</tr>
<tr>
<td>Chaloulakou et al. (2003)</td>
<td>Athens, Greece</td>
<td>Office</td>
<td>0.9</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>School</td>
<td>0.7</td>
<td></td>
</tr>
<tr>
<td>Crump et al. (1998)</td>
<td>Hertfordshire, UK</td>
<td>Residential</td>
<td>3</td>
<td>Kitchens (with gas cookers)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1</td>
<td>Kitchens (with electric cookers)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1.7</td>
<td>Living rooms and bedrooms</td>
</tr>
<tr>
<td>Kirchner et al. (2002)</td>
<td>Paris, France</td>
<td>Residential</td>
<td>1.07 – 1.04</td>
<td>Summer (without sorbing material)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1.05</td>
<td>Summer (with sorbing material)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1.01 – 1.00</td>
<td>Winter (without sorbing material)</td>
</tr>
</tbody>
</table>
1.01 Winter (with sorbing material)

Kukadia and Palmer (1998) Birmingham, UK Office 1.0 1 naturally ventilated building

Office 0.5 1 mechanically ventilated building

Ní Riain et al. (2003) London, UK Office 0.75 Background ventilation

0.83 – 0.89 With fans on

Office 0.91 Background ventilation

1.17 With fans on

University 0.51 Single-sided ventilation

0.49 Cross-ventilation

Oreszczyn et al. (1998) London, UK Residential 2.3 Kitchen

1.7 Living room

1.3 Bedroom

5.2 Particulate matter (PM$_{10}$, PM$_{2.5}$ and PM$_{1}$)

The results of a US EPA project, the Particle Total Exposure Assessment Methodology Study (PTEAM) (e.g. Wallace et al., 1993; Özkaynak et al., 1996), suggest that transport from outdoors to indoors is the primary source of particles in the indoor environment. In general, most studies find that, under normal ventilation conditions and in the absence of indoor sources, indoor particle concentrations follow closely the concentrations outdoors, with indoor levels lower than outdoors (e.g. Mark, 1999; Kingham et al., 2000; Morawska et al., 2001; Fischer et al., 2002). The ability of particles to penetrate a building shell depends not only on the factors discussed in section 1 but also on the size of the particles, since the penetration rate of smaller and larger particles will be different (Morawska et al., 2001; Ní Riain et al., 2003). Lange (1995) concluded
that little or no filtration occurs by the building fabric in the 0.1 to 10 µm size range. The size of the particles also determines their rate of deposition on indoor surfaces. Deposition velocities of particles increase with increasing size. Hill et al. (2001) found that air exchange was the dominant process affecting concentrations in the size range 1-2 µm while deposition was the dominant process in the size range 7.5 - 10 µm. Thus, I/O ratios for particulate matter are usually approximately 0.5 for PM$_{10}$ and 0.7 for PM$_{2.5}$.

Ventilation also plays a major and complex role on indoor particle levels. Koponen et al. (2001) and Chao and Tung (2001) both found that, in the absence of indoor sources, I/O ratios increased when the ventilation rate was increased, or when mechanical ventilation was switched on. Indoor levels may be further increased since, as the ventilation rate increases, particles are more likely to become re-suspended (Chao and Tung, 2001). However, forced ventilation may also lower the number of indoor particles as they can be captured within central heating systems. The fraction of outdoor particulate matter lost along air flow paths remains a source of considerable debate (Ní Riain et al., 2003).

Great variations in I/O ratios for particulate matter are reported in the literature. Studies have shown that I/O for total suspended particulate matter varies between approximately 0.2 and more than 1 (Morawska et al., 2001; Ní Riain et al., 2003). Kingham et al. (2000) measured indoor and outdoor particles in Huddersfield and observed that there was a lack of correlation between repeat measurements at the same sites and a high degree of between-day variation. This variation may be due to the effects of human activity within the buildings. In addition, further variations may be due to the nature of the electric charge carried by particles, since charged particles will have different deposition velocities to neutral ones (Chao and Tung, 2001).

As with other pollutants, correlation between indoor and outdoor particle levels has been found to improve with the addition of a time delay (e.g. Williams et al., 2000; Morawska et al., 2001; Kirchner et al., 2002). Koponen et al., (2001) determined this delay to be of 10 to 20 minutes, depending on whether the mechanical ventilation system was switched on or off, whereas Mark (1999) found the correlation of indoor and outdoor levels to be improved slightly by introduction of a 30 minute delay for a naturally ventilated building.

Another important issue is the need to distinguish between the number and mass concentration of particles. Most studies look at particle mass and concentrate little on the number of particles (Morawska et al., 2001). However, recent work suggests that adverse health effects may, in fact, depend more on the total number of particles (e.g. Kulmala et al., 1999; Koponen et al., 2001; Morawska et al., 2001). A summary of particulate I/O ratios reported in the literature is presented in Table 2, below.
Table 2. Summary of particulate matter I/O ratios reported in literature.

<table>
<thead>
<tr>
<th>Study</th>
<th>Location</th>
<th>Building type(s)</th>
<th>Mean I/O ratio</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Adgate et al. (2003)</td>
<td>Minneapolis, USA</td>
<td>Residential</td>
<td>1.6±1.1</td>
<td>PM$_{2.5}$</td>
</tr>
<tr>
<td>Bryant and Colbeck</td>
<td>Colchester, UK</td>
<td>Residential</td>
<td>1.44</td>
<td>PM$_{10}$</td>
</tr>
<tr>
<td>Chan (2002)</td>
<td>Hong Kong</td>
<td>University</td>
<td>0.7887</td>
<td>Respirable suspended particulate (RSP)</td>
</tr>
<tr>
<td>Hering et al. (2002)</td>
<td>Near Fresno, CA, USA</td>
<td>Residential</td>
<td>0.08 (PM$_{2.5}$ (6 hour average nitrate))</td>
<td>0.06 (PM$_{2.5}$ (12 hour filter nitrate))</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.53 (PM$_{2.5}$ (6 hour average sulphate))</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.51 (PM$_{2.5}$ (12 hour filter sulphate))</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.51 (PM$_{2.5}$ (6 hour average black carbon))</td>
<td></td>
</tr>
<tr>
<td>Jones et al. (2000)</td>
<td>Birmingham, UK</td>
<td>Residential</td>
<td>1.00 (PM$_{2.5}$ (1 road-side location))</td>
<td>1.00 – 2.30 (range) (PM$_{10}$ (road-side locations))</td>
</tr>
<tr>
<td>Study</td>
<td>Location</td>
<td>Type</td>
<td>PM10 (mass)</td>
<td>PM2.5 (mass)</td>
</tr>
<tr>
<td>-------------------------------</td>
<td>---------------------</td>
<td>------------</td>
<td>-------------</td>
<td>--------------</td>
</tr>
<tr>
<td>Kingham et al. (2000)</td>
<td>Huddersfield, UK</td>
<td>Residential</td>
<td>1.04</td>
<td>PM10</td>
</tr>
<tr>
<td>Kirchner et al. (2002)</td>
<td>Paris, France</td>
<td>Residential</td>
<td>0.88 – 0.78</td>
<td>Summer PM2.5</td>
</tr>
<tr>
<td>Monn et al. (1997)</td>
<td>Switzerland</td>
<td>Residential</td>
<td>0.7</td>
<td>PM10</td>
</tr>
<tr>
<td>Morawska et al. (2001)</td>
<td>Brisbane, Australia</td>
<td>Residential</td>
<td>1.07</td>
<td>SMPS (0.015 – 0.685 µm)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.97</td>
<td>APS (0.54 – 9.81 µm) under normal ventilation</td>
</tr>
<tr>
<td>Location</td>
<td>PM Type</td>
<td>Measurement Range</td>
<td>Concentration</td>
<td></td>
</tr>
<tr>
<td>---------------</td>
<td>--------------------------</td>
<td>------------------------</td>
<td>---------------</td>
<td></td>
</tr>
<tr>
<td>Office</td>
<td>CPC (0.007 – 0.808 µm)</td>
<td>under normal ventilation</td>
<td>0.89</td>
<td></td>
</tr>
<tr>
<td>London, UK</td>
<td>PM$_{2.5}$</td>
<td>under normal ventilation</td>
<td>1.01</td>
<td></td>
</tr>
<tr>
<td>Ni Riain et al. (2003)</td>
<td>APS (0.54 – 9.81 µm)</td>
<td>under minimum ventilation</td>
<td>0.95</td>
<td></td>
</tr>
<tr>
<td>Office</td>
<td>CPC (0.007 – 0.808 µm)</td>
<td>under minimum ventilation</td>
<td>0.78</td>
<td></td>
</tr>
<tr>
<td>University</td>
<td>PM$_{2.5}$</td>
<td>under minimum ventilation</td>
<td>1.08</td>
<td></td>
</tr>
<tr>
<td>Office</td>
<td>PM$_{10}$ (background ventilation)</td>
<td></td>
<td>0.60</td>
<td></td>
</tr>
<tr>
<td>University</td>
<td>PM$_{10}$ (single-sided ventilation)</td>
<td></td>
<td>0.46</td>
<td></td>
</tr>
<tr>
<td>Office</td>
<td>PM$_{10}$ (with fans on)</td>
<td></td>
<td>0.66 – 0.69</td>
<td></td>
</tr>
<tr>
<td>Office</td>
<td>PM$_{10}$ (background ventilation)</td>
<td></td>
<td>0.64</td>
<td></td>
</tr>
<tr>
<td>University</td>
<td>PM$_{10}$ (cross-ventilation)</td>
<td></td>
<td>0.67</td>
<td></td>
</tr>
<tr>
<td>University</td>
<td>PM$_{2.5}$ (single-sided ventilation)</td>
<td></td>
<td>0.71</td>
<td></td>
</tr>
<tr>
<td>Office</td>
<td>PM$_{1}$ (background ventilation)</td>
<td></td>
<td>0.62</td>
<td></td>
</tr>
<tr>
<td>University</td>
<td>PM$_{2.5}$ (cross-ventilation)</td>
<td></td>
<td>0.73</td>
<td></td>
</tr>
</tbody>
</table>
5.3 Nitrogen dioxide (NO₂)

Indoor NO₂ is more greatly influenced by indoor sources than either CO or particulate matter. Sources of NO₂, such as gas cookers, lead to considerably raised indoors levels and also to increased variation in these levels. In kitchens with gas cooking, the I/O ratio may regularly be above 1 (Dimitroulopoulou et al., 2001a). However, when no internal sources are present, indoor NO₂ is usually below ambient levels due to chemical reactions and deposition on internal surfaces. This results generally in I/O ratios of the order of 0.5 - 0.6.

Due to the importance of internal sources on indoor levels, contributions from outdoor sources will clearly be less important for NO₂ in regular buildings. Drakou et al. (1998) found that, for buildings in Athens, Greece, indoor NO₂ did not exhibit a marked diurnal variation or diurnal variations in indoor levels differed noticeably from outdoor variations. In fact, indoor levels were observed to exceed outdoor levels regularly, although with lower fluctuations than outdoors.

Despite the relative importance of indoor sources, the literature generally shows higher I/O ratios for NO₂ in cases of increased ventilation (Drakou et al., 1998). This is due to a combination of increased transport from outdoors to indoors and a lower residence time allowing less time for indoor reactions to occur (Kirchner et al., 2002). However, Dimitroulopoulou et al. (2001a) found modelled indoor NO₂ concentrations to be higher for a naturally ventilated room than a mechanically ventilated one.

Although not highly-reactive, chemical reactions may still play an important role in determining indoor NO₂ levels. There may be situations without internal sources when the I/O ratio of NO₂ may rise above 1, for example when NO from a busy road reacts with a high internal O₃ concentration. Also, rather than being simply removed by deposition, NO₂ may be converted to NO at indoor surfaces (Nazaroff and Cass, 1986). The study of Kirchner et al. (2002) concludes that there is a need to use models that account for gas-phase reactive chemistry when dealing with NO₂. A summary of NO₂ I/O ratios reported in the literature is presented in Table 3.
### Table 3. Summary of nitrogen dioxide I/O ratios reported in literature.

<table>
<thead>
<tr>
<th>Study</th>
<th>Location</th>
<th>Building type</th>
<th>Mean I/O ratio</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Berry <em>et al.</em> (1996)</td>
<td>Avon, UK</td>
<td>Residential</td>
<td>0.9</td>
<td>Seasonal mean in kitchens</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.66</td>
<td>Seasonal mean in bedrooms</td>
</tr>
<tr>
<td>Coward <em>et al.</em> (2001)</td>
<td>Across England, UK</td>
<td>Residential</td>
<td>1.04</td>
<td>In kitchens</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.57</td>
<td>In bedrooms</td>
</tr>
<tr>
<td>Coward and Ross (1999)</td>
<td>Across UK</td>
<td>Residential</td>
<td>1.2</td>
<td>In kitchens</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.55</td>
<td>In bedrooms</td>
</tr>
<tr>
<td>Crump <em>et al.</em> (1998)</td>
<td>Hertfordshire, UK</td>
<td>Residential</td>
<td>1.52</td>
<td>In kitchens (with gas cookers)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.8</td>
<td>In living rooms</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.6</td>
<td>In bedrooms</td>
</tr>
<tr>
<td>Dimitroulopoulos <em>et al.</em>, (2005)</td>
<td>South England, UK (37 homes)</td>
<td>Residential</td>
<td>0.6</td>
<td>Winter (in living room)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.8</td>
<td>Winter (in kitchen)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.7</td>
<td>Summer (in living room)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.8</td>
<td>Summer (in kitchen)</td>
</tr>
<tr>
<td>Drakou <em>et al.</em> (1998)</td>
<td>Athens, Greece</td>
<td>University</td>
<td>1.04</td>
<td>Seven day average</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.63</td>
<td>Seven day average</td>
</tr>
<tr>
<td>Kirchner <em>et al.</em> (2002)</td>
<td>Paris, France</td>
<td>Residential</td>
<td>1.20 – 1.10</td>
<td>Summer NO$_2$ (without sorbing)</td>
</tr>
<tr>
<td>Study</td>
<td>Location</td>
<td>Type</td>
<td>Season</td>
<td>NO(_2) Concentration (ppb)</td>
</tr>
<tr>
<td>------------------------------</td>
<td>---------------------------</td>
<td>---------------</td>
<td>---------------------</td>
<td>-----------------------------</td>
</tr>
<tr>
<td>Kousa et al. (2001)</td>
<td>Basel, Residential</td>
<td>Summer</td>
<td>NO(_2)</td>
<td>0.94</td>
</tr>
<tr>
<td></td>
<td>Helsinki, Residential</td>
<td>Winter</td>
<td>NO(_2)</td>
<td>1.03 – 0.99</td>
</tr>
<tr>
<td></td>
<td>Prague, Residential</td>
<td>Winter</td>
<td>NO(_2)</td>
<td>0.80</td>
</tr>
<tr>
<td>Kukadia and Palmer (1998)</td>
<td>Birmingham, Office</td>
<td>Summer</td>
<td>NO(_2)</td>
<td>1.33</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Winter</td>
<td>NO(_2)</td>
<td>1.42</td>
</tr>
<tr>
<td>Quackenboss et al. (1986)</td>
<td>Portage, WI, Residential</td>
<td>Summer</td>
<td>NO(_2)</td>
<td>2.4</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Winter</td>
<td>NO(_2)</td>
<td>0.8</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Winter</td>
<td>NO(_2)</td>
<td>3.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Winter</td>
<td>NO(_2)</td>
<td>0.6</td>
</tr>
<tr>
<td>Ross and Wilde (1999)</td>
<td>South East, Residential</td>
<td>Summer</td>
<td>NO(_2)</td>
<td>1.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Winter</td>
<td>NO(_2)</td>
<td>0.9</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Winter</td>
<td>NO(_2)</td>
<td>0.8</td>
</tr>
</tbody>
</table>
5.4 Radioactive pollutants

The transport time and indoor concentration of a radioactive cloud, for example following a nuclear accident, will depend on the duration of the outdoor peak, ventilation rates and filtration by the building (Kulmala et al., 1999). In such a case, where there is a short burst of contaminant, a model capable of time evolution is very important. Radioactive contaminants differ from conventional pollutants since they typically have more localised effects (Kulmala et al., 1999). Also, deposited radioactive substances may not be ignored, unlike in air quality studies, since the deposited material can still have damaging effects on human health. Indoor concentrations of radioactive contaminants depend very much on the nature of the particular substance. As such, when dealing with a radioactive substance, additional specific factors (such as the half-life) must be used in models (for example, see the mass-balance model for radon of Man and Yeung (1999) in section 2.2.1). A summary of radioactive contaminant I/O ratios reported in the literature is presented in Table 4, below.

Table 4. Summary of radioactive contaminant I/O ratios reported in literature.

<table>
<thead>
<tr>
<th>Study</th>
<th>Location</th>
<th>Building type</th>
<th>Mean I/O ratio</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Roed (1985)</td>
<td>Denmark</td>
<td>Residential</td>
<td>0.33</td>
<td>Cosmogenic $^{7}\text{Be}$, $^{103}\text{Ru}$ from weapons testing</td>
</tr>
<tr>
<td>Roed and Cannell (1987)</td>
<td>Denmark</td>
<td>Residential (1 house)</td>
<td>0.39</td>
<td>$^{131}\text{I}$ (particulate)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.27</td>
<td>$^{137}\text{Cs}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.49</td>
<td>$^{7}\text{Be}$</td>
</tr>
</tbody>
</table>
6 PRACTICAL GUIDANCE AND RECOMMENDATIONS

This report has summarised available models for calculating indoor air pollutant concentrations in buildings from outdoor sources and reviewed I/O field measurements. When choosing a model, it is extremely important that the choice is driven by the requirements of the work and the characteristics of the situation. Different models will be required depending on whether a long-term statistical picture is needed or whether the temporal variation associated with a short-term release is necessary. The models discussed here have a variety of different strengths and weaknesses, which must always be taken into account.

Most existing models assume a uniform concentration in the envelope surrounding the building. In cases where only long-term trends are required, the simplest method for calculating indoor concentrations from outdoor sources is the I/O ratio found by statistical regression of experimental data. The method is fast and straightforward and often the only option if little is known about the building of interest. A basic pessimistic approach may be to calculate the maximum outdoor concentration around the building (usually at street level in urban areas and due to conventional pollutants) and then apply an I/O ratio of 1, since over a reasonable time period the I/O ratio due to outdoor sources alone will not exceed this. However, such an oversimplified method cannot model the time evolution of the indoor concentration and is, hence, clearly of little use when modelling the passage of a short burst of contamination. Such a situation would require a microenvironmental, multizone or CFD model.

Microenvironmental mass-balance models (of which statistical regression models are the steady-state form) also have the advantage of being relatively simple to use. If more is known of the characteristics of a building, these models are extremely useful since they calculate indoor concentrations that may be well compared to experimental data and may be easily linked to exposure models. Microenvironmental models are generally used to predict average indoor concentrations and have sometimes been found to perform poorly where rapid fluctuations in the concentration occur. One significant recent improvement has
been the development of probabilistic models to predict frequency distributions of air pollutant concentrations.

Multizone mass-balance models provide some improvement over microenvironmental models when studying more complicated buildings (e.g. buildings with many rooms or large indoor spaces). Nevertheless, the increased complexity corresponds to an increased level of difficulty. Also, multizone models have been primarily used to model building ventilation rather than indoor air quality. The model user must decide whether a microenvironmental or multizone model is appropriate depending on the available information, such as the building geometry and whether air exchange rates are known in advance.

CFD models for indoor air quality are still only used as research tools due to their highly complex nature and the associated requirements for computational power and user expertise. Most research using CFD has thus far concentrated only on indoor airflows, ventilation and thermal comfort rather than the transport of pollution (and then only from indoor sources). It appears that the research community is moving towards the application of CFD models that use LES methods to simulate turbulence, although a great deal of further validation of the method is required. As such, CFD models remain out of the reach of users needing models for regulatory purposes.

Recently, there has been some movement towards exploiting the benefits of different model types (and overcoming model limitations) by combining several models to consider separate parts of the same problem. For example, Chang et al. (2003) attempted to overcome the limitations of both CFD and multizone modelling by developing an integrated air quality model combining both techniques. The CFD model uses an LES method for outdoor turbulent flows and pollutant transport processes while the multizone model performs indoor airflow and pollutant transport calculations. In the method, the LES model calculates pressure and pollutant concentration coefficients at each façade of the building, which are then input into the mass-balance model. The study found that the simulated indoor concentrations showed good agreement with experimentally measured indoor CO distributions. This illustrates well the benefits of CFD for calculating the distribution and time evolution of pollution in the envelope surrounding a building, the results of which may then be input into a more generally-applicable operational model.

The key conclusion of this report is that the models that are currently available do not adequately account for the spatial variations in outdoor concentration and pressure in the building envelope. Existing models generally assume a single value to represent the outdoor concentrations at a given time. This is a major limitation when considering local sources which will result in high spatial and temporal variability over the building. Measurements of concentration distributions around buildings are scarce, although several studies have been conducted using wind tunnel models (see section 1.2.1). CFD methods are more suitable than other types of models for representing this external variation and this report has described some research modelling using CFD techniques to model outdoor concentrations. However, linking of such work to CFD or other
modelling of indoor concentrations is only in the very initial stages. Therefore, this report recommends that more work is needed to study variations in pollution concentrations and pressure over buildings in different situations and environmental conditions and also to link this to internal circulation and concentrations. Only then will models for indoor concentrations due to outdoor sources be able to account satisfactorily for this potentially important factor.

7 REFERENCES


REFERENCES


## APPENDIX A

### TYPICAL MODEL PARAMETER VALUES

The following table presents typical values for the model parameters discussed in section 1 of this report.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Typical Values</th>
<th>Notes</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air exchange rate ($ACH$)</td>
<td>0.2 – 1.0 h$^{-1}$</td>
<td>Residential (Northern European)</td>
<td>AIVC (1994)</td>
</tr>
<tr>
<td></td>
<td>0.4 h$^{-1}$ (mean)</td>
<td>Residential (Southern European)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>&gt; 1 h$^{-1}$</td>
<td>Residential</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.44 h$^{-1}$</td>
<td>Winter in residential buildings (UK)</td>
<td>Crump et al. (2004)</td>
</tr>
<tr>
<td></td>
<td>0.62 h$^{-1}$</td>
<td>Summer in residential buildings (UK)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.79 h$^{-1}$</td>
<td>Residential buildings with windows closed (UK)</td>
<td>Hill et al. (2001)</td>
</tr>
<tr>
<td></td>
<td>1.37 h$^{-1}$</td>
<td>Residential buildings with windows open (UK)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.8 – 1.6 h$^{-1}$</td>
<td>Winter in a naturally ventilated office (UK)</td>
<td>Kukadia and Palmer (1996)</td>
</tr>
<tr>
<td>Deposition velocity ($v_d$)</td>
<td>Range</td>
<td>Description</td>
<td>References</td>
</tr>
<tr>
<td>-----------------------------</td>
<td>-------</td>
<td>-------------</td>
<td>------------</td>
</tr>
<tr>
<td>0.61 – 0.82 x $10^{-4}$ m s(^{-1})</td>
<td>0.5 µm particles without and with furniture present in residential buildings (Demark and UK)</td>
<td>Fogh et al. (1997)</td>
<td></td>
</tr>
<tr>
<td>1.33 – 1.73 x $10^{-4}$ m s(^{-1})</td>
<td>2.5 µm particles (Demark, UK)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.37 – 2.25 x $10^{-4}$ m s(^{-1})</td>
<td>3.0 µm particles (Demark, UK)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.88 x $10^{-4}$ m s(^{-1})</td>
<td>4.5 µm particles (Demark, UK)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.04 – 3.24 x $10^{-4}$ m s(^{-1})</td>
<td>5.5 µm particles (Demark, UK)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Range</th>
<th>Location</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4 – 1.2 h(^{-1})</td>
<td>Winter in a mechanically ventilated office (UK)</td>
<td>Rachalet et al. (1994)</td>
<td></td>
</tr>
<tr>
<td>0.3 – 0.6 h(^{-1})</td>
<td>Winter in a school (France)</td>
<td>Roed and Goddard (1990)</td>
<td></td>
</tr>
<tr>
<td>1.5 – 2.0 h(^{-1})</td>
<td>Winter in a school (France)</td>
<td>Warren and Webb (1980)</td>
<td></td>
</tr>
<tr>
<td>0.33 – 30 h(^{-1})</td>
<td>Typical residential buildings (UK)</td>
<td>Dimitroulopoulou et al. (2005)</td>
<td></td>
</tr>
<tr>
<td>0.7 h(^{-1}) (mean)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.19 – 0.68 h(^{-1})</td>
<td>37 residential buildings in winter (UK)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.44 h(^{-1}) (ar. mean)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.19 – 1.06 h(^{-1})</td>
<td>37 residential buildings in summer (UK)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Value</td>
<td>Description</td>
<td>Reference</td>
<td></td>
</tr>
<tr>
<td>---------------</td>
<td>--------------------------------------------------</td>
<td>--------------------------------</td>
<td></td>
</tr>
<tr>
<td>1.8 x 10^{-1} m h^{-1}</td>
<td>Dust in a residential building (USA)</td>
<td>Koutrakis et al. (1992)</td>
<td></td>
</tr>
<tr>
<td>10^{-1} – 10^{-2} m h^{-1}</td>
<td></td>
<td>Nazaroff and Cass (1987)</td>
<td></td>
</tr>
<tr>
<td>4.5 x 10^{-4} m s^{-1}</td>
<td>PM_{10} (USA)</td>
<td>Özkaynak et al. (1996)</td>
<td></td>
</tr>
<tr>
<td>6.4 x 10^{-5} – 7.1 x 10^{-4} m s^{-1}</td>
<td>Chernobyl aerosols</td>
<td>Roed and Cannell (1987)</td>
<td></td>
</tr>
<tr>
<td>1.66 x 10^{-4} – 2.7 x 10^{-3} m s^{-1}</td>
<td>1 – 25 µm size range in a residential building (USA)</td>
<td>Thatcher and Layton (1995)</td>
<td></td>
</tr>
<tr>
<td>3.7 x 10^{-2} m h^{-1}</td>
<td>Dust in an office (Hong Kong)</td>
<td>Tung et al. (1999)</td>
<td></td>
</tr>
</tbody>
</table>

**Loss rate (K)**

<table>
<thead>
<tr>
<th>Value</th>
<th>Description</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.18 x 10^{-3} min^{-1}</td>
<td>1 – 2 µm particles (UK)</td>
<td>Hill et al. (2001)</td>
</tr>
<tr>
<td>1.65 x 10^{-2} min^{-1}</td>
<td>2 – 5 µm particles (UK)</td>
<td></td>
</tr>
<tr>
<td>6.35 x 10^{-2} min^{-1}</td>
<td>5 – 7.5 µm particles (UK)</td>
<td></td>
</tr>
<tr>
<td>8.78 x 10^{-2} min^{-1}</td>
<td>7.5 – 10 µm particles (UK)</td>
<td></td>
</tr>
<tr>
<td>1.33 x 10^{-1} min^{-1}</td>
<td>10 – 15 µm particles (UK)</td>
<td></td>
</tr>
<tr>
<td>0.002 – 0.43 h^{-1}</td>
<td></td>
<td>Roed and Goddard (1990)</td>
</tr>
<tr>
<td>0.11 h^{-1} (mean)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Parameter</td>
<td>Value</td>
<td>Description</td>
</tr>
<tr>
<td>---------------------------</td>
<td>----------------</td>
<td>--------------------------------------------------</td>
</tr>
<tr>
<td>Mixing time</td>
<td>2.4 – 23 min</td>
<td>Unventilated, mechanically mixed room (USA)</td>
</tr>
<tr>
<td>Penetration factor ($P$)</td>
<td>1</td>
<td>PM$<em>{10}$ and PM$</em>{2.5}$ in a residential building (USA)</td>
</tr>
<tr>
<td>Penetration factor ($P$)</td>
<td>1</td>
<td>PM$<em>{10}$ and PM$</em>{2.5}$ (USA)</td>
</tr>
<tr>
<td>Resuspension rate</td>
<td>$10^{-7} – 10^{-4}$ h$^{-1}$</td>
<td>Residential building (USA)</td>
</tr>
</tbody>
</table>
Aspects of Dispersion following an Explosive Release

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ABSTRACT
This report addresses how source terms (as used in subsequent dispersion models) are defined for explosive type releases, which may result either from explosions, or from rapidly boiling releases from pressurised or refrigerated storage.

The focus of the report is on the explosive phase of the dispersion. A principal consideration within the report is how the source term energy is used within existing modelling to describe the initial gas cloud. The report provides descriptions of existing models for explosive releases, based on a wide range of literature. It shows that the initial explosive phase of dispersion immediately following an explosive release depends strongly on the energy of the explosion. The energy of explosion depends primarily on the material involved in the explosion, rather than on the material being dispersed (although it could be the same material).

Consideration is also given as to how these existing models can then be used as input into appropriate models for the subsequent dispersion. However, choice of model for the subsequent modelling is not covered.

The report concludes by summarising the issues that should be considered when deciding which model to choose, and what should be considered when interpreting the results.
EXECUTIVE SUMMARY

The initial explosive phase of dispersion immediately following an explosive release depends strongly on the energy of the explosion. The energy of explosion depends primarily on the material involved in the explosion, rather than on the material being dispersed (although it could be the same material).

Existing models for explosive releases tend to be simple first order models, or complex coupled systems. The choice of model will depend on a number of issues, including:

- the application of the results to the scenario being considered,
- the level of detail required,
- the duration and distance over which the dispersion is to be considered,
- the model assumptions, limitations, and uncertainty, and
- the level of specification of the input data for the scenario.

In this report simple models have been summarised for:

- dispersion of material following a detonation of adjacent explosive material, and
- dispersion resulting from catastrophic failure of a pressurised storage vessel,

and guidance was provided on how to address the scenarios:

- dispersion of refrigerated material following rupture of its storage vessel caused by an explosion, and
- dispersion of toxic material following rupture of its storage vessel caused by an explosion.

Several more complex models were identified and discussed, and general issues surrounding source terms were covered.

Transition to a secondary dispersion model should occur once the explosive energy has been dissipated and the pressure of the vapour is atmospheric, when other factors begin to drive the dispersion (e.g. turbulence, gravitational slumping, buoyancy, passive dispersion).

The results should be analysed in relation to the source modelling assumptions and limitations made at the start. Sensitivity to the input parameters and uncertainties in the model should be understood, and it is often necessary to undertake several iterations varying inputs and assumptions for one scenario.
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1 INTRODUCTION

1.1 Background

The dispersion of pollutants in the atmosphere (accidentally released or otherwise) can be calculated using various models, depending on the type and mode of the release. For all these models, it is necessary to specify a realistic source term in order that the dispersion is correctly modelled. For many far-field applications, the results are not strongly dependent upon the exact modelling of the source. However, for near field effects, particularly for large releases, the results can be strongly dependent upon the nature of the source term. For example, a pressure vessel failure will result in a rapidly expanding vapour cloud which entrains a significant amount of air at source, whereas an evaporating pool will give a source which has little initial dilution and covers a rather smaller area or volume. In the near field, the concentrations as material disperses from these two sources will be rather different.

There are many source term and dispersion models available in the industry, but until recently there have been gaps in some key areas, particularly for explosive releases. It is these areas that the report aims to address.

1.2 Objectives

The report aims to address several stages of dispersion and will consider the effects of the release mechanism on the initial release and dispersion.

As noted in the proposal [1], the aim was to achieve this by examining the following characteristics of the dispersion with respect to the effects of explosively generated releases:

1. The size and height of the initial plume produced by the explosion, including penetration of the boundary layer.
2. The distribution of material within the plume formed immediately after the explosive release, and the size distribution of aerosols.
3. Appropriate ways of describing the processes immediately after the initiating event including the dispersion and deposition of the resulting plume, and a review of models for such calculations.
4. The extent to which the subsequent dispersion could be predicted using simple Gaussian plume models, or how such models could be extended for this application.

1.3 Scope

This report addresses how source term, initial dispersion and passive dispersion models are combined for the following specific instances:

- dispersive consequences of explosive releases (rarely considered in literature, with primary focus usually being on resulting overpressures),
- rapidly boiling releases (e.g. from catastrophic failure of pressurised storage vessels), initially resulting in an aerosol release and a liquid pool,
• refrigerated releases (e.g. from LNG catastrophic failure of storage vessels).

The work was carried out with reference to four example events, namely:

1. high explosive combined with toxic material as in terrorist events,
2. releases from catastrophic failure of pressurised storage vessels.
3. releases from terrorist attacks on bulk shipments (e.g. LNG),
4. releases from terrorist attacks on road/train shipments of toxics.

The first scenario is the area where fewest models and papers are available. This has therefore been considered in most detail in this report, relating initial parameters (plume size, height, and material distribution) as a function of explosive yield where possible.

A comprehensive study, closely related to the second scenario, was undertaken by Atkins for the HSE in 1999 [2] and the results were published in the Journal of Hazardous Materials [3]. This work has been summarised in this report, and related to this particular scenario.

The third and fourth scenario release types are more widely discussed in the literature. However, the explosive release mechanism requires specific consideration in order to ensure that the correct source terms are calculated.

1.4 Report outline

The remainder of the report is structured as follows:

In Section 2 a general overview of dispersion modelling is given, with particular emphasis on the availability of appropriate source term descriptions. Source terms characterisation within existing passive ‘puff’ dispersion models (e.g. Atmospheric Dispersion Modelling System, ADMS [4]), and (positively or negatively) buoyant ‘puff’ models (e.g. HGSYSTEM [5]) are discussed in Section 2.2. The decision regarding choice of model for a particular scenario is also discussed. Subsequent dispersion is covered in Section 2.5, and a brief discussion of boundary layer penetration is given in Section 2.6.

Phenomenological considerations, where energy of the release is related to the different modelling scenarios, are discussed in Section 0.

More detailed aspects of the modelling are covered in Section 4. Existing literature describes many of the theoretical aspects of source and dispersion modelling, and it is not possible to cover all aspects of the modelling in this report. Therefore, Sections 4.1 to 4.4 focus on reviewing the initial dispersion and deposition following an explosion for the following mechanisms:

• Explosive charge dispersion (including boundary layer penetration), with particular emphasis on relating initial plume parameters (e.g. size, height, material distribution) to the explosive yield where possible.
• Pressurised storage vessel catastrophic failure (described in Section 4.2) resulting in a flashing liquid release which forms a cloud of vapour and droplets that may be non-symmetrical; the initial directionality depends
on the mode of failure of the vessel which in turn depends on vessel shape.

- Rapid expansion due to high vaporisation rate (for subcooled liquids stored at near ambient pressure); omni-directional expansion and a symmetrical initial cloud.

The conclusions of the study are drawn together in Section 0.
2 DISPERSION MODELLING OVERVIEW

2.1 Modelling approaches

Releases and their subsequent dispersion can be categorised according to their timescale:

a) Instantaneous – Very short timescale (usually a few seconds). Release follows large scale catastrophic failure or explosion.

b) Transient – Release rate varies over a longer period (usually minutes or tens of minutes). For example, a large pipeline failure will result in a decaying release rate as the pipeline depressurises.

c) Continuous – Release rate remains constant, or nearly so, over several tens of minutes, or even hours. A small to medium pipework rupture would give this type of release.

Since this study concerns explosive releases, the primary focus will be on instantaneous releases, and continuous releases are not considered further.

The remainder of this section gives an overview of dispersion modelling approaches, whilst Section 2.2 considers source term definition within existing models. An overview of significant instantaneous release mechanisms then follows in Sections 2.3 to 2.4, in which the important features of the release and consequences are described. Review and detailed description of existing models is left until Section 0. Subsequent dispersion modelling is discussed in Section 2.5, and a brief discussion of boundary layer penetration is given in Section 2.6.

Release of contaminant material and its subsequent dispersion can be a complex process. It can involve heating and cooling of materials, and phase changes. To an observer, other aspects of the physical behaviour will often seem more apparent than the dispersion. For example, immediately following an explosive release the blast wave will be felt, then a cloud may be seen, which may then disperse. Thus, to simplify the modelling, it is usual to break the process down into several stages, each stage reflecting a different aspect of the dispersion behaviour.

The stages of the dispersion can be determined by considering the initiating event and release mechanism. Each stage is then modelled, often by focussing on the primary behaviour governing that stage. Source terms and external conditions are used to define input parameters, with outputs of one stage to be used to calculate inputs to the next stage.

The modeller should consider the following steps when modelling the dispersion:

1. Define the initiating event and release mechanism. The mechanism of release can strongly influence the initial dispersion in terms of the rate, duration, size and momentum of the release. This in turn affects the later stages of dispersion modelling, although these stages are usually less affected by small inaccuracies in source term modelling inputs

2. Define sequence of events (stages of dispersion modelling).
3. Decide on the level of output required, and choose appropriate models and software applications. The type, level of detail and accuracy required for the chosen model will depend on the application and required output.

4. Estimate the source terms needed for input to the chosen model (e.g. material, phase (e.g. gas, liquid, powder), density, concentration, mass, momentum, energy, pressure, temperature, release velocity).

5. Describe the surrounding environmental conditions (e.g. atmospheric, meteorological and ambient conditions, terrain, obstructions) via parameters appropriate to the complexity of the modelling required.

6. Calculate and evaluate results using the chosen models, and undertake calculations to test sensitivity to variable parameters (e.g. wind speed) and uncertain parameters (e.g. amount of explosives).

7. Draw appropriate conclusions from the evaluation.

An accurate and appropriate definition of the source term is perhaps the most difficult aspect for the user. Improved source term inputs were one of the recommendations from the 2000 Maryland proceedings [6]. All models require some inputs at the start, but whilst some model the release conditions, others do not but instead require the user to describe an initial cloud or pool as the starting point. The user must choose a suitable time after the release, must provide corresponding conditions to start the modelling, and must make basic assumptions about the gas and its location. For example, when using the blast application in AutoReaGas [7] (if not run on from the explosion scenario), the user must define a rectangular box (providing appropriate dimensions) of quiescent, inviscid ideal gas as an input, also providing the material, concentration, and the contained energy (i.e. how much of it is combustible, and what is the initial internal pressure).

### 2.2 Current availability of source definitions

As noted in Section 2.1, the remainder of this document focuses on instantaneous or very short timescale releases. This section gives three examples of different publicly available source definitions within dispersion models for such release types:

a. **ADMS**: Passive or buoyant pollutant dispersion model [4].

   Inputs include choice of model, site data (including ground roughness length), source information, meteorological input, numerical grid definition for running the simulation, and choice of output format.

   A source definition always includes the height, and location. However, other inputs depend on the choice of source type, (point, line, area, volume or jet), but could also incorporate the diameter, width of line source, volume, velocity, specific heat capacity, molecular weight, temperature, density, mass or momentum fluxes, emission information, mass of water, and angle of release.
ADMS also contains a number of additional features for which further inputs are required. These include a puff model for short releases, chemistry modelling (for NO$_2$, NO$_x$ and O$_3$ only), a topography option for representing flow over hills, a radioactivity gamma ray model, and representation of (wet and dry) deposition.

b. **HGSYSTEM**: Accidental release dispersion modelling suite, with emphasis on dense gas dispersion [5].

Inputs for HGSYSTEM dispersion models can be achieved over several stages using its various sub-models.

The sub-model DATAPROP calculates material data for any given ambient conditions for materials within its database.

Source term models can be used to model a passive release, jet release or evaporating pool release, using conditions relating to the storage container, reservoir, stack or pool. The inputs are similar to those of ADMS.

Alternatively they can be by-passed and a source can be entered directly into the dispersion model, either as a continuous or ‘instantaneous’ release or as a ‘breakpoint’ (a Gaussian plume profile).

c. **CIRRUS**: Suite of models for calculating effects of accidental releases in context of production of Safety Case or Risk Assessment [8].

CIRRUS also has a range of source models, including those for momentum releases, dense releases, passive and particulate releases. The inputs required for CIRRUS are the release rate, released material, and ambient and atmospheric conditions. Like HGSYSTEM, they include information about the material (specific heat capacity and molecular weight), the ambient and atmospheric (wind and roughness data) conditions, the release conditions (release rate, temperature of the released cloud). These important parameters are required by all users; however, advanced users have further options for specifying other parameters such as flash fraction parameters (relevant to Scenario 2 in this report). These parameters are likely to have the most noticeable affect in the immediate vicinity of the release.

d. **HPAC**: HPAC is a transport and risk package.

To model the dispersion, HPAC uses a Gaussian transport model, SCIPUFF, which is based on a second order turbulence closure scheme. It uses probabilistic methods to estimate fluctuations, and then from the dispersed cloud, HPAC calculates risks to populations using population data from databases within the model.

Basic inputs can be used to provide quick hazard estimates, from which HPAC calculates representative values for the remainder of the properties. However,
more detailed inputs can be entered using a second input interface, for more specific data requirements (such as aerosol fractions).

Several sources provide comprehensive reviews of these and other models including SLAB, DEGADIS, INPUFF, DRIFT, and SCIPUFF. In particular, details of vapour cloud dispersion models are covered by CCPS [9], and both the Office of the Federal Coordinator for Meteorology [10] and States Department of Energy Emergency Management Advisory Committee Subcommittee [11], provide descriptive information and compilation information on various atmospheric dispersion computer codes, although neither of these give any detailed technical information about the physics of the models. Other in-house models or methodologies are developed for internal use only, and are not publicly available, such as models developed by Lloyds Register for LNG releases [12].

Explosive source term models are not widespread within dispersion models. However, codes such as HOTSPOT [13,14], which has a first-order source term model for short-term releases, and ADORA and NARAC, which offer source term models for more complex requirements, all incorporate some form of explosive source term models.

2.3 Explosions

2.3.1 Blasts in mining

Over the years, people working with blasts in the mining industry have contributed significantly to the knowledge of explosions and blasts. The concentrations of dust in relation to the dust concentration at which ignition is most likely, and dust deposits are sometimes discussed in these papers. Because the focus has usually been on how to optimise the blast, there is little information on the concentration of the dust after the explosion has taken place. A second difficulty in using mining blast dispersion references to model explosive dispersion is that the dust which is dispersed after the blast includes the material that has been blasted (i.e. rock face, etc.). The explosions are also either internal, or at least confined, and the releases will therefore behave differently from releases near explosives that are detonated in the open. Therefore, the papers are very specific to that particular application.

2.3.2 Explosive detonation

This section considers the detonation of explosives, which may be associated with nuclear, chemical or biological explosions, including those originating from weapons. It is important to note that a blast from a condensed phase (solid) explosion is different from an explosion caused by the ignition of a flammable gas cloud. The rate at which energy is released in the explosion differs, and the speed at which the pressure wave propagates is much faster for a condensed phase explosive detonation than for an explosion (often termed a deflagration), which is produced by the slower burning of a hydrocarbon cloud.

When explosives (usually solid) detonate, chemical (or nuclear) reactions take place producing a relatively large volume of heated gases (or a fireball), converting energy stored as mass both to change the state and also to release thermal energy. The expansion of the gases produces a pressure wave (see Figure 2-1). This impulse travels away from the explosion, radially through the
air, and a dust layer forms on the ground. As the pressure wave hits the ground it reflects upwards. The debris on the ground in the dust layer is entrained upwards causing a rising column. As the air and dust mixture loses speed some of it begins to fall back as more air and dust rises, forming a cloud. The column and cloud is sometimes referred to as a stem and cap, or a mushroom cloud.

![Figure 2-1: Energetic blast](image)

The speed and magnitude of the pressure wave and the cloud are determined by the strength and amount of the explosives and other reactants (availability of oxygen for example). They can also be affected by the surrounding environment (structures causing additional turbulence in the vicinity, or surfaces confining the pressure wave).

### 2.3.3 Volcanic eruption

In some respects the behaviour of a volcanic eruption is similar to that of an explosive blast. A comparison of a volcanic eruption with a low-altitude nuclear explosion showed similar flow regimes in the later stages of the two events [15]. However, in terms of their source terms, they are quite different from other explosives.

Whereas the majority of other explosive models only characterise the initial plume rise by the explosive energy, and then assume a point source as a starting point for the dispersion, for volcanic eruptions assumptions about the volume and temperature of the sub-surface magma provide the information to the key characteristics of the eruption, namely the release velocity, pressure, temperature and state of the material.

The magma (a mixture of molten rock, crystals and bubbles) rises through vents (conduit) to the surface, decreasing in pressure and becoming more gaseous. As it rises, it causes expansion of the material and acceleration upwards. (However, the acceleration causes widening of the vents, thereby limiting the acceleration.) The direction of the released magma is upwards, and is linear (rather than the initial radial fireball of an explosive detonation).

Ahead of the expanding magma, there is a pressure wave, causing a plume to travel along the ground behind the wave. The turbulent volcanic plume rises (also behind the pressure wave) due to the momentum of the release. The
plume is a mixture of gases and particles and, although it is very hot (about 1000°C), the presence of the particles makes it denser than the surrounding air. As it rises it loses momentum, deposits the heavier particles (fallout), air is entrained and the plume becomes buoyant causing the plume to continue to rise even once the upwards momentum is lost. The plume continues to entrain air and cool and eventually stops rising. A stem and cap cloud is formed, as shown in Figure 2-2.

![Figure 2-2: Volcanic eruption.](image)

2.3.4 Potential scenario developments following an explosive detonation
Once the explosive phase has occurred, subsequent dispersion should be modelled for the products of the reaction, un-reacted material and the nearby materials not involved in the reaction. Methods for determining the size and concentration of the cloud for input into the subsequent dispersion are discussed in Section 4.1.

2.4 Instantaneous catastrophic release of stored material
2.4.1 Release mechanism
The main feature of this release mechanism is that ‘most’ (over 50 %) of the contents of the vessel is lost ‘instantaneously’ (typically less than 1 minute, and normally only a few seconds). A storage vessel may rupture due to one of, or a combination of, an increase in internal pressure (perhaps itself caused by external heating of the vessel such as in a fire, causing a BLEVE (Boiling Liquid Expanding Vapour Explosion)), a local increase in loading, or a reduction in material strength. Failure may be caused by flawed material, fatigue, corrosion, poor manufacture, impact, or by thermal or pressures stresses. If the vessel is not pressurised, the release is unlikely to be catastrophic.

The rupture location and mechanism itself will affect the release. A ductile split will differ from a brittle break, affecting the duration of rupture, and a rupture at the top of the vessel will result in a vertically–directed initial jet, which will disperse rather differently from a release from the underside of the vessel [2].
The storage vessel could contain liquid or gas. If the vessel is pressurised and contains a material which is a vapour at atmospheric conditions, but stored as a liquid in the vessel, then the rupture often results in an aerosol cloud (2-phase release) and a liquid pool as shown in Figure 2-3 and described in Section 4.2.

Figure 2-3: Catastrophic failure of (pressure) vessel.

2.4.2 Potential scenario developments following a gas release
If the vessel contains only vapour, a gas cloud will be formed instantaneously. The consequences depend on the properties of the cloud and, for flammable materials, on the presence and strength of nearby ignition sources.

1. Dispersion of the gas cloud (with toxic effects),
2. Pressure burst (un-ignited, but resulting from the pressure of the vessel),
3. Ignition of the dispersing gas cloud leading to a flash fire,
4. Vapour cloud explosion or deflagration (ignited gas cloud in congested region),
5. Fireball (elevated ignition)

2.4.3 Potential scenario developments following a liquid release
Failure of a vessel containing liquid alone is unlikely to be catastrophic unless the vessel is pressurised, in which case a 2-phase release will occur (see Section 2.4.4). As part of a 2-phase release, a liquid pool may form, resulting in one of the following possibilities:

1. Evaporating pool (could be toxic)
2. Pool fire
3. Drain away with no effect

2.4.4 Potential consequences of a two-phase release
A two-phase release could arise from the stored material being a 2-phase mixture, or from a hole in the vessel or pipe at the liquid vapour interface (surface) so that both vapour and liquid escape through the hole. Causing either:

1. Flashing liquid release (resulting in an aerosol), or

2.4.5 Source term characterisation
A significant amount of air will be entrained following a catastrophic release, and so this will result in a turbulent cloud. The amount of turbulence and size of the gas cloud will depend upon the initial airborne fraction of the material.
(depending on the mass of the material, and the storage and ambient temperatures and pressures) and the amount of air entrained.
2.5 Subsequent dispersion

Transition to modelling the release as a passive, dense or buoyant gas will occur after the pressure generating the explosion has been equalised to ambient pressure, when the material is in an equilibrium state (not changing phase), and when the momentum of the explosion is destroyed and the turbulence is reduced to atmospheric turbulence. The transition point has been discussed for each of the scenarios separately in Sections 4.1 to 4.4.

Many different dispersion models are available for passive, dense and buoyant gases. The majority of these model the transport and growth of gas plumes, using either Gaussian or sometimes top hat profiles. Few models include the ability to model vegetative canopies, flow around buildings, and high altitude dispersion, although the more sophisticated models, such as HPAC, are addressing some of these issues. Important outputs include concentration at temporal and spatial coordinates, width and height measurements and temperature, density and velocity calculations too.

At transition from an explosive phase dispersion model to a second (dispersion) model, new source terms will be required as input to the second model. In order to make a transition to a dispersion model, the cloud properties will be required, depending on the model used. These should be found from the output to the explosive model. It will often be necessary to modify the output from one model in order to create the required form of input to the next stage of dispersion, using physical equations, conservation of mass being particularly important for dispersion calculations. Other parameters will also have to be treated as an input (e.g. temperature, concentration).

For example, to transform an output from a box model to a Gaussian profile:

The box model gives uniform concentration, \( C \), over an area described using a width and a height, \( L \).

The Gaussian model requires a centreline concentration, \( C_0 \), and a width parameter, perhaps the standard deviation, \( \sigma_x \), and a height parameter, \( \sigma_z \).

In the box model, the area of the box is width x height = \( L^2 \).

95% of the material lies within 2 standard deviations either side of the centreline.  
\[
2 \sigma_x = 2 \sigma_z = \frac{L}{2}, \quad \text{and} \quad \sigma_x = \sigma_z = \frac{L}{4}.
\]

For a Gaussian curve, the peak is at: \( \frac{1}{(\sigma_x \sigma_z (2\pi))} \), the area under the curve is 1.

Therefore, for a wind speed, \( u \), the volume flux of contaminants is \( C L^2 u \).

Therefore, the distribution should be multiplied by \( CL^2 \) to match the box model. This gives a volume flux of \( CL^2 u \) and a centreline value of \( C_0 = \frac{8C}{\pi} \).
2.6 Boundary layer penetration

For stably stratified conditions there is generally little mixing between materials above and below the upper boundary of the atmospheric boundary layer (ABL). Stratified flow is caused by a particular configuration of vertical temperature gradient which provides resistance to vertical movement. Thus, most of the material reaching the boundary layer is reflected back towards the earth, and most of the material above the boundary layer is reflected away from the earth. However, if the material has enough upwards momentum (as in the case of a large nuclear explosion, for example) it may penetrate the atmospheric boundary layer (fully or partially). Some of the material will then stay above the boundary layer. The small amount of mixing between the materials above and below the boundary layer will mean that the material which penetrates above the boundary layer will, over time, return to below the top of the boundary layer.

The height of the inversion layer varies depending on the weather (wind speed, stability class, temperature, pressures, etc.). HOTSPOT [13] assumes a default inversion layer of 5 km, above which no mixing occurs. It warns that inversion layers at 300 m - 3,000 m will significantly increase the air concentration values.

Equation 4.5 can be used to determine the amount of explosives required for the initial gas cloud to penetrate the boundary layer. A boundary layer of 1 km would require approximately $7.7 \times 10^4$ kg TNT, i.e. $3.75 \times 10^5$ MJ), so the initial mushroom cloud generated from any smaller explosion is unlikely to penetrate an inversion layer at 1 km. However, the residual buoyancy within the plume will mean that the cloud will continue to rise as it expands. Although the buoyancy will reduce as the cloud rises and expands, provided the buoyancy is strong enough, the plume could partially penetrate the layer.

Dispersion codes such as DEGADIS [16], AUSPLUME, CALPUFF, CTDMPLUS and AERMOD can also model partial penetration through the layer [17], and radioactive release codes such as NAME [18] model penetration of the atmospheric boundary layer. For partial penetration of the atmospheric boundary layer, this means (a) less material is dispersed within the atmospheric boundary layer, and (b) the material penetrating the boundary layer is either lost from within the model (for example, in the case of the ADMS code), or the material entering the upper troposphere is accounted for separately and then allowed to re-enter at some greater distance.
3 PHENOMENOLOGICAL CONSIDERATIONS

There are three main sources of energy that could lead to explosive releases [19]:

1. Stored or 'physical' energy
2. Reaction or 'chemical' energy
3. Nuclear energy.

3.1 Stored energy

Stored energy (also called 'physical energy') is that of stored material (over or under pressure of the stored material, high or low thermal energy, material stresses or strain leading to mechanical failure).

During an explosion caused by expansion of ideal gases, energy released, $E$, can be described [19, p17/25-28] as:

$$E = \frac{PV_1 - P_0V_0}{\gamma - 1}$$  \hspace{1cm} (3.1)

or using $PV^\gamma$ is constant to eliminate $V_0$ gives:

$$E = \frac{PV_1}{\gamma - 1}\left(1 - \left(\frac{P_0}{P_1}\right)^{\frac{(\gamma - 1)}{\gamma}}\right)$$  \hspace{1cm} (3.2)

where

$E$ is the energy released during expansion of an ideal gas (J),
$P$ is the pressure of the gas (kPa),
$V$ is the volume of the gas ($m^3$),
$\gamma$ is the ratio of the gas specific heats,
1 is the subscript referring to initial state,
0 is the subscript referring to atmospheric state.

The catastrophic releases considered in this review will all be of materials which are either in storage containers, or which may be attached in a discrete package to an explosive charge. In some cases, the nature of the storage will imply a large amount of stored energy. This is particularly the case for pressurised liquefied gases, such as chlorine. Materials held at ambient pressure, in gas, liquid or vapour form, will have no stored pressure energy.

If the expansion of the gas is driven by a change in thermodynamic state of the material, such as in the case of a 2-phase release of chlorine from a pressure vessel, then the energy must be estimated from the initial and final states of the fluid, under assumptions through the use of tables:

$$E = M_l(u_i - u_a)$$
$$= M_l\left(u_f - (x \ u_{ga} + (1 - x) \ u_{fa})\right)$$  \hspace{1cm} (3.4)

where
PHENOMENOLOGICAL CONSIDERATIONS

\[ E = \text{energy released by the expansion}, \]
\[ M_L = \text{initial liquid mass (kg)}, \]
\[ u_i = \text{initial specific internal energy (J/kg)}, \]
\[ u_a = \text{final specific internal energy (J/kg)}, \]
\[ u_{li} = \text{specific internal energy of the saturated liquid at pressure } P_i \text{ (J/kg)}, \]
\[ u_{fa} = \text{specific internal energy of the saturated liquid at pressure } P_a \text{ (J/kg)}, \]
\[ u_{ga} = \text{specific internal energy of the saturated vapour at pressure } P_a \text{ (J/kg)}, \]
\[ x = \text{vapour fraction at the end of the expansion (-)}, \]
\[ P_i = \text{initial pressure (vessel pressure) (Pa)}, \]
\[ P_a = \text{final pressure (ambient pressure) (Pa)}. \]

The vapour fraction is not known, but is often estimated by assuming a particular reversible thermodynamic path through conservation of some property, \( y \), of the liquid / vapour mixture (often that the material is isentropic or isenthalpic), so that:

\[ x = \frac{y_{fi} - y_{fa}}{y_{ga} - y_{fa}}. \]  (3.5)

Stored energy due to material stress or strains are not covered in this review because they are not relevant to the particular examples. In these examples, the stored vessel energy is considered only to propagate a vessel crack, and therefore does not affect the dispersion of the material.

### 3.2 Reaction energy

Reaction or ‘chemical’ energy is the energy caused by chemicals reacting (including flammable materials). These can be further divided into categories:

1. **Combinations of chemicals**: some such combinations produce thermal energy when they react (includes combustion of flammable materials).
2. **Uniform explosions**: include detonations of high explosives (where the reaction front propagates at super-sonic velocity).
3. **Propagating explosions**, including deflagration of combustible gases (where the combustion front propagates at sub-sonic velocity).

If the material is flammable, there will be stored thermal energy which may be released in the form of a fireball. In such cases, this thermal energy will only be released if the material is ignited, and it is unlikely that there would be unburned material remaining to be dispersed.

It is possible that the material involved will undergo another form of exothermic reaction. In such cases, the heat formed will cause the plume to rise initially. Both the products of this reaction, and also materials that have not been involved in the reaction, may then be dispersed downwind. Nearby materials such as powders or dusts could also be entrained into the plume. This is likely to be the case for a TNT type explosion, irrespective of any other materials which may become involved, and 1 kg TNT is expected to yield an ‘energy of explosion’ of around 4.85 MJ, of which 2.71 MJ is due to the transfer of thermal energy (termed ‘heat of explosion’) [20], (although this varies depending on the availability of excess air).
The available combustion energy in various materials can be related to the energy or weight of TNT, and are given a TNT-equivalence. The TNT equivalence method is strictly limited to high explosives. However, the TNT-equivalence method is sometimes used for Vapour Cloud Explosions with high flame speeds using an energy conversion between the heat of combustion of the gas mixture and an equivalent mass of TNT [21]. High explosives and other materials will react in different ways; e.g. deflagration, detonation, other exothermic reactions. Secondly, the internal energy is used for blast energy, thermal energy and energy for change of state, and so may not be proportional to the explosive energy. Therefore, the TNT equivalence alone cannot determine the consequences of an explosive release.

The following formula, which relates weights of fuel and heat of combustion, can be used to determine the TNT-equivalent weight, and is particularly useful for powder fuels where the volume is not easily determinable [23]:

\[
W_{\text{TNT}} = a_e \frac{W_f H_f}{H_{\text{TNT}}} = a_m W_f, \tag{3.6}
\]

where

- \(W_f\) = the weight of fuel involved (kg),
- \(W_{\text{TNT}}\) = equivalent weight of TNT or yield (kg),
- \(H_f\) = heat of combustion of the fuel in question (J/kg),
- \(H_{\text{TNT}}\) = TNT blast energy (J/kg),
- \(a_e\) = TNT equivalence based on energy (-),
- \(a_m\) = TNT equivalence based on mass (-)
- \(\gamma\) = ration of specific heats (1.4 for air).

The TNO Multi-Energy Method (22) is a similar method available for relating overpressures to combustion energy scaled distances. However, it allows for 10 categories of reactivity so that both high explosives and other gases can be accounted for, giving 10 relationships between energy and distance.

### 3.3 Nuclear energy

Nuclear explosions can release thermal energy, causing a plume to rise (a stem-and-cap, or ‘mushroom’ cloud is commonly associated with nuclear explosions). However, nuclear explosions are not considered in this report.

### 3.4 Initial plume configuration

The energy released will result in the material being propelled away from the point at which it was originally located. The shape and extent of the initial source cloud will depend upon the type and circumstances of the release, as described below:

a. Cold failure of pressure vessel

In this case, the release energy is primarily from the stored pressure energy within the pressure vessel. Although the initial spreading of the released material may take place in a preferred direction, the original rupture is likely to propagate rapidly to result in material being propelled in
all directions [2]. For a vessel at or near ground level, this is likely to give a hemi-spherical initial cloud, as assumed within the ACE model (see Section 4.2.1).

b. Hot failure of pressure vessel

This applies to any storage of liquid, whether pressurised or not, and would occur as a result of fire engulfment. The heating of the vessel above and below the liquid level will result in a large thermal gradient, as the ‘wettest’ part of the vessel surface is kept relatively cool. The thermal stresses which are set up in this way may then result in vessel burst. The fact that the vessel will already be situated in a buoyant plume (from the engulfing fire) means that there will be some initial rise of the released material.

This type of incident is known as a Boiling Liquid Expanding Vapour Explosion (23), and, where the contents of the vessel are flammable, will result in a fireball. For the purposes of calculating radiation and blast waves, the fireball is assumed to be spherical, with elevation varying over time (usually measured as height above ignition position after lift-off occurs) approximately evaluated by assuming the velocity of rise equals the rate of increase of diameter, suggesting that the level of the lower part of the cloud is fairly constant. If the vessel contents are not flammable, the high pressure induced by the boiling will ensure that material is projected in all directions. However, the thermal plume will also lift the material, so that the source could be considered to be a sphere of the same size and at the same location as the fireball.

A further effect to be considered in such cases is the potential for production of combustion products. For hydrocarbon releases, the main products of combustion are water and carbon dioxide. Although some carbon monoxide may also be generated, its toxic effects will not normally be significant compared with the thermal radiation effects. Other materials, however, may produce toxic products of combustion, whose quantities would need to be estimated as part of the source term.

c. Explosive release

As described in Sections 2.3 and 3.2, the explosion will produce a pressure wave which propagates rapidly. It will be accompanied by very rapid heat release, which will form a rising thermal plume (sometimes referred to as a stem) which will carry any entrained material aloft (the accumulating cloud is sometimes referred to as a cap), resulting in a ‘stem and cap’ or ‘mushroom’ cloud. There is likely to be some dispersion of the material as it rises, but this is a secondary effect.

The source shapes resulting from these three configurations are illustrated in Figure 3-1:
Figure 3-1: Variation of source configurations

a) Cold failure  b) Hot failure  c) Explosion
4 REVIEW OF EXISTING MODELS

In this Section, reviews of existing models that are specific to the 4 scenarios stated in Section 1.3 are given. The 4 scenarios are:

1. high explosive combined with toxic material as in terrorist events,
2. releases from catastrophic failure of pressurised storage vessels.
3. releases from terrorist attacks on bulk shipments (e.g. LNG),
4. releases from terrorist attacks on road/train shipments of toxics.

The review covered papers, text books, web-sites and discussions with contacts.

The source term modelling and initial dispersion are reviewed in Sections 4.1 to 4.4.

4.1 Releases following high explosives charge

4.1.1 Description

The majority of models in the open literature concerning energetic releases (such as explosions and blasts) focus on calculating the overpressures from the leading shock wave and the following rarefaction wave. For example, the emphasis in the HSC report on the ‘selection and use of explosion effects and consequence models for explosives’ [24], focuses on the blast overpressure wave, the kinetic energy of fragments, and thermal radiation effects. Likewise the COMEX methodology (RPA 1997 [25]) does not include any information on the initial formation of cloud, but focuses on explosive debris (for example, lead residues falling over an area) and the subsequent formation of a smoke plume.

There is little information available in the open literature linking concentrations of material and the dispersion of high explosive releases. Exceptions to this are (a) volcanic eruptions (e.g. [15]), (b) blasts in mining (e.g. [26]), as discussed in Sections 2.3.3 and 2.3.1 respectively, (c) Computational Fluid Dynamics (CFD) applications such as AutoReaGas [27], FLACS [28], EXSIM [29], CFX [30] etc., where it is necessary to assess the mass fraction of the combustible gas in order to calculate combustion for the explosion and blast modelling, and specialised CFD dispersion models such as ADORA [31], ERAD [32] and MIDAS-AT [33], and (d) ‘dirty bombs’ or RDD (Radiological Dispersion Devices) (e.g. [34, 35, 36], [37]). The CFD codes often involve complex modelling, where several physical concepts are modelled and the equations for velocity and concentration are coupled. Therefore, in order to obtain a basic understanding of the physical processes, empirical models, particularly those derived to estimate the effects of ‘dirty bombs’, can be examined.

4.1.2 Source terms and initial dispersion

The most relevant available information has come from research and papers connected with RDDs (described in references [33]-[41] and [44]) and the dispersion codes (described in references [13], [14], [42], [43] and [46]).
4.1.2.1 Rise and Disperse Models

The simplest source and dispersion models rely on the fact that the thermal rise takes place quickly, before much dispersion has occurred, and therefore entrainment of air is sometimes not considered during the rise. The initial blast wave and rainout (condensation within the cloud, forming droplets) are also neglected in most of the modelling. In the first step the initial rise, $H_e$, as shown in Figure 4-1, is calculated, and then the second step is to calculate dispersion in the normal manner from a point source.

**Figure 4-1 Cloud rise for an explosive release.**

The elevated height calculated by the HOTSPOT [13, 14] code is dependent on the explosive energy [37], and is calculated using the following equation [14] based on [13] data from Sandia National Laboratories [38]:

$$H_e = \alpha \left( 76m^{0.25} \right)$$  \hspace{1cm} (4.1)

where $H_e =$ the effective release height (m) and mid-point of dispersed plume,

$\alpha = 0.8$ (given as mid-point of dispersed plume in [14], as shown in Table 4-1, and

$m =$ the amount of explosives (lb).

Reshetin and Regens [36] also recommend an initial rise and subsequent dispersion. The height of the release is given over time:

$$H_e = \zeta \left( M^{0.25} \right) t^{1/2}$$  \hspace{1cm} (4.2)

where $H_e =$ the effective release height (m) and mid-point of dispersed plume,

$M =$ the amount of explosives (kg),

t = time from start of release (s), and

$\zeta =$ constant in range 30-50 m / (kg$^{1/4}$ sec$^{1/2}$).

Gostintsev et al. [39] state that ‘the automodel regime of movement forms in about 0.1-1.0 seconds after the explosion’, and ‘the time interval for the thermal’s rise is approximately 5-10 seconds’. ‘Automodel’ describes a property of the solution (also called ‘self-similar’ or ‘invariant’), and so the statement implies that the model described by Equation 4.2 is valid from 0.1-1.0 seconds after the explosion, and lasts until the thermal rise is complete (after approximately 5-10 seconds). Thus they calculate that, for 5-10 kg of TNT, the
effective height of the release is 50-150 m depending on the power of the explosion.

This information can be used to compare the estimates produced by Equation 4.1 with those of Equation 4.2. The effective heights of the plume after thermal rise give similar results, as shown below:

Equation 4.1 can be converted to metric units, taking $M_{kg} = 2.2 \text{ lb/kg} \times M_{kg} = 2.2M \text{ lb}$, and simplified to:

$$H_e = 74M^{0.25}$$  \hspace{1cm} (4.3)

By inspection, in Equation 4.2, values for $\zeta$ and $t$ at the lower end of the ranges will give a better comparison with Equation 4.1.

Using $\zeta = 30 \text{ m} / (\text{kg}^{0.5} \text{ s}^{0.5})$ and $t = 5 \text{ s}$, Equation 4.2 becomes:

$$H_e = 67.1M^{0.25}$$  \hspace{1cm} (4.4)

where $M$ = the amount of explosives (kg).

This suggests, according to the two formulae, that

$$H_e = 70M^{0.25}$$  \hspace{1cm} (4.5)

should give a reasonable approximation for this initial ‘plume rise’. However, this has not been compared to experimental data. Equation 4.1 is based on data obtained by Church [38], Equation 4.2 on work by Gostintsev et al. [39] and Turner [40], but with no reference to experimental data. There have been more recent experiments carried out in Germany [37] which suggest that HOTPOST over-predicts the cloud height (and indeed cloud dimensions) by an order of magnitude. It is beyond the scope of this report to examine the basis of the experimental data.

This model can be used to create simple suitable source conditions in a dispersive model where a point source is required. This method was used in an Environmental Impact Statement (EIS) [41], which compared several of these simple codes for estimating the initial post-detonation dispersion. The HOTSPOT code was used to calculate the initial rise, and then GENII [42] and MEPAS [43] (which are able to calculate radiation doses in addition to modelling transport of material) were also used to calculate the dispersion from the elevated height. HOTSPOT itself was also used to calculate the dispersion from the elevated height. All three models use straight-line Gaussian-plume passive dispersion. GENII and MEPAS assume dispersion is from a point source and were found to under-estimate the dispersion, but were able to incorporate more complex meteorological conditions than HOTSPOT.

The limitations of the model described above are that only the height is modelled, and no indication of a volume is given for the elevated source. However, HOTSPOT models dispersion from a volume source, by calculating the cloud size at the elevated height and the amount of material within the stem. This is described in Section 4.1.2.2.
4.1.2.2 Intermediate Steps

Whilst the simple models are suitable for medium to far-field dispersion results, ignoring the thermal and dispersive behaviour of the first few seconds would prove less accurate for near-field consideration. Advanced codes (discussed in Section 4.1.2.3) deal with these properties. However, an intermediate step is to model:

1. the amount of material in the stem of a stem-and-cap cloud, and
2. the size of the cloud prior to dispersion.

The HOTSPOT code does exactly this. The stem and cloud are divided into 5 regions, thereby giving an indication of the distribution of material within the plume. Each cloud region is related to the cloud rise height (discussed in detail in Section 4.1.2.1). Table 4-1 gives the heights and the amounts of material in each of the 5 regions. Note the differences to the mass distribution proposed for a fireball stem and cap model which is discussed in Section 4.1.4.1.

Using this distribution, the cloud radius (m) can be written in terms of weight of explosives (m in lbs or M in kgs):

\[
\text{cloud radius} = 0.2 \times \text{cloud top} = 15m^{0.25} = 19M^{0.25}.
\]

Table 4-1 Source distribution within stem and cap model.

<table>
<thead>
<tr>
<th>Diagrammatic representation of cloud (showing percentage of material within cloud)</th>
<th>Height (as fraction of top of cloud)</th>
<th>Height (m) (function of pounds of explosives, m)</th>
<th>Height (m) (function of kgs of explosives, M)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20%</td>
<td>1.0 (cloud top)</td>
<td>76 m^{0.25}</td>
<td>93 M^{0.25}</td>
</tr>
<tr>
<td>35%</td>
<td>0.8 (cloud mid point)</td>
<td>61 m^{0.25}</td>
<td>74 M^{0.25}</td>
</tr>
<tr>
<td>25%</td>
<td>0.6 (bottom of cloud, top of stem)</td>
<td>46 m^{0.25}</td>
<td>56 M^{0.25}</td>
</tr>
<tr>
<td>16%</td>
<td>0.4 (2/3 of height of stem)</td>
<td>30 m^{0.25}</td>
<td>37 M^{0.25}</td>
</tr>
<tr>
<td>4%</td>
<td>0.2 (1/3 of height of stem)</td>
<td>15 m^{0.25}</td>
<td>19 M^{0.25}</td>
</tr>
<tr>
<td>0</td>
<td>0 (ground height)</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

For example, 1 lb (0.454 kg) of explosives would result in an initial cloud with top at 76 m, mid-point of 61 m (0.8 x cloud top) and cloud radius of 15.2 m (0.2 x cloud top).

The main limitation of this model is that the dispersion during the explosive phase does not depend on the type of material. A powder, such as Caesium Chloride is very dispersive (think of opening up a container of talcum powder) [44, 45]. This could mean that the concentration of the material is over-predicted.
using this model, but the distance over which the material travels would be underestimated.

4.1.2.3 **Advanced codes**

There are only a handful of commercially available software applications that model the source terms and dispersion from the initiating event using explosive energy, material and external conditions.

The BlazeTech application ADORA (Atmospheric Dispersion of Reacting Agents) [46] is “the only software that couples air dispersion with chemical reactions and heat release”. Thus, it not only accounts for explosive energy, but also for reacting chemicals and other source terms appropriate to the other scenarios discussed later. Importantly for the explosion scenario, firstly, chemical reactions and thermal aspects are included right from the start (allowing accurate prediction of the height of the rise and composition of the cloud), and secondly, the properties of the stem and the cap (cloud) are modelled (size and chemical composition and are part of the output). Details of the cloud location and sizes, transition times, dosage and downwind information are also given as outputs from the model. The application is on the EPA (Environmental Protection Agency [47]) list of approved codes, and has been validated against Sandia tests and accidental releases from rocket propellants for fireballs, tests at Dugway Proving Ground and Eglin Air Force Base for chemical species and other sources for different aspects of the software as well as against validation for other widely accepted codes where capabilities match, (i.e. SLAB), and empirical data. References are not given for these tests. Explosive reactions have been considered in combination with chemicals to show the survivability of the chemical. Example calculations show the survivability for two separate cases (20kg and 2kg GB (sarin)) in a 20kg TNT explosion giving ground level hazard distance for various degrees of mixing of GB and TNT [48]. The results for the 20kg GB are given in Figure 4-2. In the same presentation (1999) it suggests a proposed link to the dispersion and consequence risk model HPAC [49]. ADORA would be used for the near-source chemical reactions (by-passing ADORA for non-reactive chemicals), and the cloud properties would then be passed on within HPAC to SCIPUFF for far-field dispersion. However, no further publications have been posted on the BlazeTech site to suggest that this has happened.

Explosive Release Atmospheric Dispersion (ERAD) [32] was specifically developed to predict near-field consequences following an explosive release of a hazardous material and its validation includes high explosive detonations [50]. It also now incorporates fires and buoyant releases. The application includes the transport and diffusion of particles in the dispersion, and uses both puff models and Monte Carlo probabilistic methods in its predictions. ERAD requires 3-D meteorological data as a function of time as part of its input. The output is given in terms of ground level dose contours, and deposition contours.

Meteorological Information and Dispersion Assessment System Anti-Terrorism (MIDAS-AT) software [33] models radiological, industrial chemical, chemical and biological agent releases. Release capability includes explosions and aerosols from tank ruptures. The software uses local tower data for the meteorological data, and updates data using the forecast every 5 minutes. MIDAS-AT, like ERAD, outputs ground level dose and deposition, and also calculates concentration.
4.1.3 Subsequent dispersion

Dispersion of the spherical cloud can be modelled using a standard model. Any appropriate dispersion model can then be used to model subsequent dispersion, provided that the concentration profile is set up correctly.

The material within the stem and cap is not uniformly distributed. Only 55% of the material is contained within the spherical cloud, and this itself is ‘bottom heavy’ (the lower half of the spherical gas cloud cap contains 35% of the released material whereas the upper half only contains 20%). Similarly, the material in the stem itself is not uniform, but is ‘top heavy’.

In order to represent the whole cloud, it is possible to model the dispersion from each segment of the stem and cloud, using 5 plume releases at 5 different elevations [25, referencing [51]].

In practice, it is simpler for subsequent modelling for the cloud and stem to be modelled as two plumes only (the spherical cloud, and the stem). It is simpler still to model the spherical cloud only, and to assume a single Gaussian profile with equal concentrations in each of the two halves, than to retain the ‘bottom heavy’ or multiple distributions. In this case, the model does not account for dispersion of the material from within the stem, and this should be noted in any discussion of the results.

HOTSPOT uses a Gaussian dispersion method to find the downwind cloud concentration. For input into the dispersion model, a Gaussian profile is required, rather than the spherical representation of the cloud. It is assumed that 95% (2 standard deviations, 2σ) of the cloud debris falls within the cloud radius:  

\[ \text{Cloud lift-off results in HF Ground concentrations} \ll 1.6 \text{ mg/m}^3 \]

\[ \text{Cloud lift-off results in GB Ground concentrations} \ll 0.06 \text{ mg/m}^3 \]
\[ \sigma_r (\text{at x=0}) = 0.5 \times \text{cloud radius} = 7.5m^{0.25} = 9.5M^{0.25}, \quad (4.7) \]
\[ \sigma_z (\text{at x=0}) = 0.5 \times \text{cloud radius} = 7.5m^{0.25} = 9.5M^{0.25}. \quad (4.8) \]

The release from the stem should be modelled in a similar way to that from the spherical cloud (cap). However, no guidance is given in the literature as to what radius should be used to calculate the standard deviation for the release.

4.1.4 Material distribution and deposition
The spherical gas cloud may contain particles. Subsequent to the initial explosion and formation of the gas cloud, deposition from a plume can occur. Particles within the gas cloud will leave by diffusion (small particles of radius < 1 \( \mu \)m) and by gravitational forces acting on the particles. This is known as diffusion sedimentation and gravitational sedimentation (also known as gravitational settling). The simple and intermediate models used to predict the cloud height dimensions that were described above, and the subsequent gas dispersion models, do not account for aerosol sedimentation, and thus may under-predict concentrations in the immediate vicinity of the explosion, but over-predict concentrations downwind.

4.1.4.1 Aerosol distribution within the plume
This section discusses the distribution of mass within the plume, and also the distribution of particle size.

Mass distribution
There is little available non-classified literature regarding aerosol distribution within a plume following an explosive release. There is, however, some limited information for an aerosol distribution in a cloud following a fireball explosion [52]. Calculations for this study investigated mass configurations for (1) total plume mass (including entrained dirt) and (2) PuO\(_2\) mass only. In the study, PuO\(_2\) made up less than 0.1%. Each calculation was carried out for 7 cases, representing different meteorological conditions and varying available energies.

The results showed that the plume could be modelled in 2 ways:

(a) the cap and stem model. This model was appropriate for 4 of the 7 total mass distributions and 2 of the 7 PuO\(_2\) mass distributions.

(b) uniformly distributed mass throughout the plume. This was applicable to the remaining cases.

The choice of model for vertical mass distribution was found to be dependent on the energy of the release relative to the mixing layer depth. If the energy is sufficient to raise the plume so that it both penetrates the inversion layer and reaches heights of 3-10 times the mixing layer depth, then the classical cap and stem approximation can be used. Otherwise it is better to assume the uniformly vertical distribution of the mass in the plume.

The stem and cap model proposed in the study represents 80% of material in the cap, and 20% in the stem. (Compare this to the distribution formulated for the explosive model in HOTSPOT, which suggests that only 55% of the material is contained within the cap, and 45% in the stem.) The model depends on the particle density (particles of higher density are more likely to be present in the lower elevations of the plume, or deposited on the ground), and on the H/D ratio.
ASPECTS OF DISPERSION FOLLOWING AN EXPLOSIVE RELEASE

(a measure of the mixing layer penetration by the plume, where $H$ is the simulated cloud height, and $D$ is the mixing layer depth). The results of the experiments are presented as a series of graphs showing dependency of mass on elevation and of fraction of mass in the stem on $H/S$. Because of the uncertainty in estimating the fraction of PuO$_2$ mass in the plume that is contained in the stem, suggested distributions were formulated in the paper to characterize the uncertainty. These are not given here, since they refer to fireballs, rather than explosive releases. The report recognises that the number of cases studied was limited, nevertheless raises some useful results on which further work can be based.

Deposition from the uniformly distributed plume was approximately 10% of the PuO$_2$ mass is deposited on the ground for the uniform PuO$_2$ distribution cases.

**Particle Size**

If it is assumed that the cloud is uniformly mixed, it is suggested that initially the fraction of aerosol particles of diameter greater than a given diameter, $R$, is modelled using the Weibull distribution:

$$F(\omega) = 1 - \exp\left(-\left(\frac{\omega}{\beta}\right)^\alpha\right), \quad 0 \leq \omega \leq \infty \quad (4.9)$$

where:

- $\omega = \text{aerosol diameter (cm)}$,
- $\beta = 0.322297 \times \text{escfrac} \times \text{rupture}$,
- $\text{escfrac} = \text{fraction of particles with 'diameter < rupture' that escape} = 1.0$,
- $\text{rupture} = \text{rupture diameter} = 1 \text{ cm}$,
- $\alpha = 0.9976$.

The Weibull parameter values of $\alpha$ and $\beta$ are given for PuO$_2$ only. Their suitability for application to other aerosols is not known.

4.1.4.2 **Ground level deposits**

The deposition density can be described as a mass per area (sometimes referred to as “deposition rate” in the literature), which decreases with distance from the release [25]:

$$\text{deposition density (kg / m}^2\text{), } L = \frac{Q_0 e^{-0.002x}}{x^2}$$

(4.10)

where

- $Q_0 = \text{released quantity (kg)}$
- $x = \text{distance from release (m)}$.

The area of a deposition, $A$, can be calculated if the angle of the plume in radians, $\theta$, is known:

$$A = \frac{1}{2} x^2 \theta.$$ (4.11)
It is possible to estimate $\theta$, using the cloud radius, $R(x)$, at a downwind distance, $x$:

$$\theta = 2 \times \tan^{-1} \left( \frac{R(x)}{x} \right)$$  \hspace{1cm} (4.12)

HOTSPOT provides an output for ground level deposition. The GENII code, for transport of radionuclides, estimates the amount of material deposited from the plume within the code. The material is not numerically removed from the plume, and is therefore double-counted. HPAC also includes a nuclear rainout sub-model.

4.1.4.3 Rate of particle or aerosol sedimentation

Sedimentation can be predicted in the following way. It is described by Resheitin and Regens in their paper on modelling $^{137}$Cs dispersion from a radiological dispersion device [36]. They adopt standard formulae to give the aerosol sedimentation characteristics:

The rate of aerosol sedimentation, $U(r)$ cm/s, is given by:

$$U(r) = FB(r)$$ \hspace{1cm} (4.13)

where

$$B(r) = \text{mobility of a particle} = B(r) = \frac{Cn(r)}{6\pi \eta r}$$ \hspace{1cm} (4.14)

$$Cn(r) = \text{Cunningham’s empirical correcting factor}$$

$$= 1 + 1.246Kn + 0.42Kn \exp \left( -\frac{0.87}{Kn} \right)$$ \hspace{1cm} (4.15)

$F$ = the force acting on the particle (g.cm/s$^2$)

$Kn = \text{Knudsen number} = l/r$ \hspace{1cm} (4.16)

($l$ = the free length of molecules of a gas)

$\eta = \text{molecular viscosity or coefficient of viscosity of a gas (g/(cm.s)})$

$r = \text{the radius of the particle (cm)}.$

For gravitational sedimentation, the force, $F$, depends on the particle size ($r^2$), and the sedimentation velocity, $U_g$, is defined by:

$$U_g(r) = \frac{2\rho g}{9\eta} r^2 Cn(r)$$ \hspace{1cm} (4.17)

$g = \text{acceleration of gravity (cm/s}^2).$

The diffusion sedimentation rate, $U_D(r)$ depends on a diffusion coefficient of the particle, $D(r)$, and the gradient of the particle concentration normal to the ground surface. However, by assuming only molecular diffusion occurs in a layer of thickness $\delta_0$ above the ground, then the rate of diffusion sedimentation becomes:

$$U_D(r) = \frac{\tilde{D}(r)}{\delta_D}$$ \hspace{1cm} (4.18)

where

$$\tilde{D}(r) = \text{diffusion coefficient} = kB(T)$$ \hspace{1cm} (4.19)

$k = \text{Boltzman constant}$

$T = \text{temperature (K)}$
giving:
\[ U_D(r) = \frac{kT}{\nu \rho_{\text{gas}} r \delta_D} \]  
(4.20)

\[ \nu = \text{kinematic viscosity} = \eta/\rho_{\text{gas}} \text{ (cm}^2/\text{s}) \]  
(4.21)

\[ \rho_s = \text{effective density of a spherical particle (g/cm}^3) \].

Unlike gravitational sedimentation, diffusion sedimentation reduces as the particle size increases.

4.1.5 Debris

All debris caused by the blast of an explosion can be assumed to fall within the 5 kPa overpressure contour, beyond which it is defined as ‘safe’ [25]. By further assuming that the deposition of the debris is uniformly distributed over this area, the amount of material deposited per 1m² of land can be found:

\[ \text{deposition of debris} = \frac{Q_{\text{debris}}}{\text{Area}} \]  
(4.22)

where

\[ Q_{\text{debris}} = \text{amount of hazardous material that will be deposited} \]
\[ A = \pi R^2, \text{ and} \]
\[ R = \text{distance to 5 kPa overpressure contour}. \]

\( R \) is related to the energy of explosion by mass of explosives and the explosivity of the material. It can be found using TNT-equivalence graphs, from the TNO multi-energy method (see Section 3.2), or using equivalent relationships of overpressure contours, relating the distance from the explosion to the size of explosion, such as the one given in Figure 4-3.

**Figure 4-3 ‘Safe’ distance regarding debris deposition for high explosives [25].**
The data for the debris limit curve in Figure 4-3 can be fitted to the equation:

\[
R_{\text{debris}} = 21.39 M^{0.3426}
\]  

(4.23)

where

\[
R_{\text{debris}} = \text{debris limit distance (m)}
\]

\[
M = \text{size of explosion (kg)}
\]

### 4.2 Catastrophic failure of pressurised storage vessels

In 1999, Atkins carried out work for the HSE (2, 3) on developing an improved and validated methodology for the characterisation of the cloud conditions following the catastrophic failure of pressurised vessels. The methodology was comprehensive and included methods for calculating the cloud volume and temperature, the internal turbulence and air entrainment, bubble nucleation and growth, flashed vapour fraction, droplet formation and behaviour, droplet size distribution, evaporation and rainout. A summary of the relevant aspects is provided here.

#### 4.2.1 Source terms and initial dispersion

The model developed by Atkins for HSE is called ACE (Airborne Concentration Estimate) [3], and it can be used to describe initial dispersion for such releases with few input source terms. ACE includes 3 sub-models to cover the stages indicated in Table 4-2. The stored internal energy is the basis for the explosive expansion phases of the model and subsequent stages. For further information about calculating the stored energy of the material in the vessel, see Section 3.1.

<table>
<thead>
<tr>
<th>Sub-model</th>
<th>Input</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Vessel rupture and</td>
<td>Storage conditions: material, material mass, initial temperature, initial pressure, and ambient conditions</td>
<td>Cloud state at end of explosive growth phase</td>
</tr>
<tr>
<td>Explosion phase.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2. Turbulent growth</td>
<td>Cloud state at end of explosive growth phase</td>
<td>Cloud state at end of turbulent growth phase</td>
</tr>
<tr>
<td>3. Slumping/transport</td>
<td>Cloud state at end of turbulent growth phase</td>
<td>Subsequent cloud state for input to dispersion model (if required)</td>
</tr>
<tr>
<td>dispersion</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The cloud state at the end of the explosion growth phase is characterised by a volume, \(V_c\). During the vessel rupture, the explosion phase, and initial stage of the turbulence phase, the radius of the gas cloud is given [53] by:

\[
R(t) = R_{\infty}(1-\exp(-t/\tau))
\]  

(4.24)

where

\[
R_{\infty} = 2.65 V_f^{1/2}
\]

\(V_f = \text{the volume of the flashed vapour} = x_v M_L / \rho_{VO}\)

\(x_v = \text{vapour fraction using isenthalpic path}\)

\(\tau = (\text{LengthVessel} + 2 \pi \text{RadiusVessel}) / (2 \times \text{speed of fracture})\)

\(\rho_{VO} = \text{density of saturated vapour at ambient conditions}\)
The maximum rupture duration, $\tau$, is the time taken for the vessel to 'unzip', i.e. for the fracture to propagate along the length of the vessel and around the end caps. It is used as a characteristic time to describe the radius of the gas cloud in Equation 4.24.

Because the cloud is spherical, the volume of the cloud, $V_c$, can be calculated as:

$$V_c = \frac{4 \pi R^3}{3} \approx 78 V_f. \quad (4.25)$$

One of the main parameters which needs to be calculated in this type of release is the amount of material which becomes airborne. The initial depressurisation on vessel failure will result in an initial flash fraction, normally of around 20% of the stored material, but varying according to its physical properties. However, the explosive nature of the release will result in additional material being entrained as droplets, and it is found that the total (vapour + droplets) is normally around 3 times the flash fraction.

The airborne fraction at the end of the explosion phase, $f_a$, gives the vapour mass of the cloud (kg), $M_V$:

$$M_V = f_a M \quad (4.26)$$

where

- $M = \text{mass of the cloud (kg)}$,
- $f_a = \min(F_a x, 1)$, where $F_a$ is a constant, and $x$ the flash fraction,
- $f_d = \text{droplet fraction} = f_a - x$,
- $f_p = \text{pool fraction} = 1 - f_a$

and mass of liquid in the pool (kg), $M_L = f_p M$.

Hence for a chlorine release, around 60% of the chlorine effectively becomes airborne, and the remainder will form an evaporating liquid pool on the ground.

Assuming that all the entrained droplets are vaporised during this phase, this cloud will effectively contain a 'contaminant' volume of around $3 V_f$. The volume concentration of this explosively dispersed cloud is therefore around $3 V_f / 78 V_f = 1 / 26 \approx 4\%$.

The remaining unknown properties (mass of air, $M_a$, and the temperature of the cloud, $T_c$), can be found from the solution of two simultaneous equations determined by combining equations for the conservation of enthalpy, the perfect gas equation, and Dalton’s Law for additivity of partial pressures.

### 4.2.2 Explosive energy

Energy released during the expansion can be calculated by considering the difference in the energy of the states of the material prior and subsequent to the release, using the equation:

$$\Delta u_h = u_{fi} - (x_h u_{ga} + (1-x_h) u_{fa}) \quad (4.27)$$

where:

- $h = \text{Specific enthalpy (J/kg)}$
- $u = \text{Specific internal energy (J/kg)}$
4.2.3 **Subsequent dispersion**

This explosion phase generates a large amount of additional turbulence, which causes the cloud to continue to grow. The turbulence length at the end of the explosion phase is:

\[ u_L = 40 \left( (\rho_a^2 \cdot x_h)/(\rho_{VT} \cdot \rho_{VO}) \right)^{1/9} \] (for butane, propane and propylene), \( (4.28) \)

where

- \( \rho_{VT} \) is the density of vapour in ambient conditions,
- \( \rho_a \) is the density of air in ambient conditions.

The ACE turbulent growth sub-model considers the decay of this turbulence, and assumes that the turbulent growth continues until the characteristic turbulence velocity has fallen to a value which is comparable with the gravitational slumping velocity. The radial growth of the turbulent gas cloud is modelled using relations derived from CFD model results. It was shown in the ACE report that the end of the turbulent phase occurred after around 5 seconds for a 30 t chlorine release, by which time the cloud volume has increased by a further factor of 6.

Subsequent dispersion modelling would then be undertaken using a standard dispersion model. The conditions calculated during these first two phases of the dispersion can be used to ensure that the source is set correctly.

4.2.4 **Material distribution and deposition**

This scenario assumes that the material is stored as a liquid in a pressurised container to keep the temperature above its boiling point. When the container ruptures and the pressure drops, the material becomes an unstable, superheated liquid which rapidly converts to a vapour. During this period vapour bubbles form and grow, and the gas becomes predominantly vapour with liquid bubbles, some of which ‘rains out’ and forms a liquid pool (deposition). The vapour and liquid fractions have been discussed in Section 4.2.1, but little is known about the nature and nucleation of the bubble nuclei following sudden depressurisation, and so more detailed models cannot be formed. However, using simplifications to existing models and assumptions about the cloud, a simple bubble nucleation sub-model was developed for ACE [2], although it was not described in the published paper [3]. ACE used a standard aerosol drop size and mass distribution presented in reference [54], which also provides a good background on aerosols for flashing releases.

Assuming the bubble was isolated, and in an infinite incompressible liquid with a constant boundary condition, a differential equation could be used to describe the bubble radius. The model was developed to predict the bubble volume, \( C_G \), and bubble radius, \( r_g \):

\[ C_G = \frac{V_G}{NM_F} \] \( (4.29) \)

\[ r_g = \left( \frac{3C_G}{4\pi} \right)^{1/3} \] \( (4.30) \)

where

- \( V_G \) = vapour volume (m\(^3\))
$N$ = number of bubbles per unit mass of fluid, assumed to be constant throughout the model (kg$^{-1}$)

$M_F$ = mass of fluid (kg)

### 4.3 Release from LNG shipment

An LNG shipment will be contained within a refrigerated container or containers. Typically LNG is refrigerated to 111K (-259ºF), and in doing so, the volume is reduced to 1/600$^{th}$ of its volume at ambient conditions [55], making its shipment much more economical.

Much of the work on releases from LNG shipments has come from the oil and shipping industries. Since 9/11 the public concern over terrorist attacks on LNG shipments leading to major hazards has increased, and put LNG tankers in the news when the LNG tanker “Matthew” was banned from entering Boston harbour on 27 September 2001; this was because of concerns over safety and security for its transit into harbour and operations at dock, with the Coast Guard stating that terrorist threats had not been fully considered in the planning [56]. Releases from LNG shipments was the subject of part of a talk by Gordon Milne, Lloyds Register [57], at a Safety & Reliability Seminar [58] in March 2005. To give an idea of the scale of the problem, it was noted that twelve attacks on LNG tankers are known to have occurred in the last 20 years [58], including attacks on “The Cole” and the double-hull tanker “MT Linburg”.

Several independent bodies from the industry (including USA government, insurance industries, shipping classification companies and consultants) have reviewed the consequences of attacks on such shipments, and the related risks. Several major reports have been written: ABS Consulting [59], Sandia National Laboratories [60], Quest [61], Fay [62], Vallejo [63] and Lehr and Simecek-Beatty [64]. These cover site-specific risk assessments for LNG shipments, guidelines on modelling LNG releases (accidental and intentional) and general LNG modelling issues. Several of these reports do not consider dispersion, (Fay, Lehr) nor explosion (Quest, Vallejo). Lloyds register has also posted articles [65] on the subject based on their years of experience in the shipping industry and development of methods specific to LNG releases, but for security reasons the reports are not openly published without confidentiality agreements [12].

#### 4.3.1 Source terms and initial dispersion

The mechanism of release should be addressed carefully in relation to definition of the source term and estimation of release size. The main influence on the LNG dispersion of an explosive charge is to affect the size of rupture of the tanker, and hence the release rate. Then, on rupture the energy from the TNT explosion can be ignored and the dispersion will be driven by the LNG release. Methods for estimating releases vary widely between the models:

- release is a percentage of the inventory. For example, this is unlikely to be the whole inventory, and is often limited to 20% for accidental releases “as of August 2004, all federal government LNG tanker safety model studies assumed a leak of only 20% of the entire LNG cargo is released.” [66].
• calculation of breach size (where it is noted that in the analysis of breach sizes, intentional releases, due to one or more attacks, could yield larger breach sizes than accidental releases),

• finite element analysis can be used to determine realistic breach from 2 colliding tankers from which releases are calculated [67],

• releases from given breach sizes calculated using empirical models,

• release is calculated using simple physics to model the dynamics (e.g. Bernoulli’s equation as a function of breach size, height of liquid level, volume and pressure. Lloyds Register has its own alternative methodology),

• release is calculated using computational fluid dynamics models,

• historical data from accidents,

• experimental tests.

Because of the wide variation, reviews of the reports focus on the initial event, the corresponding size of release, and the credibility of the scenarios. Since modern tankers are double hulled, it is important to consider the inner hole, which may be much smaller than the hole in the outer hull, when considering release following impact of the ship.

The release is generally assumed to form a pool, or spill. The LNG spread [59] can be modelled using an inertial and gravity model for a cryogenic liquid. Alternative models use the Bernoulli equation, the Webber equation [59] or empirical methods. Consideration of wave motion under the pool can limit the spread.

Evaporation from the pool of the sub-cooled liquid is then modelled, and the subsequent dispersion is often undertaken using dense gas or Gaussian models. The thermal effects can be taken into account when calculating the boiling rate from the pool. However, where an explosion has been assumed to be the initiating event causing rupture, it is also assumed that the explosion has had no subsequent involvement in the release modelling. The only secondary effect considered is that the energy of the explosion may also cause immediate ignition of the fuel. Models for the pool fire vary between reports. SANDIA bases its data on spills and extrapolates to larger pools, giving conservative results. Alternative methods would be to use established pool fire models such as Shell’s FRED [68], POOLFIRE6 [69].

None of the models include thermal effects from an initial explosion causing the impact in the calculation for the initial evaporation of the liquid. This is because (a) multiple attacks are not considered, and (b) explosions causing impact are modelled at a short distance away and are assumed to happen separately from the release and (c) nearby debris could ignite the cloud and change the event.

If the gas cloud is not ignited, it will grow and disperse until it is no longer flammable. At worst, the vapour cloud might ignite. This is not necessarily a hazard to people if the cloud is at sea. If the cloud reaches the shore, the edge
is likely to ignite quickly, and the cloud will burn before it moves to land, and will therefore not be a significant risk onshore [58].

It is possible that, on rupture, a deflagration explosion could occur for large releases with early ignition. However, there is unlikely to be any explosive behaviour because of the lack of confinement or objects generating turbulence, but rather, a liquid release that will evaporate, disperse and potentially burn (if ignited at a concentration of between 5-15%).

Subsea or below water-level releases are more complex and are not discussed here (except that immediate ignition is unlikely).

### 4.4 Release from storage vessel containing toxics

This scenario represents a terrorist attack on road or train shipments carrying a container of material. Although the release mechanism and source terms may be different from Scenarios 1 to 3, this scenario could be related to any dispersion model used in those scenarios, depending on the contents of the vessel. In order to decide which is the most appropriate model to use, the energy used in rupturing the vessel must be compared to the energy stored within the vessel. This determines the magnitude of the energy driving the dispersion.

For example,

1. A 20 tonne chlorine tanker under the conditions modelled in Scenario 2 has approximately 135 MJ of stored energy. By comparison 1kg of TNT would explode to give less than 5 MJ of energy. The TNT explosion could be assumed to cause the vessel rupture, but the energy of explosion would be insignificant compared with the 135 MJ of stored energy, and therefore would subsequently have little effect on the dispersion. Therefore, the TNT can be ignored and the scenario can proceed as for Scenario 2, in which the explosive release would be driven by the stored energy of the pressurised Chlorine within the tanker.

2. A 100 kg chloropicrin cylinder has no stored energy since it is not transported under pressure (chloropicrin is liquid at ambient temperature and pressure). Therefore, the TNT explosion would be used to model the initial dispersion using the stem and cap model described in Scenario 1. This would be a conservative approach because some of the TNT energy would be used to cause vessel rupture. In this particular case, it is possible that a proportion of the explosive energy will cause the material to vaporise. Therefore the source term will be some proportion of the inventory instantaneously released within the stem and cap, rather than a slowly evaporating pool at ground level.

An additional consideration for non pressurised liquid vessels is in relation to the vaporisation of the liquid from the pool. Whereas in normal conditions following a fracture of the vessel a pool may have formed that would evaporate slowly over time, following an explosive rupture, it is possible that a proportion of the explosive energy will cause the material to vaporise. In this instance a
proportion of the inventory instantaneously released within the stem and cap can be used as the source term for the dispersion.

4.4.1 Source terms and initial dispersion
Terrorist attacks on a storage vessel would possibly take the form of some impact, fire or blast, leading to a catastrophic release or continuous fixed duration release.

• Catastrophic releases are often modelled by assuming that the contents of the vessel are released at once, conserving mass and volume and taking the aspect ratio of the vessel to model the shape of the released cloud. Instead of using models in Scenarios 1 and 2, other models can be used or approximations made. Sometimes, the initial air entrainment (e.g. 10 times the mass) is assumed to have already occurred before using the models. In that case it is assumed that it will all be mixed, because of the significant amount of turbulence caused by the rupture.

• For continuous releases, knowledge of the release rate, release diameter, and material properties is required. This requires the user to estimate the effective duration of the release. Typically a sensitivity study could be carried out, perhaps taking 1 minute and 10 minute release durations as examples.
5 CONCLUSIONS

The report has summarised methods for predicting dispersive consequences following an explosive release. They have been compiled from existing models available in the public domain. Three scenarios were addressed in detail:

- detonation of high explosives
- rapidly boiling releases from a pressurised storage vessel
- refrigerated releases from an LNG tank following an explosive release

Consideration was also given to the scenario of a terrorist attack on a road or train shipment of toxics.

Due to the limited resource for the project, it has not been possible to compare the models with experiments, or to undertake full reviews of the models. Where possible, references to experimental data and reviews were provided.

For the first scenario (dispersion of releases following an explosive detonation), there was a good amount of material, with focus on RDDs in many papers. The models fell into 2 main categories: (i) the complex CFD codes that solve coupled equations to predict detailed scenarios, and (ii) simple models that capture the characteristics of the dispersion. Papers on the simple models have described many of the areas of interest to this study:

1. The size and height of the initial plume produced by the explosion can be related to the $\frac{1}{4}$ power of the energy of the release (expressed as TNT-equivalent mass of explosives). Penetration of the boundary layer following explosive releases is not always modelled, and little detailed information is published. Where it is modelled, codes use simple models, assuming loss of the material that penetrates the layer, or tracing the material above and below the layer separately and allowing for re-entry to the atmosphere at a later stage in the model.

2. Reference to distribution of the material within the plume and the size distribution of aerosols is fairly limited in the literature. Simple models could assume a uniform mass distribution, or more commonly a stem and cap model, with a specified mass fraction to be contained within the cap.

3. Most models predict the deposition from the plume, although not all remove this quantity from the plume, thus double counting for the material.

4. Transition to a Gaussian plume model can be made by assuming a Gaussian volume concentration profile within the cap, and a separate profile in the stem. In practice, this can be simplified by considering the cap only, or made more detailed by further breaking down the material distribution.
The model presented for the rapidly boiling release was primarily provided from one study [2 & 3]. Although the expansion of the cloud is driven by the energy of release, the size of the cloud depends on the mass of the stored material and the storage conditions in the proposed model. The energy of release can be calculated, but requires assumptions about the thermodynamic paths to be made and does not add value to the method.

1. The size and height of the initial plume produced by the explosion, including penetration of the boundary layer, are given by the model.

2. Very little is known about bubble nucleation and growth following a sudden depressurisation. A simple model for the bubble radius is given, based on several assumptions and simplifications.

3. Rainout can be inferred through the flash fraction of the material to give the mass of the liquid pool that may form. More detailed information about deposition from the cloud is not known.

4. Following the initial expansion, a turbulent phase of the dispersion occurs. Relationships describing the growth of the cloud can be found using CFD analysis. These provide inputs into a standard dispersion model.

The literature suggests that it is common practice to model LNG releases using standard source term and dispersion models. Vaporisation of the liquid will be rapid, and its rate will increase with a rise in ambient temperature. The thermal effects of a nearby plume resulting from an explosive release are not accounted for in the literature reviewed for this study. The consideration of explosives was only studied in the context of estimating the size of rupture, which affects the release size.

The brief analysis of the fourth scenario involved comparison of energy of release and energy of explosion. This then indicated which of the methodologies of the other three (more detailed) scenarios could be used for this final scenario.
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