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HSE CONTRACT RESEARCH REPORT No. 70/1994

DISPERSION OF RELEASES OF HAZARDOUS MATERIALS IN THE VICINITY OF BUILDINGS

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The requirements of the CIMAH regulations for major hazard sites have resulted in the provision of 'Safety Cases', most of which have included some quantification of the consequences of credible major accidents. The gas dispersion models which have been applied hitherto generally deal with idealised, level, unobstructed terrain rather than the more realistic case where buildings and obstructions may have a significant effect. In order to understand these effects better, a research programme into the dispersion of hazardous releases in the vicinity of buildings has been initiated by HSE; this report presents the results of the first phase of this programme.

The primary objective of this phase has been to identify and review the current status of airflow and dispersion modelling around buildings. Information was obtained for both CFD modelling of this problem, and also for full scale and model scale tests. As a result of this review, requirements for future efforts in CFD development have been proposed. The report therefore includes a specification for Phase II of the project, which will involve the application of a suitable CFD code to a series of test cases, together with the parallel development of 'simpler' models (eg. zone models) bearing in mind HSE's ultimate requirements in relation to safety case review.

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CONTENTS

1.0 INTRODUCTION

1.1 Background

There are many major hazard sites within the UK which handle hazardous materials in sufficient quantities that they fall within the requirements of the CIMAH regulations. The requirement for a Safety Case for these sites will mean that not only should hazardous scenarios be identified, but that their consequences should also be assessed. This will typically include source term calculation, gas dispersion calculation and an assessment of toxic or flammable effects.

The Major Hazards Assessment Unit of HSE is also responsible for advising local planning authorities on the desirability of significant developments in the vicinity of major hazard installations. This advice is given on the basis of a risk calculation from the activities at the hazardous installation. The effect of building proximity on releases from toxic gas installations could mitigate risks at some distance from the installation and influence the decisions HSE makes in such cases.

Although significant advances have been made in the calculation of gas dispersion in the last decade or so, the weakest point in the analysis often remains the ability to provide a realistic characterisation of source conditions. The significance of source modelling has been realised, and some recent effort put towards improving our understanding of the mechanisms at work. One area in which some uncertainty remains, however, is the magnitude of the potential beneficial 'buffer' effect of a release in the vicinity of a building. The application in this case is particularly important for toxics, such as chlorine, which are frequently stored in substantial quantities within buildings. Not only does this offer a limited level of 'containment', as described in the companion study 'Dispersion of Releases of Toxic Materials Within Buildings', but it also implies that releases will be discharged either into the wake, or into a region otherwise affected by the building.

The HSE have been at the forefront of the development of gas dispersion models, and the obtaining of full scale validation data in the past 12 years or so **(McQuaid & Roebuck, 1985)**. Most of this work has been directed towards the dispersion of dense gases in open flat terrain. Some effort, however, has been expended in seeking to improve the understanding and prediction of dispersion flows affected by obstructions. The problem under consideration here was tackled by **Brighton (1986)**, funded by HSE. This study gave some useful guidelines for risk assessment purposes, based upon 'zone' type models, which assume complete mixing of the released gas within each zone. More recently, **Porter (1991)** has utilised a simple source adjustment to reflect the cross-sectional area of the building in realistic scenarios and has demonstrated the potential benefit, in terms of reduced hazard ranges, in storage of toxic materials inside buildings.

In view of the lack of coherent current methodology, HSE considered it appropriate to revisit this particular subject and address it in a slightly less simplistic manner. This report therefore presents the findings of the first phase of a study to assess the building wake and other flow effects much more accurately, primarily by using CFD modelling of the external flows.

Contents

1.2 Scope of Work

The main objectives of the overall research project are as follows:

- To identify the range of parameters which need to be considered.
- To determine and, if necessary, develop an appropriate computational tool to enable the problem to be addressed sufficiently accurately.
- To validate the methodology and apply it over an agreed range of parameters.
- To produce a computer model to enable HSE to calculate the effects of turbulence and other flow effects in the vicinity of buildings on the source configuration from the vicinity of the building with reasonable confidence.

The project has been divided into 4 distinct parts in order that progress can be monitored adequately. These are:

a) Feasibility study
b) Methodology development
c) Application of methodology
d) Development of a usable tool

This report presents the results of the feasibility study, which has included an extensive information gathering exercise. This has been undertaken both by personal contacts and by formal literature review, with the objectives of identifying appropriate computational models and test data for validation of those models. The output from this first phase, as reported here, covers the results of the various reviews, and also gives recommendations for the scope for Phase II of the study.

1.3 Test Cases

The first part of this study has involved consultations with HSE to ensure that the problem to be considered is well defined. The starting point was an understanding of the required range of applications, and the way in which the results of the study would actually be used.

It is clear that a primary application will be to undertake a test case which links this project with the parallel study 'Dispersion of Releases of Hazardous Materials Within Buildings'. Output from that study will be a time-varying release rate and concentration of gas entering the wake or other area adjacent to the building (eg. from a roof vent). One of the main cases under consideration in that study is the effects of release of around 3kg/s of chlorine into a building of volume of order $1000m^3$.

Further potential applications which were discussed at the kick-off meeting include liquid chlorine releases from tanker deliveries adjacent to a building. In this case, there is likely to be an evaporating pool which will release chlorine at low momentum into the wake. Releases from bunded vessels are also included, giving the more symmetrical wake flow patterns associated with a circular cylinder, and possibly including the effects of a bund wall on the turbulence, and on the pool evaporation.

Contents

In all these cases, releases may be continuous or instantaneous, but are more likely to be time-varying. This will be an important requirement for any model which is developed.

After the release rate, the next most significant parameters relate to the geometry of the building from or near which the release occurs. In order to ensure that realistic conditions are used, it was decided to use actual chlorine storage buildings as examples. At an early stage of the project, two such buildings were identified, both of which were on water treatment (chlorination) sites for which WS Atkins had provided significant input to the CIMAH Safety Cases. These buildings are rather different in their sizes and locations relative to other parts of the sites, and are described briefly below:

Site A

The site in the Midlands, adjacent to a motorway. The chlorine room, containing 2 x 30t chlorine tanks, is located in the central portion of a large 'U' shaped building of overall length 120m. This building is set about 100m to the East of a reservoir, whose edge is raised a few metres relative to the ground around the building. The motorway passes about 60m to the East of the building, on an embankment of about 2m height. The nearest residential areas are just beyond the motorway, to the East.

Site B

This site is located in the North West, on the edge of a residential area. The chlorine room is located near one corner of a block-shaped irregular building whose overall dimensions are around 50m x 50m. The room itself is a cuboid about 10m x 10m x 8m high, containing 2 x 30t chlorine tanks. Immediately adjacent to the chlorine room is a tanker unloading bay. This area is about 5m x 10m, and can be closed by the operation of a roller-shutter door at one end during unloading. The building is set approximately 200m to the East of a raised covered reservoir. The site is very open to the South, whilst to the North-east, the remaining site buildings give way to an extensive residential area within about 200m.

1.4 Report Outline

The next section describes the methodology which has been used in this review, and this is followed, in Section 3, by a detailed review of the information and data which has been obtained. Although the identification of CFD models was the primary objective of this part of the study, the review also identified some simpler analytical or empirical models which could be adapted to the scenarios under consideration; these are discussed in Section 4. The main review of CFD modelling and relevant applications is given in Section 5, whilst the recommendations, including the programme for Phase II, are given in Section 6. Section 7 completes this phase of the study by presenting conclusions.

Contents

2. METHODOLOGY

2.1 Areas of Interest

This phase of the study aimed to identify relevant information, and to provide a review of that which was considered appropriate to the subsequent phases of the study. Whilst the CFD modelling aspect was a key part of the study, there were other areas of interest which were also considered and drawn into the review. These relate to the acquisition of validation data, and the identification of 'simple' models. The objectives of the information gathering exercise in each of these areas are discussed below:

Data acquisition

It is clear, from even a cursory scan of the relevant literature, that many papers have been written giving CFD predictions for flows around buildings, but very few have provided adequate validation. Indeed, one of the main charges levelled against CFD is that it is frequently used beyond its range of validation. One of the primary objectives of this phase of the study was therefore to identify useful sources of validation data which would be appropriate to the development of a CFD model for dispersion in the vicinity of buildings. The following types of data were reviewed, as discussed in Sections 3.2-3.4:

- flow around 2D obstacles
- wind tunnel data for cubes
- wind tunnel data for various building shapes and topography
- studies of dense and buoyant releases near buildings
- field and full scale measurements of flow and dispersion around buildings.

The notation adopted when discussing the data is illustrated in Figure 2.1. The length (l) of the building is taken to be the along-wind dimension, the width (w) the across-wind dimension, and the height is h. For a cube, l=w=h whilst, for a quasi-2D obstruction, $w >> l$. For non-normal incidence, the distinction between l and w is less clear. However, most studies for which data for a non-normal flow direction is included also give results for normal incidence, enabling l and w to be defined.

Simple models

There are some specific areas of application where the presence of a large amount of wind tunnel data has enabled semi-empirical models to be developed. In other areas, field data have led to the development of empirical or semi-empirical models. Relevant areas where such models exist have been highlighted, and those which could usefully be extended to the problem under consideration identified.

CFD modelling

One of the main objectives of this phase was to review the current status of CFD modelling, and to assess the requirements for further modelling in the subsequent phases. As noted above, there are many papers published giving CFD applications, most of which utilise standard, general purpose, computer codes. The review has therefore been selective, and covered only those of greatest interest to this problem.

Contents

However, the review has also covered those applications which, whilst not directly applicable in all respects, have covered some parts of the problem. These have included:

- dense gas dispersion
- flows around buildings and obstructions
- atmospheric boundary layer simulation
- predictions of surface pressures on buildings

2.2 Identification of Work in Progress

In order to ensure that the results of this study were as useful as possible, it was considered appropriate to identify researchers in relevant fields, and to ascertain the current status of their research. Appropriate contacts were made, either those already known personally to the WS Atkins project officer, or to the HSE responsible officer, or those identified from them. In most cases visits were made to the appropriate institutions and a summary of the outcome of these visits is presented below in Table 2.1.

Organisation	Contact	Subject	Classification			
			E		M	
			S	F	E	N
Cambridge CUED	Dr R.E. Britter	Dense gas dispersion	✓		✓	✓
Surrey University	Dr. A.G. Robins	Dispersion in building wakes	✓			
Warren Spring Lab	Dr. D.J. Hall	Dispersion in building wakes	✓			
Silsoe	Dr. R.P. Hoxey	Dispersion in building wakes		✓		
Shell Research	Dr. P.T. Roberts	Roughness effects on dispersion	✓			✓
BP Research	Dr. T. Moros	Smoke dispersion offshore		✓		✓
Hertford Univ.	Dr. A.E. Holdo	Smoke dispersion offshore	✓	✓		✓
UMIST	Dr. H.L. Higson	Concentration fluctuations in wakes		✓		

Table 2.1 Summary of relevant current research

Note: The classification columns follow those used in the 'Dispersion Within Buildings' report (WSA/8005). i.e.

Experimental - small scale
- field or full scale
Modelling - empirical or integral
- numerical

2.3 Literature Review

Although the subject of CFD modelling of wake releases had not previously been studied in any research contract funded by HSE, a large amount of relevant work has been undertaken, notably by SRD. Recent CEC/HSE funded studies have resulted in reports by **Brighton et al (1993)** and by **Jones et al (1991)**, both of which relate to dense gas dispersion affected by obstacles. The first of these provides a particularly useful review of relevant data, some of which was obtained for this study.

Contents

A literature search was also undertaken, which involved collecting published information and assessing it technically to provide an overview of recent research and to make recommendations. Information was collated from a number of sources, as indicated in Sections 2.2 and 2.4.

In view of the fairly well defined areas of interest, it was found that existing information held by WS Atkins, and references provided by the contacts noted in Section 2.2, yielded a large amount of useful data. This was supplemented by reference to journals which were expected to contain a high proportion of relevant papers, such as the Journal of Wind Engineering and Industrial Aerodynamics. Conference proceedings, from recent events focusing on gas dispersion, consequence modelling and risk assessment, were also scanned for relevant information.

In addition, searches were conducted on the following on-line computerised database systems;
- BRE 'BRIX/FLAIR'
- 'COMPENDEX'

A range of selected keywords, as shown in Appendix 1, was applied to each on-line computerised database. Appendix 2 gives the resulting list of references, including those which were generated from these searches, those already held by WS Atkins, and those identified through the contacts indicated in Table 2.1.

2.4 Information from Software Vendors

One of the objectives of this phase of the study was to recommend an appropriate CFD model for further use and development within the subsequent phases. In order to ensure that the most up-to-date information was obtained, the following software vendors were approached:

Vendor	CFD code
CHAM	PHOENICS
Fluent Europe	FLUENT
Flomerics	FLOVENT
Harwell CFDS	CFDS-FLOW3D
CD	STARCD
Flow Science	FLOW-3D
ACE	FIDAP
Nuclear Electric	FEAT
ESI GmBH	PAM-FLUID

A standard letter was sent to the relevant contact in each organisation, requesting sufficient information to enable WS Atkins to ascertain the suitability of each code for the problem under consideration.

The information provided by vendors varied in both quality and quantity. However, for some of the codes mentioned in this study, namely FLUENT, STAR-CD, FLOW-3D (Flow Science) and FEAT, being codes familiar to WS Atkins staff from past CFD projects, it was supplemented by user manuals.

The review of this information and conclusions are presented in Sections 5.3 and 6.2 respectively.

Contents

3.0 DATA ACQUISITION

In this section, a brief review is given of the data sources which have been examined to determine how useful they might be in providing validation for any CFD modelling undertaken in this project. The summary begins by identifying the work currently being undertaken by researchers in the United Kingdom, and continues with a review of published data in the open literature.

Many authors have produced reviews of data available from laboratory, field and full scale experiments on dispersion in the vicinity of buildings. Notably, **Foster & Robins (1986)** provided a detailed review of the effects of buildings on low-level discharges, generally aimed at the assessment of releases from nuclear power stations. **Benodekar et al (1985)** produced a report which described the CEC programme for developing a general computer method to predict flow and dispersion around buildings, with consideration given to the buoyancy of the release and atmospheric stratification. Tables 1 and 2 from this report provide an excellent summary of many of the wind tunnel and field experiments up until around 1983 on flow and dispersion around bluff bodies.

Section 3.1 covers current research, whilst the following sections (3.2-3.4) present details on some of the experimental data which is considered to be of most relevance to the current project. The conclusion of Section 3 is a short summary of those data sources which are considered to be of most relevance to the current project, particularly in terms of validation for CFD modelling.

3.1 Current Research

There are a number of people and organisations within the United Kingdom who are currently interested in dispersion in the vicinity of buildings. These people have been contacted to determine the nature of their current research and the potential for useful data being made available.

<u>Central Electricity Generating Board/Surrey University</u>

Over the years, the Central Electricity Generating Board (CEGB) conducted a considerable amount of work to investigate the effects of buildings. Dr Alan Robins of Surrey University, formerly of the CEGB, provided a substantial amount of useful information on his previous work, but at present he is heavily involved in setting up the new ENFLO facilities at Surrey University. The wind tunnel and towing tank are currently being commissioned, and there is a significant amount of work that will be undertaken using these facilities. This includes a project for British Nuclear Fuels (BNF) plc to investigate the dispersion of releases over a complex site, such as that at Sellafield. The effects of atmospheric stability will be investigated using the stratified flow wind tunnel to extend work previously undertaken for neutral conditions. Dr Ian Teasdale of BNF plc is currently working on the analysis of previous wind tunnel studies at BMT, which concentrated on stack releases, usually at greater than 1½ building heights in neutral conditions. The results are being reviewed and compared with the predictions of simple models such as R-91 and UK-ADMS. This work will not be reported until later this year. BNF plc are not using any CFD modelling to investigate these topics, nor do they have any definite plans for field/full scale tests.

Contents

Warren Spring Laboratory

Dr David Hall of the Warren Spring Laboratory was also contacted as he has done a considerable amount of work in this area over the last 15 to 20 years. He is currently completing two EC projects, one of which is specifically concerned with the dispersion of plumes from fires. Some preliminary results from this work were presented at the WS Atkins / IChemE symposium on CIMAH Safety Reports for Warehouses at Chester in March 1993, and more detailed results should be available shortly. Wind tunnel results are being obtained for three different building configurations:

i) Smoke released through small openings
ii) Roof vents removed
iii) Roof disintegrated

There is a limit to the heat release in the plume depending on the degree of ventilation. For i) it is of the order of 1 MW. For other cases, the relative effects of buoyancy and momentum differ, and for all cases the presence of the building has some effect. Measurements are mainly in the near / medium field.

Dr Hall also undertook some wind tunnel work about 9 years ago which has not been fully reported. This involved buildings of square cross-section, but of varying cross-wind dimensions, in order to assess the effect of building width. For $w/h < 3$, the wake was found to be 3-dimensional, whereas for $w/h > 7$ the wake becomes quasi 2-dimensional and is more closed in form, with fresh air only able to enter at the edges, and resulting in higher concentrations near the centre line than expected. The effect of building orientation to the flow was also considered.

Chemical, Biological and Defence Establishment and UMIST

Dr Chris Jones of the Chemical, Biological and Defence Establishment at Porton Down informed us that they are sponsoring field trials at UMIST by Professor Richard Griffiths and Dr Helen Higson, who have provided some useful information. In addition to their reported work (see Section 3.3.1 for details) they have recently undertaken further experiments, using a 2m cube as the model building, which were conducted at Dugway Proving Ground in Utah, USA. Propylene tracer gas was released at various locations close to the cube, to investigate the effect of sources inside and outside the recirculating region.

A series of experiments during 1993 at Altcar were conducted using a continuous point source of propylene, released either above the centre of the roof of the rotatable building, or at ground level at the centre of the rear face of the building. The mean flow direction was normal to either the long or the short face of the building. Detectors were located across the wake at downwind distances varying from 2h to 20h, where h is the height of the building.

The future programme of work involves mapping the concentration field around the main rectangular structure of the Altcar rotatable building. Propylene will be used as the source (simulating a non-buoyant release) with UVICs as the detectors. The UVICs have a response time of approximately 1/50 second and are therefore able to detect concentration fluctuations. A variety of source locations will be considered, including upwind sources, sources in the wake region and sources above the roof.

Contents

Several orientations of the building relative to the mean flow direction will be considered.

Cambridge University Engineering Department

Dr R.E. Britter has been active in the field of dense gas dispersion for a number of years, with much of his work funded by HSE. His current interests include both CFD and simpler modelling using the shallow water equations. This latter work is aimed at the problem of dense gas dispersion over complex terrain, for which relatively shallow gradients will ensure that the wake effects, as produced by buildings, will not be evident.

The CFD modelling is currently following 2 avenues. Direct Numerical Simulation is being used to represent the McQuaid experiment on dense gas injection into a boundary layer. Whilst DNS has been considered in this review (see comments in the CFD guide) it is not considered appropriate to the building wake problem in its current state of development. The other area of research which is more relevant is the modification of the k-ϵ model to 'mimic' the Reynolds Stress model for smoke dispersion applications.

Silsoe Research Institute

SRI are currently undertaking a range of dispersion studies both inside and outside buildings. These are led by Dr. R.P. Hoxey, with Dr. B. Harral undertaking CFD development and Mr. C. Boon performing experiments. Whilst most of the work so far has been for internal flows, it is intended to undertake full scale tests of dispersion from a building during 1994. The primary application is to odours from pig houses, and the releases will represent buoyant gases such as methane and ammonia.

The experimental studies are being supplemented by CFD development. This is currently leading to the consideration of Reynolds Stress Modelling, at least for internal flow applications, in order to resolve the observed anisotropies in the turbulence field.

Shell Research

The dispersion group at the Thornton Research Centre, led by Dr. P.T. Roberts, is active in a range of areas, including dense gas dispersion and smoke movement around offshore platforms. Much of their recent work on obstructions has been in the characterisation of building complexes as roughness, and the significant effects of that roughness on the dispersion of dense gases.

BP Research

Dr T. Moros of BP Research Sunbury is heavily involved in the current series of studies of smoke dispersion on offshore platforms. This includes field studies (releases on actual platforms), wind tunnel tests and CFD. It was found that W/T and CFD gave about the same levels of accuracy when compared with full scale, with slightly greater variability of concentrations in the wind tunnel case. The CFD has been undertaken using FLUENT with the standard k-ϵ turbulence model. They have also used CFD to model flows over a floating roof storage tank, in which the greatest inaccuracies occur when the lid is at the top, and there is no recirculating cavity.

Contents

University of Hertfordshire

The primary applications of the work of Dr. A. E. Holdo is the ventilation of offshore modules. However, his interests also extend to smoke dispersion offshore, and he has undertaken small scale experiments and CFD modelling. The FIDAP code has been used for CFD, and studies have included tests on the sensitivity of results to inlet conditions of k and ϵ, primarily for internal flow configurations.

Building Research Establishment

Richard Walker and Martin Smith of the Building Research Establishment (BRE) were also contacted, but most of their work relates to dispersion inside buildings. However, BRE are doing some related work such as looking at the effects of the proximity of nearby buildings on cigarette smoke movement inside a room. They are also undertaking measurements which will link internal flows with external wind measurements.

WS Atkins et al

WS Atkins, Surrey University, HSE, EdF and NCSR Demokritos are currently involved in a joint CEC project to investigate uncertainties in dispersion modelling, which may also generate useful data for use in CFD validation. The project aims to study the variation of results from computer models and wind tunnel tests used in consequence analysis studies as part of safety investigations. The project will focus on near-field gas dispersion, including dense gas dispersion in the wake of buildings or process plant.

3.2 Experimental Laboratory Data

Wind tunnels have provided the largest source of data for the study of dispersion in the vicinity of buildings. This is undoubtedly because they provide a controlled environment in which to conduct experiments, in contrast to the real atmosphere which is constantly varying. Furthermore, studies in wind tunnels tend to be more cost effective, although it should not be forgotten that they do not always correspond to reality so well as field experiments or full scale data. There have been some studies using water flumes and towing tanks, which are particularly useful for stratified flows at low wind speed, but in general, wind tunnels have produced the most interesting results. In the following subsections, a review of relevant data, principally from wind tunnels, is presented. The literature has been divided into various topics, and it is noted that some data is relevant to more than one topic.

3.2.1 2D Obstacles and Cubes

2-Dimensional Objects

There is a considerable body of work which considers the flow and dispersion around 2-dimensional obstacles, such as a simple fence (see for example **Meroney (1993)**). Whilst such work is of interest, and is well suited to simple modelling (both in the laboratory and in CFD modelling), it is not directly relevant to the current study which is principally aimed at the flow and dispersion around 3-dimensional buildings. However, it should be noted that there are some buildings, such as that at Site A, which are almost 2 dimensional for certain wind directions in that their width (cross-

Contents

wind) is considerably greater than their length or height, and so a 2-dimensional analysis may be appropriate in these cases.

However, it is evident that, even for obstructions which are effectively 2 dimensional for a particular wind direction, there will be a range of other wind directions for which 3D effects are important. Vertical cylinders evidently give 3D flow effects but have no directional dependence. Since this is an unlikely shape for a typical building obstruction (although it may represent such plant items as storage tanks), attention is next focused upon the simplest 3D building shape, a cube.

Wind Tunnel Data for Cubes

A wide variety of building shapes have been investigated in wind-tunnel studies, but the most commonly studied 3 dimensional object is a simple cube.

Ogawa et al (1983) conducted wind tunnel experiments on flow and diffusion around a cube. Non-buoyant tracer gas was released from the centre of the cube roof at low exhaust velocity. The experimental program considered four roughness cases, and five wind directions (0°, 10°, 20°, 30° and 45°), although not all the results are presented. The results include normalised concentration contours on the ground and on the cube surfaces.

Robins & Castro (1977b) describe an investigation of dispersion in the vicinity of a cube mounted in an atmospheric boundary layer. The following cases were considered:

i) releases from a porous cube;
ii) releases from sources in the surface of the cube;
iii) releases from stacks (at 1.5 h in centre of roof).

The releases from the surface of a solid cube were as follows:

a) low level point source (at a height of 0.125h);
b) high level point source (at a height of 0.875h);
c) roof centre point source

The ground level centreline concentrations were measured for a wide range of wind directions, effectively giving releases on upwind, downwind and side faces, and concentration contours are given for the stack release case.

Robins (1975) reports the above work in more detail, including concentration contours on the centreline and at ground level for the rooftop release at 0 and 45° building orientations. **Robins (1985a)** discusses the effect of source location in greater depth and considers the influence of stability effects.

Fackrell (1984a) describes a data set produced by Dean & Robins in the Marchwood Engineering Laboratories wind tunnel using a 1.2 m neutral boundary layer with rural type roughness. A number of rectangular building shapes were considered, including simple cubes. One such cube was chosen for consideration by Fackrell, i.e a 27 m cube (full scale at 1:300) with release heights of 0, 27 and 38 m. Wind directions normal and at 45° to the faces were considered.

Contents

Fackrell also considers the data set produced by **Hatcher & Meroney (1977)** for a 1:200 scale model of the EOCR reactor at Idaho Falls. The reactor is approximately represented by a 23 m cube. Ground level concentrations were measured for three release points and at 45° intervals over the complete range of wind angles for neutral, stable and unstable flow conditions.

Hunt & Castro (1984) investigated cubic models with a range of equivalent full-scale sizes from 50 to 200 m. The cubes used in the wind tunnel were of dimensions 25, 50, and 100 mm. A light-scattering technique was used to measure the residence time of a particulate tracer within the building wake, but no concentration measurements were made.

Li & Meroney (1983a&b) examined the dispersion of effluent plumes emitted from roof vents for a cubical model building. The study was undertaken in a wind tunnel with a neutrally stratified shear layer, and mean concentration measurements were made on the 5 cm model building for three different roof vent locations and three different building orientations. Results are given in the form of concentration isopleths on the building faces. The three roof vent release locations considered were:

i) at the centre of the roof;
ii) near the upwind edge of the roof;
iii) near the downwind edge of the roof.

The orientations considered were with the building face at 0°, 22.5° and 45° to the direction of the incident wind. In addition to the building surface concentration measurements, transverse concentration contours are given at 1 to 5 building heights downwind for the central roof vent release, and longitudinal centreline concentration isopleths are also given for this case. Details are also given of vertical mean concentration profiles in the near wake region for the central roof vent release at building orientations of 0° and 45°.

Dawson et al (1987) report measurements made by Thompson & Lombardi of the concentration field resulting from a roof top emission from an isolated cubic building in the EPA meterological wind tunnel. The model was a 0.18m cube placed in a 1.8m deep simulated neutral atmospheric boundary layer. The release was emitted with negligible momentum and negligible buoyancy. Vertical and lateral (ground level) concentration profiles are given at 2, 5 and 8 building heights downwind.

Robins & Fackrell (1983), in their Figure 6, provide non-dimensionalised ground level concentrations contours for a cube at 0° and 45° orientations to the wind. The sources were located immediately downwind of the buildings at a height of h/4, and the emissions were directed towards the building.

Wind tunnel data for cubes are also presented by **Barrett et al (1978)**. This study demonstrated the variation in the effective stack height of a chimney located at various distances downwind of a cube set at 45° to the flow. This included velocity and turbulence profiles downwind on the building centreline. The height of the chimneys varied between 1 and 2 building heights, and they were located at up to 24 building heights downwind of the cube. The study demonstrated the short stacks close to the building result in the highest ground level concentration, and that the

Contents

building influence is still evident at downwind distances as great as 24 building heights.

Koga & Way (1979) also investigated the effect of stack height and position on dispersion in the building wake of a cube using smoke visualisation and concentration measurements. Various release locations on the surface of the cube were studied, and shown to have a significant effect on the local ground level concentrations. Centreline profiles of ground level concentration are given for roof vents located at the upwind and leeward edge of a cube at 0° to the flow, and also for 4 different roof vent locations with the flow at 45° to the building.

Olivara & Babuska (1990) demonstrated the use of a video camera and digital image processing for the analysis of dispersion in the wake of a cube in a wind tunnel. Smoke releases were made from a central roof vent, and a laser sheet was used to provide instantaneous or time averaged concentration patterns in selected vertical and horizontal planes.

Thompson (1993) presented wind tunnel results for dispersion around cubes and other simple cuboid shapes. The primary objective of the study was to determine downwash effects on elevated plumes; other relevant effects are discussed further in the next section.

3.2.2 Simple Building Shapes

Since it is relatively uncommon for real buildings to be shaped as simple cubes, many wind tunnel studies have been aimed at an assessment of simple rectangular cuboid buildings, which are more likely to correspond to real structures.

Fackrell (1984a) reports the experiments by Dean & Robins conducted in the Marchwood Engineering Laboratories wind tunnel using a 1.2m neutral boundary layer with a rural type roughness. The buildings examined were of simple rectangular shape: three were of square plan form with ratios of width (and hence, in this case, also length) to height of 1/3, 1 and 3 and the rest were of square section transverse to the flow of various cross-flow widths from ½ to 8. Releases were made from a roof top source or a stack located in the centre of the building roof, or from a ground level source immediately behind the building. The cases reported by Fackrell are summarised in Table 3.1 below.

Fackrell (1984a) also reports the wind tunnel study for an AGR nuclear power station (by Fackrell & Robins) conducted in the same boundary layer flow as the above. At full scale, the reactor building is 70m high and 40 by 110m wide. Although there are other smaller buildings nearby, the reactor hall is assumed to dominate the flow. Concentration measurements were obtained for a complete range of wind directions at 45° intervals and Fackrell provides graphs of how the centreline ground level concentration varies with distance downwind.

Contents

Building w x 1 x h (m full scale at 1:300)	Release Heights	Orientations
9 x 9 x 27	0, 27, 38	0, 45°
27 x 27 x 27	"	"
81 x 81 x 27	"	"
13.5 x 27 x 27	0, 27, 40.5	0°
54 x 27 x 27	"	"
135 x 27 x 27	"	"

Table 3.1 Wind tunnel cases studied by Fackrell (1984a)

Robins & Fackrell (1983) in their Figures 7 and 8, provide ground level concentration contours for square cross-section buildings of length 2h and 4h for building orientations of 0°, 45° and 90° to the flow. The sources were located just downwind of the buildings, at a height of h/4, and emissions were directed towards the building.

Vergison et al (1989) describe a study carried out at the Von Karman Institute for Fluid Dynamics and the Solvay Research Laboratory in Brussels. The main purpose was to develop a mathematical model to describe downwind dispersion of gaseous release, employing both theoretical and experimental study. Some validation work was done for simple 2-dimensional and 3-dimensional obstacles, and factors such as release at various points on the building surface.

Hunt & Castro (1984) report experiments with sharp edged flat plates, cubes and wedges with the apex pointing upstream. Residence times for material released into the wake were measured, but no direct measurements of dispersion were made.

Hall (in **Robins (1985b)**) describes a series of wind tunnel experiments using simple block shape buildings of dimensions h x h x w, for aspect ratios (w/h), in the range from 1 to 25, where w = cross-flow width. The passive source was located in the centre of the rear face and concentration measurements were made at ground level along a line parallel to the rear face and h/2 from it. Experiments were undertaken for wind directions between 0° and 45° (normal to the long face).

Huber (1989) presents the results of a wind tunnel study on the influence of building width and orientation on the concentration profiles in the near wake of a building. The effects of building widths were examined for aspect ratios (w/h) from 2 to 22 and for building orientations from -30° to 60°. The release was either at ground level or 1.5h at the centre of the lee side of the building.

Huber (1991) describes wind tunnel studies on various square cross-section buildings with a crosswind width of twice the building height. Four building sizes were investigated, from 0.05m to 0.3m in height, in both a low-turbulence and a simulated atmospheric boundary layer with four different flow speeds. All measurements were made with the flow normal to the long building face. Details are given of the velocity and turbulence profiles at various locations. Plume centreline concentrations and profiles are presented for ground level tracer releases from the centre of the leeward face. The effects of the relative building size and the different boundary layer flows were demonstrated.

Higson (1993) and **Higson et al (1993)** describe some wind tunnel work by Hall which was undertaken to provide a comparison with the field data being collected by UMIST, which is outlined in Section 3.2.2 below. The wind tunnel data include non-dimensionalised mean concentrations for a number of locations on the building surface for four different building orientations. The releases were at 3 different distances upwind of the building, and the reported data refer to the cuboid building with the L shaped penthouse mounted on the roof.

Lee et al (1991) describe a video image analysis system to measure the vertically integrated concentration downwind of various model building shapes in a wind tunnel. The smoke concentrations were calibrated using an ethane tracer. The basic building geometry was a 10cm cube, but nine variations were also tested in which the building was made taller (h=20, 30 and 40cm), longer in the flow direction (L=20, 30 and 40cm), and wider in the crosswind direction (W=20, 30 and 40cm). Three source locations were tested for each building geometry:

i) source at ground level downstream of the building;
ii) source at ground level upstream of the building;
iii) source at top centre of the building.

Time averaged contour plots are presented for selected cases, as are some instantaneous results.

Wilson & Britter (1982) present results for the building surface concentrations for a variety of cuboid shaped buildings for the following source locations:

i) upwind sources;
ii) surface sources;
iii) downwind sources in the near wake;
iv) short roof-mounted stacks.

Huber & Snyder (1982) used a wind tunnel simulation to investigate the effect of various release heights for stacks located at the centre of the lee face of a cuboid building with it length equal to twice its height and width. Longitudinal and lateral ground level concentration profiles are presented.

Thompson (1993) reports wind tunnel results for cuboid buildings varying from a simple cube to aspect ratio w/1 = w/h = 4. Results are presented in terms of the 'building amplification factor', which provides a measure of the downwash effect. The release locatio was varied, with the minimum release height being h/2, and the closest downwind location being a distance h from the rear face. Results from this release configuration, for each of the 4 building shapes used, were presented in non-dimensional form, and, with suitable interpretation, shown to conform to the simple model of **Wilson & Britter (1982)**.

Contents

3.2.3 Wind Tunnel Data for Complex Building Shapes

Wind tunnel modelling is commonly used to assess the flow and dispersion around particular buildings. The data from these studies may be of limited use as they refer to very specific building geometries, but nevertheless, some details of the sort of data available are presented below. Many of the studies have concentrated on dispersion in the vicinity of power stations, particularly nuclear power stations. These studies have been aimed at improving our understanding of both the normal continuous releases and accidental discharges from sources close to large buildings.

Baechlin & Plate (1986) and **Baechlin et al (1991 & 1992)** have described the dispersion of accidentally released gases in a built up area. A 1:500 model of 6.6km^2 of industrial plant was placed in a thick boundary layer wind tunnel and passive releases were made at various source heights within the complex. Concentration measurements were made and compared with the results obtained using uniform surface roughness.

Hatcher & Meroney (1977) report wind tunnel studies on a 1:200 model of the reactor building and nearby structures at the Idaho National Engineering laboratory. The study consisted of releases from the base of one face, centre rooftop and a low level stack. In each case the release rate was maintained at low rates such that no appreciable jetting or plume rise was present. The measurement programme was repeated for cases of moderately unstable, neutral, moderately stable and stable conditions in the wind tunnel, in 8 wind directions. Concentration distributions in the wake were obtained and compared with the predictions of several analytical and semi-analytical models.

Diener (1991) provides some details on wind tunnel tests of fences and vapour boxes, as part of an HF mitigation programme. One objective of this work was to assess the effect that obstacles in an industrial plant could have on the dispersion of a heavier than air cloud. The results are unlikely to be of much use in the present study as they do not relate specifically to buildings.

Fackrell (1984a) summarises some of the work by **Hatcher et al (1978)** and that by **Fackrell & Robins (1981)**, both of which consider building wake dispersion at nuclear power station sites.

Fackrell & Robins (1981) describe the wind tunnel tests carried out for an AGR site. Most of the releases considered were passive, from roof top and ground level sources. Detailed ground level concentration measurements, and vertical profiles were obtained for different wind directions. Some consideration is also given to the effects of source momentum, buoyancy, transient releases and concentration fluctuations.

Robins & Fackrell (1983) present some wind tunnel results of the variation of the concentration at a few fixed receptors for a complete range of building orientations for three particular source locations. The building used for this study was relatively simple block model of a power station, including just the reactor building and turbine hall. This work is described in more detail in **Fackrell & Robins (1981)**, as discussed above.

Robins (1985a) gives details on the variation of concentration with wind direction, source location and fetch for Oldbury Power Station, based on wind tunnel studies.

Contents

Further details are given in **Foster & Robins (1986)**. **Foster & Robins (1985 & 1986)** describe the full scale and wind tunnel experiments carried out for Oldbury Magnox nuclear power station. As for the AGR study, detailed ground level concentration measurements and vertical profiles were obtained for different wind directions and a variety of source locations. The results are compared with field measurements. **Robins (1985b)** presents some selected result from the Oldbury study.

Hoydysh & Dabberdt (1992) describe studies on a rectangular power plant model in an atmospheric boundary layer wind tunnel. Neutrally buoyant gas mixtures were released from two locations at the ground surface in the centre of the leeward face, and from the centre of the mid-level roof. Concentrations were required at the ground surface along six arcs and along two vertical profiles in the centreline of the wake. Results are given in terms of normalised downwind concentrations and plume spreads.

Janssen (1979) investigated the dispersion of odours in the vicinity of pig houses using a model in a boundary layer wind tunnel. Results are given for various combinations of boundary layer conditions, emission heights and conditions. Some consideration is also given to the effect of surrounding houses. Results are given in terms of the variation of non-dimensionalised concentrations with distance downwind.

MacDonald et al (1988) describe the wind tunnel experiments for Hinkley Point power station carried out with buoyant and non-buoyant releases. Ground level concentration profiles were measured at a range of locations for various wind directions, and the results compared with full scale measurements.

Thuillier (1981) describes a wind tunnel simulation of the Duane Arnold Energy Centre nuclear power plant, to complement full scale observations. Various release locations within the complex building structure were considered, and the results were compared with standard empirical models and full scale measurements.

Dispersion Influenced by Topographic Effects

A significant amount of research work has been conducted to investigate the effect of terrain on dispersion, and models have been developed for such situations. Some of this work is of interest when considering the effect of buildings, but it is generally not directly relevant to the scope of the present study, one reason being that sharp edged buildings will induce flow separation, which is not generally a characteristic of flow over terrain.

Examples of terrain influence dispersion studies can be found in **Ohba et al (1988)**, **Robins (1985b)** and **Snyder (1990)**.

3.2.4 Density Effects

Denser-than-air gases

Many toxic and flammable gases are denser than air, either because of their high molecular weight, because they are cold or because they form an aerosol. When the concentration of such gases is sufficiently high, they behave in a significantly different manner to passive emissions, often tending to remain close to the ground, and usually altering the general flow field, particularly close to the source. it is therefore important to consider the influence that building wakes may have on the dispersion of dense gases, and data relevant to this situation are identified below.

Dirkmaat (1981) describes a wind tunnel study to investigate the extent of the heavy LPG cloud resulting from 800,000m^3 spill after a pipeline fracture. The influence of wind speed, surface roughness and simple rectangular block shaped building are considered, and the results are given in the form of 2% (LEL) concentration isopleths at ground level. Some conclusions are drawn on the effect of the building and its position in relation to the source, but they are somewhat qualitative and not likely to be relevant to the type of releases being considered in this study.

White (1986) describes a wind tunnel study of the dispersion of carbon dioxide past a square section 2 dimensional obstacle in an atmospheric boundary layer. This included measurements of the flow field and concentration profiles at various locations, for a ground level area source located just upwind of the obstacle.

Guldemond (1986) presents the results of a wind tunnel study to model the dispersion of the cloud formed after the release of 15 tons of pressurised liquid ammonia on an industrial site. Results are given in terms of flow visualisation and concentration measurements.

Brighton (1986) summarises some wind tunnel experiments by Britter in which a heavy gas was emitted from a ground-level area source of dimensions 50 x 50 mm directly in the wake of flat metal plates mounted normal to a turbulent boundary layer flow. Three obstacles were used with $h = w = 50$, 100 and 150mm. The character of the flow was assessed using smoke visualisation techniques and mean ground level concentration sat distances $x = h$ and 2h on the centreline behind the plate. **Britter (1989)** gives further details of these experiments.

McQuaid (1986) reviews the effects of obstructions on the dispersion of heavy gas clouds, with particular reference to the field trials at Thorney Island and associated small-scale simulation studies.

Heidorn et al (1992) described wind tunnel observations of the spread of a heavy gas cloud with various obstacle configurations, some of which were based on the Thorney Island trials. The cases investigated included buildings upwind and downwind of the release location, as well as a fence, trench, and uniform block array.

Hall et al (1991) describe wind tunnel results for the dispersion of dense gas clouds over fences, based on a 1/100 scale model of the Thorney Island trials. Various source gas densities and fence heights were used. The results include flow visualisations using smoke and concentration measurements at fixed detectors. Fifty repeat experiments were made to determine the variability of the results.

Krogstad & Pettersen (1986) describe wind tunnel experiments for a continuous dense gas release. The resulting gas cloud was investigated both with an unobstructed flow, and with various sizes of rectangular building placed in the dense gas plume, either perpendicular of along the flow. Flow visualisations using smoke provide a good indication of the building effects, and quantitative concentration measurements on the surface of the buildings are also given.

Contents

Meroney & Neff (1982) describe wind tunnel simulations of the China Lake LNG spills. The wind tunnel studies used 1:85 and 1:170 scale models of the China Lake topography and the release was simulated by an argon release in a circular-area source mounted in the model pond. Ground contour plots of peak concentration are given for a number of trials. These experiments did not examine the effect of buildings, but the effects of the circular pond/bund may be relevant to this project.

Buoyant Releases

Some releases in the vicinity of buildings may behave as buoyant emissions. These would include releases of gases with lower molecular weights than air, and also hot emissions, such as those produced in a fire. Generally speaking, buoyant releases are less hazardous than passive or dense gas releases as they tend not to be concentrated at ground level, but it may still be important to assess the effect of the building and to determine the extent of entrainment, lift-off and final rise of buoyant plume.

Hall et al (1980) describe wind tunnel experiments on a release of buoyant gas from a model building 167 x 167 x 333mm in size set with the longest face across the flow. The buoyant gas source was a uniformly emitting rectangle of 167 x 333mm set either in a face of the building or in the ground adjacent to the building. Ten sets of experimental conditions were used to model the required range of windspeeds and buoyancy fluxes. For each set of conditions, ground level centreline dimensionless concentrations are given for the following source locations:

i) source on ground behind building;
ii) source on rear face of building;
iii) source on roof of building;
iv) source on upwind face of building.

Vertical concentration profiles are also given at two downwind distances.

Hall & Waters (1986) extended the above wind tunnel work with a further series of experiments. These included experiments with a cube and with a building with a width of three building heights. Experiments were performed at smaller scales to provide concentrations at extended distances and also with the sources restricted to just a fraction of their original size. The effect of orientating the building at various angles to the flow was also investigated. A number of flow visualisations and concentration contours are provided for selected cases.

Robins (1975 & 1985a) briefly considers releases of varying momentum and buoyancy in the vicinity of a cube. **Fackrell & Robins (1981)** assess the effects of buoyancy and momentum for releases from a ground level source adjacent to a 1/300 scale AGR model. Three source densities and two source diameters were used with various release rates to give a range of buoyancy and momentum fluxes.

Hall et al (1993) describe some of the features of atmospheric dispersion associated with plumes from warehouse fires. The effects of heat release rate, momentum, release location and aerodynamic disturbances around the building were investigated in a series of wind tunnel tests. Ground level centreline concentrations are presented to show the variations with plume buoyancy, plume momentum and various discharge conditions.

Contents

3.2.5 Concentration Fluctuations

Concentrations at a point are usually described in terms of the average concentration over a specified period. Where the concentration does not vary significantly over time, or where the effects of interest only depend on the average concentration, this information may be sufficient. However, there are many cases where the effects, such as the toxic effects of a gas such as chlorine, depends on the toxic load, defined as $\int C^n dt$, where C is the concentration and n is an integer typically between 1 and 2. In cases, where n=2, for example chlorine, the effect of exposure to a particular mean concentration will depend crucially on the fluctuation and intermittency. There have been relatively few studies of such concentration fluctuations in the vicinity of buildings, but some of the principal data are identified below.

Li & Meroney (1983b) described a wind tunnel study using a cubic building in a neutral boundary layer in which concentration fluctuations were measured. The releases were from a central roof vent for buildings with 0° and 45° orientations, and from a downwind roof vent for a building with 0° orientation. The study provided data on the concentration fluctuation intensity at various locations and gave upper limits for the peak-to-mean concentration ratio near the ground behind a model building.

Concentration fluctuations around an isolated building are currently being investigated at UMIST. This work is described in Section 3.3.1 below.

Boreham (1986) describes a preliminary investigation into the feasibility of using bipolar space charge to study the dispersion of pollutants in the wake flow region behind isolated model buildings in a wind tunnel. The effect of the presence of trees was also studied. Measurements were made using a fast response time ion detector and results are given in terms of horizontal and vertical flux profiles at various locations.

Jones & Griffiths (1984) have described full-scale experiments around an isolated hut, using an ionized air tracer technique. This enabled very rapid response concentration measurements to be made, both for a continuous and a pulsed source.

Concentration fluctuations have also been described in **Hinds (1969)** and **Guenther et al (1990)**, and their effects discussed in **Griffiths and Harper (1985)**.

3.3 Field and Full-Scale Experiments

3.3.1 Field experiments

Field experiments provide an additional source of data. The experiments are conducted in the atmospheric boundary layer, and thus may correspond to reality somewhat better than wind tunnel studies in which the boundary layer has to be simulated. However, field trials are less easy to control than wind tunnel studies, and the data is therefore more difficult to collect and may be harder to interpret.

Britter & McQuaid (1988) present some simple algorithms for the assessment of the influence of buildings on dense gas dispersion, and review some of the relevant experiments and field trials. **McQuaid (1984)** provides a brief review of field experimentation on heavy gas dispersion, but none of the studies were specifically

Contents

aimed at investigating the influence of buildings. It is noted that the Thorney Island trials did, however, give some consideration to the effect of barriers and simple building shapes on dispersion. **Havens (1992)** also summarises the dense gas dispersion field experiments undertaken over the last decade, but again, none of the studies, except those at Thorney Island, explicitly considered buildings in a way that would be directly useful in the present study. **Meroney (1993)** describes field and laboratory data on the influence of bluff bodies, such as 2-D fences on the transport and diffusion of hazardous gases, particularly dense gases. Specific data is not given, but many of the main results from related studies are summarised.

Relatively few field experiments have been conducted to investigate the flow and dispersion in the vicinity of a building. A selection of the most notable are mentioned below.

The most recent field experiments include the work currently under way at UMIST, described by **Higson (1993)** and **Higson et al (1993)**. The experiments are being conducted using an isolated rectangular building (1.56 x 4.24 x 10.96 m) with a small L shaped penthouse on the building roof at a flat site near Southport in the north west of England. This building can be rotated relatively easily to place it in the required orientation to the wind. Most of the work has concentrated on passive releases at various locations upwind of the building, with concentrations being measured at a number of positions on the surface of the building. Concentration measurements have been made over 5 minute periods, using a detector system with a response time of about one second. The results provide the concentration fluctuations as well as mean concentrations. **Higson (1993)** showed that concentration fluctuations in the field were greater than those in the wind tunnel, and demonstrated the need for measurement of the turbulent flow field. Details of the comparison of wind tunnel and field data are given in **Higson et al (1993)**.

Current work at UMIST involves the use of sonic anemometers to assess the flow field, as well as concentration detectors with a significantly improved response time. This work should demonstrate the influence of the turbulence scales. The current work is based on the simple cuboid building, without any additional attachments. Section 3.1 gives some further details.

Additional work has recently been conducted in the USA by **Higson et al (1994)** using a 2m cube in flat terrain, with a detector system with a response time of about 1/50 second. Comparisons were made of a range of statistical parameters of the concentration distribution around the building, but this work has yet to be reported.

The upwind building trial of Thorney Island Phase II was discussed by **Deaves (1985)**. In Trial 29 ,the mobile 9m cubic building was placed 27m upwind of the spill point, which was at the centre of the cylindrical gas tent. Some encouraging agreement between 3-D model predictions and full scale results was demonstrated.

Nielsen (1991) describes some dense gas field experiments with obstacles. The preliminary results presented showed that a solid wall perpendicular to the wind direction had a general diluting effect on the gas cloud, but at some positions above ground level the concentration was increased in the presence of the obstacle as a result of increased cloud height. Some limited data and mean gas concentration profiles are given.

Contents

Ogawa et al (1983) and **Ogawa & Oikawa (1982)** report field and wind tunnel studies of the flow and dispersion around a cube in flat terrain. The field studies were conducted using a 1.8m cube, placed on casters to facilitate rotation. The source was of 18cm diameter flush with the surface at the centre of the roof for the emission of SF_6 tracer gas. The results include a number of flow visualisations for varying orientations of the cube, as well as normalised concentration contours on the building surfaces and at ground level from one to four building heights downwind.

Many field experiments have been aimed at assessing the wind loading on a structure. Much of this work has been described in the Journal of Wind Engineering and Industrial Aerodynamics, but as this lies outside the scope of this project it will not be discussed further here.

3.3.2 Full Scale Measurements of Dispersion

There have been relatively few studies of dispersion around full scale buildings, and even fewer which include comprehensive measurements of both the flow field and the concentration field. The studies often relate to specific buildings, and therefore many of the results are not generally applicable and may not be of much use when considering other building configurations. However, the results provide a true indication of the complexity of dispersion phenomena in the real world and do not involve any of the problems associated with smaller scale experiments. It is therefore important that such studies should be included in this review, even if the data is not directly applicable.

Start et al (1977) describe the results of 23 full scale gaseous tracer release tests conducted at the Rancho Seco Nuclear Power Station in California, which is a relatively complex building structure with some nearby topography. Tests were conducted for various windspeeds, directions and atmospheric stabilities with concentration measurements being made on arcs at 100, 200, 400 and 800 m. Significant discrepancies were shown between the measurements and the results of simple analytical models (such as those described in Section 5.2), particularly in the region close to the buildings.

Thuiller (1981) describes two studies on the dispersion of roof vent effluents in the immediate vicinity of nuclear power plants. The studies were conducted at the Millstone Nuclear Power Station (MPNS) in 1974 and the Duane Arnold Energy Center (DAEC) in 1978, and the results were compared with the results of simple analytical models and a wind tunnel simulation of the DAEC experiment. The general conclusion was that popular approaches to modelling dispersion performed poorly for the two sites in question.

Robins & Fackrell (1983), in their Figure 10, summarise the stability effects on near field dispersion of ground level emissions near buildings in full scale field trials. This is also compared with some wind tunnel data.

Fackrell (1984a) provides some brief details on full scale data, concentrating principally on the data produced by Start et al at the EOCR reactor at Idaho Falls. This data has been described above.

Foster & Robins (1985 & 1986) describe work carried out as part of the CEGB building wake study. This included analytical studies, wind tunnel and full scale

Contents

experiments. The full scale data were conducted at Oldbury Nuclear Power Station (approx 150 x 50 x 54 m high). About 20 tracer releases were made, including some from ground level, some from roof height and some from pile cap height (25 m). Concentration measurements were made from 125 m to 700 m and plume profiles were obtained using lidar.

Ramsdell (1990) developed a time-based model for predicting ground level centreline concentrations in the wake of buildings as a result of low level releases. The model is compared against standard wake models and is validated using seven sets of data from nuclear reactor sites.

Moros & Akhurst (1993) have assessed the dispersion of hydrocarbons in tank farms. The quantity of hydrocarbon that leaks from large floating roof storage tanks depends on the pressure distribution and the flow patterns in the vicinity of the tank. Measurements were made at full scale of the hydrocarbon losses from such tanks, and CFD calculations have been made to investigate the flow patterns around the tanks.

Moros et al (1992) of BP have studied the dispersion of smoke from simulations of fires on offshore installations. They have performed a comparison of full scale trials using artificial smoke releases on a North Sea platform with the results of a CFD model. Comparisons were made of both the windspeed and concentrations at selected measuring points.

Huber (1984) provides a useful summary of some full scale experiments on dispersion around buildings. The predictions of three simple analytical models are compared with the results produced in ten different sets of experiments, namely those by:

Islitzer (1965)
Martin (1965)
Dickson et al (1967)
Munn and Cole (1967) (two papers)
Cagnetti (1975)
Johnson et al (1975)
Thuiller and Mancuso (1980)
Start et al (1980)
Engineering Science (1980)

Comparisons are made of the concentration variation with downwind distance. However, most of the above work relates to large structures, such as reactor buildings with very case specific dimensions and release conditions, and it is not considered that the data would be directly relevant to the current project.

Drivas & Shair (1974) report dispersion measurements made in the wake of the three-story Caltech Spalding Laboratory, which is 12m high, 17m in width and 64m long. Concentration measurements were made on the roof for a releases at 6, 12 and 18 m downwind and 0.3 or 1.2 m above ground level.

Hinds (1969) provides normalised ground level concentration contours around a fairly large rectangular building (24 x 35 x 11 m). Comparisons were made between the peak-to mean concentration ratios in unobstructed flow and in the lee of the building.

Contents

Guenther e al (1990) report SF_6 tracer experiments carried out near a large oil gathering facility in the Prudhoe Bay, Alaska, oilfield reservation. At this site, the atmospheric stability and wind speed profiles are influenced by the smooth surface, but the near field dispersion from the site is dominated by the effect of buildings. The study concentrated on the 39 m turbine stack adjacent to a 34 m high building, and so the releases had considerable momentum and buoyancy.

3.4 Wind Tunnel and Full Scale Measurements of Flow Characteristics

In the preceding sections, emphasis has been placed on the concentration data that is available in order to quantify the degree of dispersion. However, the degree of dispersion depends on the nature of the flow field in which the release takes place, including the velocity and turbulence characteristics of the flow. Therefore, many of the better experimental studies provide measurements of the velocity and turbulence at various locations. Such results can be compared between full scale, wind tunnel and CFD predictions, in order to demonstrate whether the features of the flow have been correctly modelled. Information on flows is also often investigated using flow visualisation techniques, and data on parameters such as recirculation lengths and times are sometimes presented.

The table of references in Appendix 1 (Category 11) indicates those authors who have included data on the flow field for their experiments. However, the data is usually fairly brief and of limited value to this current project. The studies identified below present sufficient data to be reasonably useful.

Castro (1973) provides details of the flow around a surface mounted cube in a free stream, whilst **Castro & Robins (1975)** consider the flow around a cube for a thick incident boundary layer. This work is also reported in **Castro & Robins (1977)** and **Robins & Castro (1977a)**.

Huber (1991) provides details of the flow characteristics in the wake of rectangular buildings, both for the low-turbulence boundary layer and for the atmospheric boundary layer.

Ogawa et al (1983) present flow measurements around a cube in both field trials and in a wind tunnel with various surface roughnesses.

3.5 Relevant Data Sets

One of the principal aims of Phase 1 of this project is to identify any data sets which would be suitable for the purposes of validating CFD modelling work. From the preceding sections, there is clearly a wealth of data available but relatively little is likely to be of direct use for the purposes of this project. The main criteria which have been used in assessing the suitability of data have been identified, and are outlined below:

i) The building shape or shapes used in the experiments should correspond to the sort of building configurations of interest (see Section 1.3).
ii) The release locations should be at typical positions of interest.
iii) Release momentum and buoyancy should be well specified.

Contents

iv) The windspeed and turbulence characteristics of the approach flow should be well specified.

v) Measurements of the concentration field should be made in all 3 dimensions. Mean values and concentration fluctuations should be given.

vi) Details of the turbulent flow field around the building should be provided.

There are no data sets currently available which meet all of the above criteria completely, and so it is inevitable that certain compromises must be made, particularly in the case of field trials where the above criteria are virtually impossible to meet fully. In particular, the very few measurements of concentration fluctuations will mean that the latter part of criterion (v) is likely to have to be relaxed. Furthermore, it is clearly necessary to use different data sets depending on which particular configuration is being investigated.

Most of the useful data sets are from wind tunnel studies on cubes and simple cuboid buildings. Cubes are relatively uncommon in terms of the shape of real buildings of interest, and so we shall concentrate on data for simple cuboid buildings. Such shapes are still fairly general, but can be used to approximate many building configurations that occur in industry. Furthermore, the cube is merely a special case for cuboid buildings with $w = l = h$.

Relevant data for passive releases in the vicinity of cuboid shaped buildings are given in the following references:

Robins & Fackrell (1983)
Fackrell (1984a)
Huber (1989 and 1991)
Hall (in Robins (1985b))
Hall (unpublished work, see Section 3.1)

Of these, the work of Huber is perhaps the most interesting.

There does not appear to be any full scale data that would be directly applicable, but the field trials being undertaken by UMIST would seem to be ideally suited to the project requirements. This may involve the use of currently unpublished data from UMIST or may necessitate additional tests to be carried out to a given specification.

For dense gas releases, there is significantly less data available, but the work of **Krogstad & Pettersen (1986)** is of particular interest, as are the Thorney Island Phase 2 trials, reported by **McQuaid & Roebuck (1985)** and **Davies & Singh (1985)**.

Similarly, there is little available good quality data for buoyant releases near buildings, the best currently available being that of **Hall et al (1980)**, **Hall & Waters (1986)** and **Hall et al (1993)**.

The data sets identified above are not intended to represent a complete list of all the work that may be of relevance. Other references may be of use in specific areas and so should not be neglected altogether.

Contents

4.0 SIMPLE MODELS

4.1 Wake Structures

The structure of building wakes has been of interest for some time, with obvious applications to dispersion. The nature of the turbulence enhancement, and the rate of velocity defect recovery downwind have also been studied, with a view to characterising the overall effect of a building, or indeed of a group of buildings, on the incident flow.

A leading figure in this particular field of research has been Prof. J.C.R. Hunt, formerly of the University of Cambridge and currently Chief Executive of the Meteorological Office. Some early studies in this area were reported in **Britter et al (1976)**, in which theoretical considerations of flow and turbulence structures around buildings and hills led to simple predictive methods for dispersion from near wakes, as well as in elevated plumes affected by nearby buildings. Kinematical studies of a more general nature, describing the detailed structure of 3D building wakes, were presented in **Hunt et al (1978)**.

This general description of wake structure was developed further in **Hunt (1981)**, which gave qualitative representations of streamline displacement, vorticity generation etc in relation to buildings and road embankments. The paper also included quantitative results of velocity profiles, velocity defects and turbulence quantities in a range of building shape wakes, including cubes and cylinders. These results are combined with other theoretical considerations to provide simple models of concentration in the wake. **Hunt & Robins (1982)** gave further discussions of wake structure, with particular emphasis on the increased downwash due to delta wing vortices which are generated for non-normal flow incidence (ie. wind angle >15° from normal to a face). They then gave details of modifications to Gaussian plume models for releases on top of or above the building.

Further studies in the late 1970's by **Vincent (1977, 1978)** were undertaken by observing the decay of concentration within the wakes of blocks. Normalised residence times and wake lengths were measured for a range of flow speeds, block sizes and turbulence conditions, enabling a picture of the wake structure to be built up, and a simple wake dispersion model to be developed.

An excellent recent review of the flow characteristics around surface mounted obstacles has been given by **Schofield & Logan (1990)**. Although much of the paper is devoted to 2D wakes, there is a very useful discussion of 3D wakes, particularly emphasising their differences from 2D, such as non-closed recirculation regimes. A very useful schematic diagram of the streamline around a 3D cuboid is given, with suggested vortex generation patterns based primarily upon flow visualisation studies, due to the lack of detailed 3D flow measurements. The paper also provides some discussion of the effects of multiple buildings, on the wake structure.

The final paper considered in this section is **Ramsdell (1990)**. Although this is primarily aimed at providing a wake dispersion model, it does so by considering the detailed turbulence structures of the wake, and is thus unlike any reviewed in Section 4.2. However, the use of this more sophisticated approach is not backed up by experimental validation of the turbulence properties, and validation is only given in terms of rather coarse concentration measurements from power station emissions.

Contents

Furthermore, discussion of this paper by **Briggs et al (1992)** suggests that there is little support for Ramsdell's approach from the main body of the gas dispersion modelling fraternity.

4.2 Passive Releases

One of the most common types of atmospheric dispersion model currently in use is the simple Gaussian plume model, as described by **Jones (1983)**. This type of model is often used to assess dispersion from point sources in an unobstructed flow. The plume is assumed to have a Gaussian profile in both the horizontal and vertical directions with the spreads given by σ_y and σ_z, both of which are functions of the distance downwind as well as factors such as the surface roughness and atmospheric stability. This kind of simple model can be modified to assess dispersion from an area source, such as a building wake, by assuming that the release is from a virtual source some distance upwind of the actual source location. ie the parameters σ_y and σ_z are increased to allow for dispersion in the wake of a building.

Jones (1983) also reviews several aspects of atmospheric dispersion modelling and includes a brief survey of the simple models available for the dispersion of material near a building. Plume rise from a building wake is considered, but no new data or simple models are presented, although some equations for the final rise of the plume are suggested.

Fackrell (1984b) provides an excellent summary of some of the simple theoretical models for building influenced dispersion. These are presented in Table 4.1.

NAME	THEORY	COMMENTS
Gifford (1960)	$C = \dfrac{Q}{(\pi\sigma_y\sigma_z + cA)U}$	A is projected area of building c lies between 0.5 and 2. Only applicable to centreline glc.
Turner (1969)	$\sigma'_{yo} = W/4.3$ $\sigma'_{zo} = h/2.15$	Virtual source height is 0 or h
Barker (1982)	$\sigma'_{yo} = W/3$ $\sigma'_{zo} = h/3$	Virtual source height = h/3 If W > 3h then $\sigma'_{yo} = h$
Ferrari & Cagnetti (1980)	$\sigma_y' = \sigma_y + w/a$ $\sigma_z' = \sigma_z + h/b$	a = b = 2.507 (F&C) a = 2.83, b = 2.36 (Dutch National Model)
Huber & Snyder (1976)	$\sigma_y' = 0.35\ w = (x-3h)/15$ $\sigma_z' = 0.7h + (x-3h)/15$	Valid in region $3h < x < 10h$ For x > 10h a virtual source model is used with the spread matched at 10h

Table 4.1 Simple models presented by Fackrell (1984b)

Contents

Petersen & Ratcliff (1987) have developed an integral plume rise algorithm with modified dispersion coefficients to account for the presence of building wakes. This model has been assessed against relevant data sets and the authors claim that it should perform better than the original Industrial Source Complex model. The ISC models were developed by the Environmental Protection Agency (EPA) in the United States and are one of the most commonly used sets of models throughout the world for the assessment of dispersion from industrial sources.

All the above models are, essentially, simple modifications to the basic Gaussian plume model for unobstructed terrain. An alternative approach is often adopted for concentrations within the recirculating wake downwind of the building (see **Jones (1983), Foster & Robins (1986)** and **Duijm & Webber (1994)**). The concentration (C) within the recirculation zone, length L, is given by:

$$CU_hA / Q = 0.5\,\tau / \lambda \qquad \text{for } x \leq L$$

where τ and λ represent the normalised residence time and length respectively and are given by the following formulae:

$$\tau = \frac{U_h t_r}{h} = \frac{11(b/h)^{1.5}}{1+0.6(b/h)^{1.5}}$$

$$\lambda = \frac{L}{h} = \frac{1.8(b/h)}{(d/h)^{0.3}(1+0.24b/h)}$$

where b and d are the building width and length in the flow direction, and h is the building height.

For b/h < 0.3 the result for b/h = 0.3 should be used, and similarly for b/h > 3 the result for b/h = 3 should be used.

For the main wake region, x ≥ 5h, downwind of the recirculation zone, a virtual source gaussian plume is generally used, with linear interpolation in the intermediate region L < x < 5h.

An excellent review has also been given by **Meroney (1982)**. This discusses the structure of the wake and the influence of source location on the subsequent dispersion. In particular, it provides details of building wake dispersion models which incorporate estimates of concentration distribution *within* the wake, as a function of the 'taut string' distance between the emission and target points. A number of such simple models are presented, along with the appropriate ranges of model parameters.

The review of **Cooper (1984)** was undertaken with specific reference to the requirements of the nuclear industry. It therefore concentrates upon the effects of buildings on elevated passive releases over the medium to far field ranges.

A rather different approach has been adopted by **Ramsdell (1990)**. This involved postulating a parametric equation for the concentration downwind of a building, incorporating the key variables such as windspeed, stability,and then using statistical

Contents

analysis to find the best possible coefficients required to fit the data available. The result was:

$$\text{Normalised centreline concentration} = 84.5\, x^{-1.13}\, A^{-1.25}\, U^{0.72}\, S^{0.473}$$

where x = distance from release point
A = projected building area
U = windspeed at 10 m
S = atmospheric stability class (1=A, 2=B, ...)

This approach has been called into question, particularly because the variables are not all independent, and also one would expect an inverse proportionality to the windspeed.

Another type of model relates specifically to the calculation of building surface concentrations. For example, **Wilson & Britter (1982)** describe a number of empirical relationships to calculate surface concentrations for releases from the following source locations:

i) upwind sources;
ii) surface sources;
iii) downwind sources in the near wake;
iv) short roof-mounted stacks.

More sophisticated models have been developed than those described above, but in general, all these simple analytical models tend to fail in that they are unable satisfactorily to take into account factors such as:

i) the building shape;
ii) the release location;
iii) the building orientation to the wind;
iv) release momentum and buoyancy;

For example, it is well known that ground level concentrations are significantly higher when the incident flow is diagonal to the building rather than normal to it, but most simple analytical models, such as the virtual source Gaussian plume models, fail to take any account of such factors.

Furthermore, such models tend only to predict the mean concentration, and not the nature and extent of concentration fluctuations.

4.3 Non-Passive Releases

There are very few authors who have attempted to produce simple models for the complex phenomena associated with a buoyant, dense or momentum dominated release in the vicinity of a building. The United Kingdom Atmospheric Dispersion Modelling Group (**Jones (1983)**) felt that it was not possible to give a formula for plume rise from a building wake, for plumes emitted either with significant vertical momentum or with significant buoyancy.

Contents

Britter & McQuaid (1988) provide a number of non-dimensionalised relationships which are of interest when considering non-passive releases. For example, suggestions are given as to the criteria which determine the transition between dense and passive behaviour for a gaseous release, and the effect of a fence on an upwind dense gas release is discussed.

Brighton (1986) has suggested a model for dense gas behaviour near a building which involves two layers in the recirculation zone: a lower heavy layer which spreads due to gravity forces, and a less dense upper layer. It is based on an extension of Vincent's simple wake model and involves the use of flux conservation relations in the two-layer wake, as well as some simple assumptions about the turbulent transfer processes and mean flow structure. The model enables calculation of the concentrations in both the upper and lower layer, but requires knowledge of various mixing coefficients.

Tatom (1986) discusses the downwash on buoyant plumes due to the wake produced by structures, but the study concentrates on downwash due to stacks, and does not consider the effect of buildings.

More recently, **Brighton et al (1993)** and **Jones et al (1991)** have reported the results of an extensive CEC/HSE funded exercise on the effects of obstacles on dense gas dispersion. In the event, the emphasis of this work shifted away from buildings and focused upon the effects of fences, and on the changes to dense gas dispersion induced by sloping terrain. The 'simple' modelling which was undertaken for the sloping terrain example included both integral (or 'box') modelling, and use of the shallow water equations.

In addition to their review, **Duijm & Webber (1994)** produced a simple method for assessing the effects of fences on dense gas dispersion. This depends upon the use of a standard 'box-model' for unobstructed dispersion, and matches the height of the plume to that of the fence to give a virtual source. This is clearly limited in application, and makes no allowance for the width of the fence or its porosity, nor even for the density of the cloud, given that a denser cloud is more likely to be blocked.

Contents

5.0 CFD MODELLING

In this section, a brief review is given of CFD modelling applications of wind flows and gas dispersion around buildings. Since much of the terminology is explained in the companion 'Guide to CFD', that report should be referred to where a fuller description is required. A brief explanation of some of the terms relating to turbulence modelling is, however, given in Section 5.3 of this report

5.1 Applications for Flows around Buildings

General Reviews

Laurence & Mattei (1993) review the different approaches for solving turbulent flows from the eddy viscosity approach to large eddy simulation and Reynolds stress transport modelling. They point out that some of the key modelling hypotheses may be violated in the problems of practical interest. For example, for modelling purposes, turbulent flows are commonly assumed to be locally homogeneous, ie. length and time scales >> those of turbulence, but in wind engineering situations it is evident that the scales of gusts may be larger than that of a building.

A number of 'standard' test cases are described, including:

- the backward facing step is probably the most extensively computed test case for turbulent flows, following the ASOFR-HTTM Stanford Conference in 1980. The standard k-ϵ model under-predicts the reattachment length. Improvements can be obtained by adopting Reynolds stress modelling, but have also been demonstrated for the k-ϵ approach by using a low Reynolds number version **(Abe et al, 1993)** or a non-linear k-ϵ model **(Bassara & Younis, 1992)**.

- the surface mounted cube is becoming an increasingly popular test case, using the experimental data of **Castro & Robins (1977)**. **Murakami (1993)** describes a thorough study and shows that the k-ϵ model is inadequate especially on the impinging side, improvements are obtained using a Reynolds stress model, but the most reliable approach is Large Eddy Simulation (LES). The cost ratio between LES and conventional Reynolds Averaged Navier Stokes (RANS) solvers is probably from 100 to 1000. Many of the characteristics of the cube (such as impinging flow on upwind face, separation on top and wake re-attachment) can be found on a 2-D square rib configuration. **Obi et al (1990)** have shown that mesh refinement up to 240 x 120 cells was necessary to reduce the discretisation error to 1%, so it is doubtful that 3-D solutions are always spatially converged.

- the Texas Tech building provides a simple geometry (9 x 14 x 4m rectangular box) which has been investigated in both field and wind tunnel studies. Solutions have been presented by **Selvam & Konduru (1993)** for the k-ϵ model, and by **Mochida et al (1993)** for both k-ϵ and LES models. Correlations were used with the k-ϵ model calculations to estimate the fluctuating pressure coefficient C_p'.

There is little evidence of test cases involving time dependent mean flows.

Contents

As an example application, the results obtained with the finite element code N3S (k-ϵ turbulence model) for air flows around an urban area in Nantes are presented. The model includes a domed-church with five streets leading to the square in front of the church. It was concluded that although there may be uncertainty on the exact size of eddies, the intensity of the wind can be predicted to within about 10% which is sufficient for evaluation of nuisance to pedestrians.

Other general reviews of CFD modelling of flows past bluff bodies are given by **Rodi (1993)** and **Leschziner (1993)**.

Flow over a cube

Murakami and co-workers have undertaken detailed studies of the turbulent flow around a cubic building using the k-ϵ, algebraic stress model (second moment closure) and large eddy simulation approaches for turbulence modelling. For example, **Murakami & Mochida (1989)** reported the use of the k-ϵ model. The issue of mesh refinement was addressed by using both coarse and fine meshes, the second-order QUICK differencing scheme, and by actually estimating the truncation errors by Richardson extrapolation. More recently, **Murakami (1993)** compared the performance of the k-ϵ, algebraic stress model (ASM) (second moment closure) and large eddy simulation (LES) approaches for turbulence modelling. A distinctive feature of the flow field is the highly anisotropic distribution of strain rates, with steep velocity gradients in the streamwise direction as well as in the vertical direction. The k-ϵ model overestimates turbulence energy, giving rise to a large eddy viscosity and an excessive mixing effect. The separation zone near the top leading edge is poorly predicted and the surface pressure is in error. In comparison, the separated flow, turbulence energy and surface pressures predicted by ASM are in much better agreement with the wind tunnel results. With regard to prediction of turbulence statistics, LES performed better than ASM but at a much greater cost.

Numerous other workers have tackled the cube problem. For example, **Zhang et al (1993)** looked at the effect of the incident wind shear and turbulence level; **Kawamoto et al (1993)** applied a finite element Reynolds stress transport model and concluded like Murakami that a dramatic improvement is found in comparison to the k-ϵ model. At the Wind Engineering conference held recently in Guernsey, papers were presented by **Delaunay et al (1993)** and by **Mikkelsen & Livesey (1993)** which included solutions for the flow past a cube problem. Both solutions were obtained with the k-ϵ turbulence model.

The results of **Delaunay et al (1993)** for the cube problem comprise pressure coefficients on the cube faces, for the 'normal wind' case only. The results are generally in good agreement with the **Castro & Robins (1977)** data except for the leeward face; here, pressure is slightly underestimated.

Mikkelsen & Livesey (1993) compared their predictions of cube surface pressures with wind tunnel results for wind directions of 0°, 5°, 15°, 25°, 35° and 45°; the predicted C_p's were slightly higher than the experimental in both pressure and suction areas.

Contents

Flow over other building shapes

The Texas Tech building is a case being tackled by several workers, due to the availability of field data as well as wind tunnel results. The building measures 9m x 14m x 4m. The computation of surface pressures was described by **Selvam (1992)** for winds normal to the long side of the building. The CFD code used the k-ϵ turbulence model. **Selvam & Konduru (1993)** presented CFD predictions of roof corner pressures for wind directions at 20° intervals over the full 360° range. Two grid resolutions were used; the building occupied 13 x 17 x 9 grid cells in the 'fine' grid and 7 x 10 x 9 cells in the 'coarse' grid. Mean surface pressure coefficients were predicted, and peak pressure coefficients then estimated using an empirical correlation. The computed mean pressure coefficients at upwind corners of the roof were under-predicted by as much as 60%, and it was concluded that other turbulence models needed investigation.

Another useful case for CFD validation of flows around buildings is the Silsoe Structures Building (24m x 12.9m x 5.3m). Computational modelling of wind flow around this building was described by **Richards & Hoxey (1992)** using the PHOENICS code. The inlet conditions were based on the **Harris & Deaves (1981)** model of the atmospheric boundary layer. The ground was treated as a rough wall and appropriate wall functions used. This combination resulted in an equilibrium boundary layer which in the absence of the building gave outlet conditions almost identical to the inlet conditions. A body-fitted grid was employed. The overall domain was 48 h wide x 48 h long x 16 h high (where h was the building ridge height). The main conclusions from the study were that the CFD model failed to reproduce the 'delta-wing' vortices near the gable ends with oblique flows, but in general adequately represented the variations of pressure coefficients with direction.

Haggkvist et al (1989) presented simulations of pressure fields around buildings using the PHOENICS code with the k-ϵ turbulence model. A Cartesian geometry (stepped) representation of a low-rise house with pitched roof was studied. In one case, the inlet variables were specified using measured (wind tunnel) values. In a second case, cyclic boundary conditions were used for the house surrounded by other houses. Discrepancies between predicted and measured pressure fields were felt to be due to inadequate specification of the boundary conditions.

Delaunay et al (1993) simulated the wind flow over a house with a pitched roof. The results were compared to the wind tunnel measurements of **Wiren (1983)**. Pressures on the leeward roof and gable walls of the building were underestimated by about 35% of the pressure difference between the upwind and downwind sides.

Atmospheric conditions

The modelling of turbulent flows in the atmosphere has received a significant amount of attention. To illustrate some of the directions taken, a couple of relevant papers are outlined below.

Bartzis (1989) reported the modelling of turbulent diffusion for wind flow and dispersion analysis, with an anisotropic eddy viscosity model. The eddy viscosity in the ith direction was given by

$$K_i = C_\mu k^{1/2} l_i$$

Contents

where C_μ is a constant and l_i is an effective length scale. These length scales are derived from consideration of the proximity of solid boundaries, the global pressure gradient field and local stability conditions. Test examples included a 1-D neutral boundary layer height problem, a triangular ridge wind tunnel problem, and a time dependent boundary layer growth problem (ie. rise of inversion). More recent applications are described by **Andronopoulos et al (1993)**.

Bottema et al (1991) compared the results of CFD modelling with wind tunnel experiments and full-scale measurements for a thin 2-D obstacle. The CFD simulations were carried out using FLUENT with a second-order algebraic stress model of turbulence.

5.2 Dispersion Applications

Passive and buoyant releases

Benodekar et al (1985) described a study undertaken with very similar aims as to the current project, except that the particular applications of interest were limited to nuclear facilities.

The report describes the development of two and three-dimensional CFD codes for predicting the flow and dispersion in the vicinity of buildings, taking account of release buoyancy and atmospheric stratification. The 3-D code employed the k-ϵ turbulence model with modifications for curvature and stratification, the QUICK algorithm with modifications to suppress spurious numerical 'wiggles', and a modified PISO scheme. An embedded analytical model was used for point source releases.

The codes were first tested on the 2-D problems of flow over a surface mounted square rib and flow over a thin rib. Predictions of 3-D flows and plume dispersion were then carried out for:

- a cube in a neutral atmosphere with passive releases, using the data of **Castro & Robins (1977)**, and **Robins & Castro (1977a&b)**;

- the rectangular prism investigated by **Hall et al (1980)**.

Flow predictions were qualitatively in good agreement with measurements, except for the upwind edges of the roof and side walls. The pressure field was poorly predicted at the rear of the buildings; this was attributed to insufficient mesh refinement and the turbulence model.

The predicted concentrations for the cube were generally in satisfactory agreement with measurements, but discrepancies were noted in the recirculation region. The isotropic turbulence model and insufficient mesh resolution were blamed for these problems. For the rectangular shape, agreement with experimental values was less satisfactory, particularly for the buoyant releases where a different form of vertical concentration profile was obtained. The treatment of non-isotropic effects was again considered to be the primary cause of error.

Dawson et al (1987) presented CFD results for the flow field and concentrations in the vicinity of a cubic building in a neutral atmosphere. A release with negligible momentum and buoyancy was considered. The flow field was computed first, and the

Contents

results passed onto the scalar concentration solver. The k-ϵ model was employed with a modified value for the constant C_μ (used in the calculation of eddy viscosity, given by $\mu_t = C_\mu \rho k^2/\epsilon$). Instead of the standard value of 0.09, a value of 0.026 was deduced from reported atmospheric boundary layer measurements. In addition, the constant $C_{1\epsilon}$ in the dissipation equation was modified to be a function of a characteristic scale for the atmospheric boundary layer. A rather coarse mesh was employed with the building occupying only 3 cells across x 3 cells along x 6 cells high. In view of this, it is not surprising that there were some significant differences between predicted and measured concentrations.

Kot (1990) discussed the modelling of contaminant dispersion, noting that although the k-ϵ model is well established for computation of turbulent flows past bluff bodies, a model of turbulent diffusion is still not standardised yet. Kot described the use of additional transport equations for scalar flux and scalar fluctuation respectively. Difficulties arise in particular with the extra detailed boundary conditions needed. Large eddy simulation techniques for dispersion modelling were also discussed.

Mestayer et al (1993) used the k-ϵ model to predict flows over and within a street canyon of infinite length. Wind directions normal and at 60° to the street were modelled. Particle trajectory plots illustrated the helicoidal flow patterns within the street canyon. Passive scalar concentrations were predicted.

Moros et al (1992) and **Moros & Akhurst (1993)** presented CFD predictions of fugitive hydrocarbon emissions from oil storage tanks. In such tanks the roof floats on the oil, thus when the oil level is low the roof is down, forming a cavity. The amount of hydrocarbon which escapes via the circumferential seals depends upon the pressure distribution and the flow patterns in the cavity. The tank under examination was 20m high and 25m in diameter. Three different heights of the roof below the top of the tank were examined. FLUENT/BFC was used for the CFD modelling.

Dense gas releases

In addition to the Thorney Island, Trial 29 comparisons (**Deaves, 1985**), discussed in Section 3.3.1, **Deaves (1987a)** also considers other Thorney Island data and demonstrates how the data was used to improve heavy gas dispersion models. In particular, a comparison is made between model predictions and the results of Trial 21, which involved dense gas dispersion over a 2-dimensional fence.

Deaves (1987b) presented the results of 3-D simulations of the dispersion of chlorine gas around a building. A continuous release of 5 kg/s was considered in 2 m/s, F stability conditions. A downwind building measuring 50m x 10m x 10m high was modelled. Two runs were undertaken, with the distance from the source to the front of the building being 50m and 100m respectively. The simulations were carried out using the k-ϵ turbulence model, modified to take account of the effect of buoyancy.

The development of a computational model for predicting the dispersion of toxic gases in complex environments was described by **Vergison et al (1989)**. A key simplification was that the turbulent flow field was not affected by the pollutant release, thus allowing the flow and concentrations calculations to be conducted separately. Predictions were compared with wind tunnel and full-scale results for free-field situations. The influence of release duration was examined by modelling durations of 10, 60, 300 and 1200 seconds of a 10 kg/s release of chlorine. The influence of 2-D buildings was considered. For 3-D buildings an empirical correction had to be applied within the 2-D code to take account of the tendency of plumes to split and pass either side of 3-D buildings for small width-to-height ratios. A 3-D version of the code was reported to be under development.

Witlox (1990) reviewed various mathematical models for simulation of the dispersion of dense gases, and considered the different turbulence models, numerical solution strategies and some of the programs available. Results were presented for the finite element programs FEM3 and FEMSET and the finite volume code CFDS-FLOW3D. FEM3 incorporated a zero-equation turbulence model with diffusion coefficients, k_h and k_v, depending on a local Richardson number. Both FEMSET and CFDS-FLOW3D used versions of the k-ϵ model. The results were compared with wind tunnel results for a two-dimensional steady-state release over flat ground. The most accurate results were predicted by CFDS-FLOW3D using a buoyancy extended k-ϵ turbulence model.

Betts & Haroutunian (1988) described the development of a finite element code based on the k-ϵ model but incorporating an algebraic anisotropic eddy viscosity model. The effects of buoyancy were included in the k and ϵ equations. The anisotropic eddy viscosities were determined by first calculating the local vertical and lateral turbulent velocity variances. Streamwise diffusion was assumed to equal lateral (crosswind) diffusion. This approach is similar to that described by **Deaves (1985)**. Results were presented for a flat ground simulation of the Burro 8 LNG spill in which gravitational effects were significant. Some problems were encountered due to the over-simplified thermal boundary condition at the ground and numerical instability.

Andronopoulos et al (1993) present results obtained with their anisotropic eddy viscosity turbulence model for dense gas dispersion test cases including both flat terrain problems and dispersion over simple 2-D obstructions.

A number of test cases were examined from the Thorney Island heavy gas dispersion trials (**McQuaid & Roebuck (1985)**) including Trial 8 of Phase I (instantaneous release without obstacle), Trial 21 of Phase II (instantaneous release with obstacle). A further case involving a continuous two-phase release with an obstacle, based upon Trial 55 of the CEC experiment reported by **Heinrich & Scherwinski (1990)**, has also been considered.

Dispersion around offshore platforms

Several offshore CFD applications have been reported recently in the literature. These have been concerned with air flow regimes and gas build up in naturally ventilated modules, and exhaust dispersion and smoke movement around the topsides.

Dr Holdo and co-workers at the University of Hertfordshire have undertaken a number of CFD studies into flow and dispersion around offshore platforms. Using the FIDAP finite element code, **Holdo (1993)** modelled a complete platform with about 30,000 elements. The predictions were compared with wind tunnel results obtained using a 1/200 scale model of a platform with similar proportions. On the windward side of the platform, the predicted and measured pressures agreed to within about 7%, while in the leeward regions there was a difference of about 20-25%. The dispersion of gas turbine exhaust fumes was also presented. One other reported aspect was the

Contents

time dependent simulation of an exhaust plume. A cosine model of a gust was used with a minimum at 0.8 of the mean longitudinal velocity and a maximum at 1.2 of the mean longitudinal velocity. A lateral velocity component at a peak to peak amplitude at 0.2 of the mean longitudinal inlet velocity was also modelled. **Mariathasan (1993)** investigated the natural ventilation of a module on an offshore platform. Full-scale measurements were undertaken for comparison with the CFD predictions, again obtained using the FIDAP finite element program with the k-ϵ turbulence model. Qualitative agreement between predicted and measured velocities was observed.

Whittle et al (1993) reported the prediction of wind-induced ventilation velocities, and fire and smoke movement on an offshore production platform using CFD. A Cartesian geometry representation of a whole platform was employed. Two wind directions were modelled; for the South-westerly direction the incident wind was perpendicular to the platform, while the Northerly direction corresponded to winds striking the platform at an angle of 45°. Comparisons with measurements were not reported.

Ronold (1993) described the modelling of ventilation flows within petroleum process plants on an offshore platform. The whole platform was represented with a Cartesian geometry model (comprising 50,000 cells) and flow predictions made for three wind speeds and eight wind directions. These results were combined with wind frequency data to provide an estimate of the frequency of occurrence of the number of air changes in all areas of the installation considered, An example of a major gas release (100kg/s) in the wellhead area of an offshore platform and the subsequent dispersion were also presented, although no comparisons with measurements were reported.

Moros et al (1994) gave a comparison of CFD modelling and field experiments conducted on an offshore platform. Artificial smoke releases were undertaken from different locations. Air flow velocities were measured using a hand held vane anemometer, and optical smoke sensors were used to measure smoke concentrations. FLUENT was used for a model with 140,000 computational cells. At the solid platform boundaries, a roughness of 0.5m was used to account for stair cases, etc. Obstacles such as louvre walls and chimney arrays were treated as porous structures. On average, the predicted wind speeds were within a factor of 2 of the measured values and in some areas to within 50%. The predicted concentrations were to within a factor of three of the measured values at almost all the monitoring points.

5.3 Turbulence Modelling

Taking account of turbulence involves the modelling of the effect of fluctuations in the flow at a wide range of different scales. The fluctuations are difficult to calculate using simulation techniques, largely owing to a need for sufficient computer speed and memory capacity to allow the resolution of flow features at all significant length scales at high Reynolds numbers. In order to overcome this difficulty, various ways of modelling the effects of turbulence on the mean flow characteristics have been developed, and many are in use in engineering CFD codes.

The majority of turbulence models used in engineering calculations rely first on the use of Reynolds averaging to derive conservation equations for mean flow quantities from the Navier Stokes equations, within which are contained additional terms

Contents

representing turbulence in the form of stresses or modifications to the local effective viscosity. Typical CFD models of turbulence are as follows:

Zero equation models: The Reynolds averaged momentum transport equations use an empirically derived eddy viscosity. Scalar equations may use eddy diffusivities (or 'K' values) to calculate turbulent fluxes. This gives the opportunity for non-isotropic formulations to be applied, but is clearly limited in application.

One Equation models: An additional scalar transport equation for the turbulent kinetic energy is solved. This is combined with an empirical relationship for the turbulence length scale and the eddy viscosity hypothesis to calculate a distribution of effective turbulent viscosity.

Two Equation Models: Two additional scalar transport equations are used, one for the turbulent kinetic energy (k) and one for either its rate of dissipation (ϵ), or (less commonly) the length scale (l). The transport equations also contain a number of modelling constants whose values have been established by experiment. The values of k and ϵ at each grid node are used to calculate an eddy viscosity using the relationship:

$$\mu_t = \rho C_\mu \frac{k^2}{\epsilon}$$

Where the constant C_μ is generally given the value 0.09, consistent with the assumption of turbulent equilibrium. Finally, it should be noted that the k-ϵ approach is consistent with the k-l model only in the limit of high Reynolds number, where the relationship:

$$\epsilon = k^{3/2}/l$$

allows the derivation of the equation for the eddy viscosity.

RNG Formulation of k-ϵ: Recently, the application of Re-Normalisation Group theory to the derivation of turbulence models has led to the development of a range of modifications. In the case of the standard k-ϵ model, this entails changes to the constants used, and the addition of a term to the dissipation equation (the so called $\Re$ term) related to the total rate of fluid strain and the turbulent viscosity. It is claimed that the RNG formulation of the two equation approach is more accurate, although this has so far only been confirmed for certain flows. It is perhaps of more benefit to note that its range of applicability extends to lower Reynolds numbers than the standard k-ϵ model.

Non-Linear k-ϵ models: These models **(Speziale, 1987)** are based upon solutions of the k-ϵ transport equations (in standard or RNG form), but use non-linear relationships to compute Reynolds stresses from rates of fluid strain and the eddy viscosity. The gradients of these Reynolds stresses are used in the momentum equations to allow the modelling of non-isotropic turbulence.

Algebraic Stress Models: An algebraic stress model seeks to calculate the Reynolds stresses from a set of equations derived from the Reynolds stress transport equations. The chief assumptions are that each component of the Reynolds stress tensor is transported and diffused at the same rate as the turbulent kinetic energy, and scales like the turbulent kinetic energy. The result is a quadratic equation for each of the

Contents

Reynolds stresses. The main advantage of the approach is that it provides a model of non-isotropic turbulence, which is closely related to the Reynolds stress transport model, but without the complication or computational effort associated with its solution. The main disadvantage is that it is often not clear which of the two roots of the quadratic equations for the Reynolds stresses is the admissible solution.

Reynolds Stress Transport Models: The solution of the Reynolds stress transport equations leads directly to values for each component of the Reynolds stress tensor, which may then be used in the momentum equations. Their main advantage is that they provide a model of turbulence which is sensitive to factors such as streamline curvature and swirl, allows non-isotropic solutions and may be used at quite low Reynolds numbers. Their main disadvantages lie in the increased computational effort required, the need for further empiricism for certain of the terms (and hence "calibration"), and complexities in the formulation of boundary conditions. Despite this, numerous studies have shown the RSM approach to provide more accurate solutions than standard k-ϵ for impinging jet flows, flows with strong swirl, flows driven by buoyancy etc.

Large Eddy Simulation: The large eddy simulation approach differs somewhat from the above in that the Navier Stokes equations are averaged in space only, and that the averaging is carried out using a Gaussian filter, rather than by assuming small perturbations about some mean flow value. The resulting momentum equations are unsteady, and employ a model for the Reynolds stresses which involve a turbulent viscosity proportional to the width of the Gaussian filter used. It is assumed that the width of the filter can be related to the grid size used in the simulation of the flow field. Thus the large eddy approach can be summarised as one which simulates the transport of flow field fluctuations of large length scale (large scale vortices), and models the effect of fluctuations at sub-grid length scales.

The range of turbulence models available in commercial CFD codes covers most practical options, and also includes approaches still under active research. All codes offer the standard k-ϵ two equation model, with an eddy viscosity and experimentally derived coefficients. This model has grown popular due to its robustness, and qualitatively good performance over a range of engineering flow problems. More recently, the standard k-ϵ formulation has been augmented with RNG derived models in a number of CFD codes. The RNG derived model appears to perform more accurately for some flows, but less well for others. Its main strength is that it appears better suited to low Reynolds number flow regions, and can therefore be used without additional empiricism for near wall flows. RNG type formulations appear in FLOW-3D, FLUENT, STAR-CD and CFDS-FLOW3D, PHOENICS-2.

The implementation of the k-ϵ approach within finite element codes was at first found to be difficult. This appears to have been due in part to a lack in robustness of the Galerkin formulation of the k-ϵ equations, the coupling of k and ϵ via the eddy viscosity, and the method by which boundary conditions were chosen and implemented. Thus most finite element codes feature alternative two equation models which, with experience, appear to be offering robust solution schemes.

Simpler mixing-length based models are available in most codes, as are one equation formulations, wherein a scalar transport equation for k, the turbulent kinetic energy is solved in conjunction with an empirical formulation for the length scale. This approach is particularly useful in boundary layer flows, where the variation of the

Contents

length scale with distance from the wall can be derived from experimental data, and the high Reynolds number assumptions made in the k-ϵ approach are in any case invalid.

The solution of the Reynolds stress transport equations or their equivalent flux based formulation is also now featured in codes such as FLUENT, CFDS-FLOW3D and STAR-CD. These approaches have been shown to be superior to k-ϵ for some applications, particularly those involving strong streamline curvature and non-homogenous turbulence. However, RSM also contains empiricism, can be less well behaved numerically, and requires more computational effort. Therefore this approach appears to be best applied to problems for which inhomogeneity in the turbulent flow field is an important factor.

Finally, large-eddy turbulence models are gaining in popularity, and some codes offer simple formulations to suit. The Flow Science FLOW-3D code is one such example, which, since it is a code which has been written to handle predominantly unsteady flows is well suited to this approach. Considerable research is still required into using LES, particularly with respect to the application of near wall boundary conditions, before the technique can be applied with the levels of reliability to match more conventional modelling methods.

Application to flows and dispersion around buildings

The k-ϵ turbulence model has been applied to single isolated buildings and groups of buildings. With the standard model, poor agreement with wind tunnel and full-scale data is reported for features such as separation or 'delta wing' vortices at upwind edges of flat roofs. In addition, the reattachment length and the pressure in the wake of a building are generally underestimated. Nevertheless, the velocity field in the wake is predicted quite well.

Some optimisation of the k-ϵ model may be appropriate for atmospheric flows, eg. modification of some of some of the model constants **(Bottema et al 1992)**

To improve the predictions, a number of different approaches have been adopted, for example:

- non-linear k-ϵ model **(Bassara & Younis, 1992)**
- low Reynolds number k-ϵ model **(Abe et al, 1993)**
- Reynolds stress transport models **(Laurence & Mattei, 1993)**

Almost all reported computations of gas dispersion have been carried out using the k-ϵ model. It appears that there is no standard approach to turbulent diffusion modelling. Approaches have included, isotropic treatment of eddy diffusivity and anisotropic eddy diffusivities (eg. **Benodekar et al, 1985**, **Betts & Haroutunian, 1988)**.

There is little evidence of the application of the more recent and advanced turbulence models to the problem of dispersion around buildings.

Contents

5.4 Comparison of Commercial Codes

In this section, an overview of the range of possible modelling features available in commercial CFD codes is given. For the purpose of this section, only "general purpose" CFD codes will be examined. There are many examples of problem or industry specific codes which may be licensed. However, the feature which distinguishes such software from better known general purpose codes, is that the numerical models are based upon specific formulations. Such codes may be well validated, though only over a narrow range of geometries and flow parameters.

Discretisation

Table 5.1 lists the proprietary CFD codes whose features have been examined during this review. These general purpose codes vary in the type of numerical discretisation and solution approach taken. However, it is noticeable that the finite difference method, with associated non-conservative equations and need for numerical mapping to complex domains, is not well represented amongst the major codes.

A further important aspect when considering the general usefulness of a CFD code is the form of mesh structure employed. In principle, unstructured meshes of the Finite Element type provide the user with the highest level of flexibility. However, some finite volume codes have also been written to allow the use of unstructured meshes, as shown in Table 5.1.

Code	Authors/Vendors	Discretisation	Mesh type
ASTEC	AEA Harwell	Finite volume	Unstructured
CFDS-FLOW3D	AEA Harwell	Finite volume	Structured (Multiblock)
ESTET	EDF-SIMULOG	Finite volume	Unstructured
FEAT	Nuclear Electric	Finite element	Unstructured
FIDAP	FDI/ACE	Finite element	Unstructured
FLOW-3D	Flow Science	Finite difference/ volume	Structured
FLUENT	Fluent Europe	Finite volume	Structured
FLOVENT	Flomerics	Finite volume	Structured
N3S	EDF-SIMULOG	Finite element	Unstructured
PAM-FLUID	ESI GMBH	Finite element	Unstructured
PHOENICS-2	CHAM	Finite volume or Finite element	Structured or unstructured
STAR-CD	Computational Dynamics	Finite volume	Unstructured

Table 5.1 Discretisation features of commercial CFD codes

Contents

The representation of complex geometry using structured grids may be approached in a number of ways. The simplest method, which has been in use since the beginning of commercial CFD development, represents solid objects embedded in the mesh with "obstructions" or "blockages". These are regions, generally bounded by grid planes, within which nodes are excluded from calculations, and whose surfaces provide boundary conditions via their bounding mesh planes. Where grid structures are rectangular Cartesian, then only rectangular blockages can be defined. For certain applications this does not present any problems, and in certain codes such as PHOENICS, FLUENT and FLOVENT, this approach still finds considerable use.

The definition of obstructions bounded by grid planes is retained within body-fitted mesh versions of structured codes and, in certain cases, this allows more complex objects to be represented with a reasonable degree of realism. It is also possible to represent smooth curved boundaries within a rectangular mesh structure by taking special account of computational cells which contain a portion of the obstruction as well as fluid. One example of this is the FAVOR algorithm used in the Flow Science FLOW-3D code. Such approaches cannot provide the level of near-wall mesh resolution required for accurate boundary layer predictions, but their strength lies in their versatility and ease of use.

In some fluid flow problems, it is convenient to be able to deal with changing geometry and/or mesh, either to allow grid adaption, or simply because the domain geometry is subject to change. The representative codes given in Table 5.1 are able to handle such problems in different ways.

First, codes such as PHOENICS and STAR-CD, which have been applied to Internal Combustion engine in-cylinder combustion problems, have for some time allowed for the cyclic movement of grid planes to simulate a moving piston or valve. More recently certain codes have been extended to allow certain mesh zones to move relative to one another. This is particularly useful in the representation of rotor-stator blade rows in gas turbines, and stirred tanks.

A more difficult test of grid adaptation is presented by the modelling of liquid free surfaces. This is a problem typical of simulations of casting processes and finite element codes such as FIDAP have been used in such cases with some success. In practice, free surface flow of liquids is more often modelled using volume-fraction (VOF) techniques such as in FLOW-3D, PHOENICS and ASTEC. In the VOF method, the grid remains stationary with respect to the flow and the movement of the free surface is modelled using an advection equation for the fluid fraction. This preference is based upon the experience that large amplitude fluid motions can lead to severe finite element mesh distortion and badly conditioned solutions if the former approach is adopted.

Flow modelling

All of the codes cited in Table 5.1 seek solutions of the Navier-Stokes (laminar) or Reynolds Averaged Navier Stokes equations. This sets a very broad band upon the type of fluid behaviour which can be modelled.

The basis of most of these codes is the incompressible form of the N-S or RANS equations. All of the codes allow small variations in density via the Boussinesq approximation such that thermally buoyant flows may be modelled. This

Contents

approximation is based upon the assumption that changes in density are not brought about by changes in pressure, but by differences in temperature and concentration only. The word 'small' is thus relative, but one might assume a rule-of-thumb in which changes in density caused by changes in pressure would be at least an order of magnitude smaller than those produced by temperature differences alone. It can be argued that this is not the case for, for example, heavy gas slumping, but the convenience of the Boussinesq model is hard to ignore. The alternative is to assume fully compressible flow. However, for the low Mach numbers considered here, and the increase in difficulty associated with turbulence modelling in such cases, this approach is problematical. Certain of the codes, for example STAR-CD, CFDS-FLOW3D and FLOW-3D permit the calculation of fully compressible flow, but are relatively untried in this context.

The basic assumption that the flow is Newtonian applies to all of the codes cited. However some are capable of modelling certain types of non-Newtonian behaviour, through the addition of non-linear shear-stress terms. PHOENICS, FLUENT and FLOW-3D have this feature, although, in practice, there are many non-Newtonian flows for which this approach is inappropriate.

The modelling of multi-phase flow is an area which attracts considerable interest, and for which a large number of alternative approaches exist. The most common treatment is for so-called dispersed phases, in which the evolution of the concentration of one fluid contained within another is represented by a scalar transport and diffusion equation. For each additional fluid component, further scalar transport and diffusion equations may be added. The coupling with the overall momentum and continuity equation is usually made through the density and a Boussinesq assumption. This particular approach is the most popular choice for modelling dense gas dispersion, and has been used in most research codes (FEM3 & FEMSET) as well as the commercial software listed above, and is the most likely choice for further studies in this project.

An alternative approach is to model the dispersed phase as Lagrangian "particles" of particular mass. The particles are transported using interpolated velocities found directly from the grid, and diffused by the random-walk approach, with diffusivities computed using the local turbulence solution. The concentration of the dispersed phase is then found directly from the number of particles contained within each computational grid cell. This particle tracking approach is most frequently applied to positive buoyant gas plumes.

Finally, it is also possible to compute flows containing components with widely varying densities by using so-called volume fraction techniques. For this approach to be useful, the phases must be "non-dispersed", i.e. there must be large regions within the computational domain for which the concentration of each component is unity. This is the case, for example, during the early phases of slumping of a dense gas. The volume-fraction approach was originally developed to model free-surface flows and so, in principle, is able to maintain reasonably sharp interfaces between two fluids. In practice, some numerical diffusion is often present in such calculations, such that no truly sharp interface between fluids exists. Codes such as FLOW-3D, ASTEC and PHOENICS contain this type of algorithm.

Contents

6. RECOMMENDATIONS

6.1 Discussion of CFD Requirements

Accurate simulation of the release of hazardous material in the vicinity of a building requires detailed consideration of the following:

- the geometry of the building and other nearby buildings and obstructions;
- atmospheric boundary layer conditions and ground conditions;
- the size of the computational domain; this depends on the buildings and external wind flow regime and needs to extend sufficiently far from the region of interest to minimise the influence of the boundaries;
- prevailing wind conditions; these need to be simulated prior to the release of any hazardous material;
- transformation of the local flow regime by the release of gas; this may occur if there are significant momentum and buoyancy effects.

Most of these issues have been considered by the applications described earlier. In the light of the reported experience, it is concluded that there are only two particular requirements of the CFD code:

i. the CFD code should employ an unstructured or body-fitted coordinate mesh system;

ii. the available turbulence models should include not just the standard k-ϵ model but also appropriate modified models (eg. a non-linear k-ϵ model), and a Reynolds/algebraic stress model.

Both these particular needs can be met by a number of the currently available commercial CFD codes. This is discussed below in the next section.

6.2 Appropriate CFD Models

The review of dispersion modelling undertaken during this project allowed the following modelling features to be identified as being important to the outcome of the work:

Turbulence Modelling: It was considered to be important that the CFD code chosen would need to allow levels of turbulence closure up to Reynolds stress modelling. The 'standard' k-ϵ model poorly predicts features such as the separation at the upwind edge of a flat roof and reattachment in the wake. Hence there is likely to be a need for more advanced turbulence models.

Mesh Structure: Although it is not thought that highly complex geometries will be modelled, it is considered to be a minimum requirement to model curved boundaries accurately. Some form of body-fitted mesh system is therefore required.

Contents

Flow Physics: The modelling of the dispersed phase fluid, and the effects of buoyancy are two important aspects of this work. The key to choosing the most appropriate code is therefore that of versatility.

An initial review of code capabilities led to the elimination of codes such as ASTEC, FIDAP, FEAT, N3S, PAM-FLUID and FLOVENT, since these codes appear to lack the general flexibility in turbulence modelling deemed necessary.

This left the following codes from which to make a choice

CFDS - FLOW3D	CFDS - HARWELL
FLOW-3D	Flow Science Inc
FLUENT	Fluent Europe
PHOENICS	CHAM
STAR-CD	Computational Dynamics

The Flow-Science FLOW-3D code is an extremely versatile transient flow solver for multi-fluid problems with complex physics. However, it is eliminated from further consideration largely as a result of lacking a Reynolds stress modelling capability and its treatment of obstructions as blockages within a regular non-body-fitted mesh. Its treatment of dispersed phases is unique to FLOW-3D and therefore difficult to compare with other codes.

The PHOENICS code was also eliminated. In practice, it is likely to be of similar capability to FLUENT, but no evidence of its use in these problems was made available to us.

The remaining codes, CFDS-FLOW3D, FLUENT AND STAR-CD have all of the features required of this study. It would appear that any of these codes would be suitable for further consideration. Further consultation with the vendors, and with HSE, will be taken prior to making a final recommendation. If available, further evidence based upon past usage of the code, not so far provided by vendors, will also be examined.

6.3 Suggested Test Cases for Validation

The test cases suggested for validation purposes are:

- flow and dispersion of passive/buoyant releases over a cube;
- flow and dispersion of passive/buoyant releases over a rectangular block with dimensions 2h x h x h (where h is the height of the building);
- dense gas dispersion over a fence.

Experimental results for the cube were presented by **Castro & Robins (1977)** for the flow field, and by **Robins & Castro (1977b)** for dispersion. The dispersion data covers a range of release conditions, including both area and point sources. The flow problem has been used for validation of CFD by several authors, including **Murakami (1993)**.

Contents

For the second case, there is experimental data for passive and buoyant releases for various release conditions and locations around the building **(Hall et al, 1980, Hall & Waters, 1986)**. The problem was used for CFD validation by **Benodekar et al, (1985)**. Alternatively, it may be considered advantageous to utilise the full scale results from the UMIST Altcar experiments.

The first two cases deal with the complex flow effects in the vicinity of 3-D buildings. Experimental data exists for these cases for passive and buoyant releases, but unfortunately there appears to be no similar experimental (model-scale or full-scale) data for dense gas releases. The dispersion of dense gas is an important issue in this study; therefore, in the absence of a fully 3-D test case, it is suggested that the test case involving dense gas dispersion over a fence is examined.

Dense gas dispersion over a fence was examined experimentally in some of field trials organised by the Health and Safety Executive at Thorney Island **(McQuaid & Roebuck, 1985)**. Trial 21 (Phase II) involved an instantaneous release of a cylindrical dense gas cloud of 2000 m^3 volume and density 2.02 relative to the air. The cloud was released at the centre of a semi-circular fence of 5m height and 50m radius. The wind was blowing towards the fence and neutral stability conditions prevailed. This case was used for CFD validation by **Andronopoulos et al (1993)**.

6.4 Programme for Phase II

The original warrant proposal for this study (D4010.070/T8000/P2) outlined the anticipated scope for Phase II of this project. This section provides an update to the original scope in the light of the findings of Phase I. The proposed approach for Phase II is outlined below, and costings have been provided separately.

a) Test case definition

The review has revealed a large quantity of data relating to dispersion near buildings. By far the greatest body of data is for wind tunnel tests, and simple shapes such as cubes have been tested extensively. In addition, some full scale data is also available for cubes. It is therefore suggested that a cube is used as one of the test cases. Once this simple geometry has been set up, it will be relatively straightforward to obtain results for non-normal incidence, and hence to check that flow patterns are reasonably predicted.

It is also recommended that three further test cases will be used. One would be a cuboid building (possibly to correspond to the Altcar tests - see Section 3.1). There are measurements of dispersion of material released at various positions around the building which can be used for validation. A simpler case, of the fence in the Thorney Island Trial 21, will be used to test the modelling of dense gas effects. The final test case would be one of the buildings identified in Section 1.3, probably Site B, with a vaporising chlorine pool as the source, representing a spill from tanker offloading operations.

b) CFD model development

The CFD code selected will be set up for the three test cases chosen. This will involve the determination of an appropriate level of grid refinement in each region of the computational domain, based upon the anticipated flow

Contents

patterns, turbulence generation effects etc. It may also include the modification of turbulence models to enable them to model the important effects of buoyancy, impingement and entrainment correctly. This activity will require a significant effort in testing and refining the models to ensure that the features are modelled correctly, that sufficient accuracy can be obtained and that computational efficiency can be achieved.

c) CFD model validation

At this stage, the simpler test cases - the cube and the Altcar building - will be used and run for a range of release rates and configurations to match those available from the various experiments. Although data on dense gases is available from the Thorney Island Phase II dataset, the instantaneous nature of these releases makes them less useful than the continuous releases chosen. If it appears useful, it may be possible to replace the Altcar test case by one of Trials 26-29 from Thorney Island.

This validation study will allow the identification of any areas in which the features of the modelling may need to be modified in order to give a correct representation. It will also enable studies to be undertaken on the optimal grid arrangements and the overall efficiency of the numerical procedures. This validation study would also act as a test case for different turbulence models, although the level of detail of such a study will be limited by the lack of turbulence data.

d) CFD sensitivity study

Although the validation study will allow certain checks on sensitivity, the main sensitivity studies will be undertaken on the Site B test case. The main parameters to be varied will include the following:

- release rate
- release momentum and buoyancy
- release position
- building orientation

In each case, although the overall sensitivity of predicted flow patterns is clearly of interest, the main consideration will be the variation of the concentration of gas just downwind of the building near wake.

e) Simple model development

Simple models exist for the definition of the size of the near wake, and for the residence time of material within it. For neutrally buoyant releases, the assumptions of complete mixing within the wake enables these models to be extended to allow the calculation of concentration. This type of simple model could be extended in a number of ways to supplement the CFD modelling being undertaken. These include:

i) Non-normal incidence
ii) Dense gas releases
iii) Jet releases

Contents

For (i) and (ii), information identified in this report will be utilised to extend the current simple models. For (iii), parametric studies using the WS Atkins computer program PLUME will also be undertaken.

f) Interim report

A report will be provided to HSE detailing the work undertaken in this phase, presenting results of CFD simulation, and assessing the usefulness of zone modelling. The report will also provide recommendations for the subsequent phase of the work, which will be the application of the CFD methodology.

Contents

7. CONCLUSIONS

The modelling of external flows using CFD is an area of current interest for a range of applications. The two main areas in which such studies are being undertaken are the calculation of pressure loadings on buildings, and the prediction of the movement of smoke on offshore platforms. Dispersion is clearly of interest in this latter case, and has been modelled for some simulations. However, the very complex nature of an offshore structure, the generally higher prevailing wind conditions (at some 30-50m above the sea), and the positive buoyancy of the smoke all provide significant differences from the case of dense gas dispersion near buildings. For flows around surface-mounted buildings, some CFD studies have been undertaken, although the emphasis is more clearly on pressure distribution predictions.

The first phase of the study has therefore enabled all relevant CFD applications to be reviewed, and has given recommendations for the future development of CFD modelling for the specific building wake scenarios of interest. It is apparent that CFD has both great potential, and also some limitations and has to be used with great care, particularly for the types of problem under consideration here.

The review, and contacts with various research organisations, has also identified simpler empirical models which, whilst not directly addressing the problem under consideration, have the potential to be developed further in parallel with the CFD modelling. The work which has been recommended in Phase II covers both these areas and should advance the HSE's understanding of the effects of building wakes on near-field dispersion.

Contents

APPENDIX 1

Selected Keywords Used in the On-line Database Search

Contents

SELECTED KEYWORDS USED IN THE ON-LINE DATABASE SEARCH

1. DISPERSION?
2. DISPERSION EXPERIMENTS?
3. OBSTACLE FLOWS?
4. WAKES?
5. DISPERSION EQUATIONS?
6. DISPERSION AROUND BUILDINGS?
7. GAS DISPERSION AROUND BUILDINGS?
8. DISPERSION AROUND OBSTACLES?
9. DISPERSION WITH WAKES?
10. DISPERSION IN WAKES?
11. WIND TUNNEL EXPERIMENTAL DATA?
12. WIND TUNNEL TESTS?
13. TURBULENCE MODELS/MODELLING?
14. GAS RELEASE?
15. GAS DISPERSION?
16. GAS DISPERSION FROM BUILDINGS OR OFFICE OR WAREHOUSE?
17. FLOWS AROUND OBSTACLES?
18. GAS DISPERSION MODELS/MODELLING?

Contents

APPENDIX 2

References

Contents

Specific Topics Considered in Literature Review

Each reference examined during the course of the literature review has been briefly assessed to determine its usefulness and relevance to the current project. This was done by identifying a number of key topics, and assessing which topics were addressed by each reference. The topics used, together with their code numbers are listed below. The Table of References on the following pages gives the relevant code numbers for each reference

1. Reviews of models for the effects of buildings on dispersion and general discussions.
2. Wind tunnel studies of dispersion influenced by a cube.
3. Wind tunnel studies of dispersion influenced by simple building shapes.
4. Wind tunnel studies of dispersion influenced by complex building shapes.
5. Wind tunnel studies of dispersion influenced by topography.
6. Studies of concentration fluctuations near buildings.
7. Studies of dense gas dispersion around buildings.
8. Studies of buoyant releases and plume rise in the vicinity of buildings.
9. Field trials of dispersion around buildings.
10. Full scale measurements of dispersion around buildings.
11. Wind tunnel and full scale flow measurements around buildings.
12. CFD modelling of flow and dispersion around buildings.

Arrangement of Appendix

A large number of references were obtained, not all of which have been cited in the text. This appendix therefore includes 2 lists:

List 1 References cited in the text
List 2 Additional relevant references

Contents

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Contents

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