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Review of FLACS version 9.0

Dispersion modelling capabilities

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Dispersion modelling capabilities

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FLame ACceleration Simulator (FLACS) is a commercial Computational Fluid Dynamics (CFD) code developed and marketed by Global Explosion Consultants (GexCon), based in Bergen, Norway. The software has been developed to model the dispersion and combustion of flammable liquids, gases and dust clouds in open and bounded geometries.

The first version of FLACS, released in 1986, was developed by CMI (Christian Michelsen Research Institute). CMI continued the development of FLACS until 1992 at which time its development was passed to CMR (Christian Michelsen Research). GexCon was established in 1998 to manage the consultancy activities of CMR and in 2000 it took full responsibility for the development of FLACS. At present the company employs around 35 people, many of whom are involved in the development of the software. The present release of FLACS is Version 9.0, which forms the subject of the present review.

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EXECUTIVE SUMMARY

Objectives:

The principle objective of this report is to review the suitability of FLACS for modelling dispersion by examining the underlying theoretical basis of the model and its verification and validation.

Main Findings:

A survey of the literature and user manuals has shown that FLACS is based mainly on established CFD modelling techniques and has been demonstrated by GexCon to produce good predictions for a wide range of dispersion scenarios. However, the code has limitations, in particular its use of a Cartesian grid, which make it unsuitable for modelling certain flows such as dense gas dispersion over sloping or undulating terrain. A number of the validation cases reported in the literature are also not described in sufficient detail to provide confidence that the results are repeatable if, for example, a finer grid is used. A summary of the strengths and weaknesses of the model is given below.

Strengths:

1. FLACS has been tested for a wide range of different dispersion scenarios including releases of dense, passive and buoyant gases in open, obstructed and enclosed spaces. In most of these tests, FLACS is shown to produce reasonably good predictions (within a factor of two for more than half of the time in nearly all cases).

2. FLACS features a distributed porosity model for small sub-grid scale obstacles, a semi-automated process for creating complex flow geometry and a simple Cartesian grid that enables simulations to be produced rapidly compared to other general-purpose CFD codes.

3. Source models for high-pressure gas releases, flashing releases and evaporating pools are provided.

4. Atmospheric conditions at inlet boundaries can be specified which take into account upstream surface roughness and atmospheric stability.

5. FLACS uses a well-established turbulence model and some proven solution methods.

6. Training courses and support are provided for the software by GexCon.

7. FLACS can also be used to model vapour and dust explosions.

Weaknesses:

1. Many of the validation studies reported for FLACS do not provide sufficient details to be confident that the results are repeatable if, for example, a finer grid is used. Often the results are shown for only one grid and no grid-sensitivity tests are reported. The version number of FLACS is usually not provided.

2. Documentation of FLACS version 9.0 is poor. Despite it having been released in April 2008, a draft version of the User's Manual was only provided to the authors of this report, following some discussion, in January 2009. A new user manual for FLACS

version 9.0 was released in February 2009. The manuals also lack a description of some of the sub-models.

3. It appears that some underlying mathematical models have changed between FLACS versions 8.1 and 9.0. It is unclear how this affects its predictions.

4. FLACS uses a single-block Cartesian grid. This may lead to unreliable predictions of dense gas dispersion over sloping or undulating terrain due to the overly high dissipation of momentum from modelling a stepped surface. To simulate such flows, a body-fitted curvilinear or unstructured grid, or cut-cell approach, is needed. A single-block Cartesian grid also introduces limitations in the approach that can be used to model gas jets. Since the code is not yet parallelised, grids cannot contain a very large number of cells.

5. FLACS lacks choice in its sub-models. Only one turbulence model is provided which, although well-established, has certain limitations, and the code lacks a Lagrangian model or an inhomogeneous Eulerian model for simulations of sprays or particles.

6. The scientific basis of the wind meandering model for atmospheric dispersion simulations is unclear.

7. The application of the distributed porosity concept to dispersion modelling is gaining acceptance but is still not fully-established. Much of the development of the distributed porosity model was undertaken for explosion-driven flows. There is a lack of validation data examining the accuracy of dispersion predictions across a range of different grid resolutions, modelling obstacles as either solid obstructions or as sub-grid porosities.

The quality of the results produced by FLACS will be determined to a large extent by the way in which the code is used and by the skill and judgement of the CFD practitioner, although this is common to all CFD codes, not just FLACS. GexCon provides some guidance on best-practice use of FLACS in its User's Manuals. It is recommended that FLACS users also consult guidance produced by, for example, the European Research Community on Flow Turbulence and Combustion (Casey & Wintergerste, 2000; Franke *et al*. 2007).

FLACS is under continual development and it is therefore recommended that this review be repeated in two to four years time. GexCon are aware of the issues with the FLACS documentation and have started to improve this. For the last two years, work has been ongoing on the development of improved treatments for sloping or curved geometry, and a parallel version of FLACS is under development. In addition, it is planned to implement a Lagrangian model for sprays and particulate-laden flows, and improvements have been made in the flashing release and the pool-spread models. GexCon have also recently performed simulations using FLACS of all of the test cases documented in the "Validation Database for Evaluating Vapor Dispersion Models for Safety Analysis of LNG Facilities" (Ivings *et al*., 2007; Coldrick *et al*., 2009), although the results from this study have yet to be published in the open literature (Olav Hansen, Private Communication, September 2009).

1 INTRODUCTION

1.1 BRIEF OVERVIEW OF FLACS

FLame ACceleration Simulator (FLACS) is a commercial Computational Fluid Dynamics (CFD) code developed and marketed by Global Explosion Consultants (GexCon), based in Bergen, Norway. The software has been developed to model the dispersion and combustion of flammable liquids, gases and dust clouds in open and bounded geometries.

The first version of FLACS, released in 1986, was developed by CMI (Christian Michelsen Research Institute). CMI continued the development of FLACS until 1992 at which time its development was passed to CMR (Christian Michelsen Research). GexCon was established in 1998 to manage the consultancy activities of CMR and in 2000 it took full responsibility for the development of FLACS. At present the company employs around 35 people, many of whom are involved in the development of the software. The present release of FLACS is Version 9.0, which forms the subject of the present review.

FLACS was initially developed for modelling vapour cloud explosions. GexCon later integrated a dispersion model within the code in order to predict the extent of the vapour cloud, prior to modelling its combustion. GexCon promote the latest version of FLACS as being suitable for simulating a diverse range of dispersion and explosion related flows, including the dispersion of dissolved chemical species, homogeneous gas mixtures and suspensions of solid particles. Furthermore, FLACS version 9.0 is described as being suitable for modelling dispersion over sloping and undulating surfaces, and through complex geometries. The main focus of the present review will be on the dispersion modelling capabilities.

A number of previous studies have reviewed aspects of FLACS. GexCon have been involved in many of these reviews, recent examples including Hanna *et al.* (2004) and Hansen *et al.* (2008). Independent reviews undertaken by the Health and Safety Laboratory include those of Deevy and Ledin (2004) on the FLACS dust explosion model (DESC), and the review by Ledin (2008) on the gas explosion model.

1.2 THE MODEL EVALUATION PROCESS

The model evaluation approach adopted in the present investigation is based on that outlined by Ivings *et al*. (2007). In that work, a Model Evaluation Protocol (MEP) was developed that can be used to assess the suitability of dispersion models for predicting hazards associated with spills of LNG. The protocol is based on that developed by the EU SMEDIS project for dense gas dispersion (Carissimo *et al*., 2001; Daish *et al*., 2000).

The MEP developed by Ivings *et al.* (2007) addresses three distinct aspects: scientific assessment, model verification and model validation. To carry out the scientific assessment, detailed information on the mathematical and numerical basis of the model is required. This information is obtained using a Model Evaluation Questionnaire (MEQ), which is completed in collaboration with the model developers.

In the present study the MEQ developed by Ivings *et al.* (2007) was modified for general dispersion and completed in collaboration with GexCon. The information contained in the MEQ was then used to write this report. In addition to the questionnaire, one of the authors of this report attended the FLACS training course, run by GexCon, and there have been numerous private communications with GexCon to clarify various issues. By obtaining information directly from GexCon, the factual information upon which this review is based should be as accurate as possible.

1.3 OUTLINE OF THIS REPORT

In order to review the dispersion modelling capabilities of FLACS, it is important to understand the types of dispersion problem that FLACS might be used to model. Furthermore, it is necessary to understand the key physics of dispersion. These two aspects are discussed briefly in Section 2.

In Section 3 the scientific basis of FLACS is reviewed. The review essentially takes the factual details contained within the MEQ and provides a critical analysis of the approaches taken in FLACS.

Section 4 addresses the verification of FLACS, which includes checks that have been performed to ensure that the equations are coded and solved correctly.

In Section 5, the validation of FLACS is discussed, which includes analysis of the evidence that FLACS produces physically accurate predictions.

Finally, the conclusions from the review, including the main strengths and weaknesses of FLACS, are presented in Section 6.

2 DISPERSION FUNDAMENTALS

2.1 KEY PHYSICS OF DISPERSION

Dispersion is defined as the process by which a material is spread within a fluid. Typically, a material is dispersed from regions containing higher concentrations to regions with lower concentrations. The process of dispersion can occur in gases or liquids and the material that is dispersed can be gaseous, liquid or solid (particulate).

The two principal physical mechanisms that control dispersion are diffusion and convection. Diffusion includes the effect of random molecular motion (Brownian motion) and fluid turbulence (turbulent diffusion), whilst convection is related to the effects of fluid inertia (forced convection) and buoyancy (natural convection). Once the material becomes diluted into a mixture, for example when a contaminant gas is released into the air, the material cannot become “un-mixed” and the mean contaminant concentration increase without work being done on the mixture.

Diffusion and convection processes are influenced by a number of factors. Firstly, the geometry of the flow and the presence of walls or solid obstructions. For example, dense gases tend to flow downhill, complex obstacles may trap fluid and rough boundaries may enhance mixing. Diffusion and convection are also affected by fluid composition (i.e. the concentration of the dispersed material) and fluid temperature, both of which may result in density variations. If a fluid is stably stratified, with density increasing with depth, mixing can be suppressed as the vertical density gradient acts to damp vertical turbulent motions. Conversely, if a fluid is unstably stratified this will typically result in enhanced mixing.

Factors that may be important in affecting the dispersion of material in the open atmosphere include the atmospheric conditions (wind speed, direction, turbulence intensity, atmospheric stability), the properties of the material being dispersed (e.g. density, viscosity, thermal conductivity) and details of the site over which the dispersion is taking place (topography, surface roughness and the presence of obstacles).

In modelling dispersion it is important to properly account for the source conditions, i.e. the way in which the material is first released. For instance, a high-momentum jet typically entrains a significant quantity of surrounding fluid, which can rapidly dilute the mixture.

In some cases, there may be an increase or decrease in the quantity of material being dispersed due to phase change or chemical reactions. For example, in a high-pressure carbon dioxide release, dry-ice particles may sublimate some distance downstream from the release point producing additional gaseous CO_2.

There are numerous works which describe in more detail the underlying flow mechanisms and the different approaches for modelling dispersion. These include the books by Hanna *et al*. (1982), DeVaull *et al*. (1995), Blackadar (1998) and Hanna & Britter (2002) for atmospheric dispersion, the works edited by Puttock (1988) and Castro & Rockliff (1994) on dense gas dispersion and stably stratified flows, and the more general text books by Etheridge & Sandberg (1996) and Goodfellow & Tähti (2001) on industrial ventilation. A summary of the factors influencing indoor dispersion of contaminants is given by Gant *et al*. (2006).

2.2 MODELLING APPROACHES

To model dispersion there exist a variety of approaches of varying degrees of complexity, ranging from simple empirical models to integral and shallow-layer models (for gravity currents) and finally to fully three-dimensional computational fluid dynamics (CFD) models. A summary of the capabilities and limitations of these approaches can be found in Ivings *et al*. (2007).

FLACS is a three-dimensional CFD model aimed at modelling dispersion and vapour or dust cloud explosions. It has some flexibility in terms of the types of flows that can be studied, but does not offer many of the features of other general-purpose CFD codes such as ANSYS-CFX[1], Fluent[2], Star-CCM+[2] or OpenFOAM[3]. For instance, most commercial CFD codes have significant flexibility in the design of the computational grid and a range of sub-models for turbulence, combustion, radiation and multiphase flow. FLACS offers a far more restricted set of approaches but is tailored to certain applications, offering source models for high-momentum jet sources, catastrophic failures and evaporating liquid pools, for example.

Best practice guidance for the use of CFD models such as FLACS is provided by the European Research Community on Flow Turbulence and Combustion, ERCOFTAC (Casey & Wintergerste, 2000). Specific guidance for CFD simulations of flows in the urban environment are also provided by Franke *et al*. (2007).

2.3 DISPERSION APPLICATIONS

The dispersion-modelling element of FLACS was initially developed in the 1980's and 1990's for dispersion of natural gas on offshore platforms (Olav Hansen, Private Communication, April 2008). Savvides *et al*. (2001a) presented the FLACS validation for gas dispersion in an offshore module as part of the Blast and Fire Engineering for Topside Structures project, which followed on from the Piper Alpha incident. In the last decade, work has focussed on other application areas including hydrogen, tracer gases and chlorine. GexCon was a partner in the HySafe project[4], which ran from 2004 to 2009, and involved a number of validation exercises. FLACS was also one of the CFD codes examined as part of a U.S. Department of Homeland Security study of atmospheric dispersion in Manhattan (Flaherty *et al*., 2007).

For modelling explosions, FLACS has been used widely, including in the investigations into the Piper Alpha and West Vanguard incidents and the assessment of the vapour cloud explosion at the onshore process plant at Beek, Holland. More recently, FLACS has been used in investigations of the Petrobras P-36, Buncefield and BP Texas City incidents.

[1] *http://www.ansys.com, accessed January 2009.*
[2] *http://www.cd-adapco.com, accessed January 2008.*
[3] *http://www.opencfd.co.uk, accessed January 2008.*
[4] *http://www.hysafe.org, accessed January 2009.*

3 THE SCIENTIFIC BASIS OF FLACS

3.1 INTRODUCTION

The purpose of this section is to critically review the scientific basis of FLACS in order to understand the capabilities and limitations of the software, based on its underlying mathematical models and numerical implementation.

3.2 INFORMATION SOURCES

A summary of the different versions of FLACS and their release dates is given in Table 1. The present review considers the current version of FLACS (version 9.0), which was released in April 2008. When the present review of FLACS was started, there was no technical documentation available for this version. HSL was advised by GexCon that documentation was provided as an integral part of the FLACS Regular Training Course. One of this report’s authors (James Hoyes) attended the training course in June 2008 and material presented at that course is referenced here as FLACS RTC (2008). In addition to the course material, further technical information was extracted from the FLACS version 8 User Guide, which also provided information on an earlier version of the code, FLACS98, and this is referenced as FLACSv8 User’s Guide (1998). Technical information was also obtained from the FLACS version 8.1 Release Notes, which are referenced as Hansen *et al*. (2005).

Using information obtained from these various sources, a Model Evaluation Questionnaire was completed by HSL as part of the review process. This was reviewed by GexCon, who added comments and provided corrections. This is referenced as MEQ (2008). Further clarification of various sub-models used in FLACS were obtained subsequently from GexCon via email (referenced as private communications) and in January 2009 a draft version of the FLACS version 9.0 User’s Manual was provided to HSL by GexCon. This is referenced as FLACSv9 Draft User’s Manual (2009).

3.3 GEOMETRY AND MESH

In FLACS version 9.0 geometries are created using the pre-solver CASD6 by manipulating simple shapes such as cuboids, cylinders and spheres (FLACS RTC, 2008). Objects can be added or subtracted from one another such that a wide variety of geometries can be constructed.

However, complex geometries such as pipe bends or undulating ground are difficult to generate using CASD6 (FLACS RTC, 2008). Many CFD models have sophisticated design tools that can be used to create highly intricate shapes. In comparison to some design tools, the functionality of CASD6 is limited.

Geometries can also be imported from a CAD file using the FLACS function ‘geo2flacs’ (FLACS RTC, 2008). When importing geometries from a CAD file, geo2flacs converts the geometry objects in the original CAD file into cuboids and cylinders. Furthermore, these shapes are by default rotated to coincide with the Cartesian coordinate system (FLACS RTC, 2008). The alterations made by geo2flacs means the original CAD geometries can become misrepresented in FLACS version 9.0 (FLACS RTC, 2008). For example, a cylinder which is slanting in the original CAD geometry may be represented in the FLACS geometry with its axis aligned to the Cartesian axes. Considerable care is therefore required when using geo2flacs.

Table 1 FLACS Versions and Release Dates[5] (source: Olav Hansen, Private Communication, March 2009)

Release	***Version***	***Date***
FLACS_v9.0	Flacs2.2.6 & Flacs2.2.7	January 2009
	Flacs2.2.6 & Flacs2.2.7	April 2008
FLACS_v8.1	Flacs2.2.6 (inc. DESC_1.0)	July 2006
	Flacs2.2.6 (inc. DESC_1.0B3)	July 2005
	Flacs2.2.6	March 2005
FLACS_v8.0	Flacs2.2.5	February 2004
	Flacs2.2.5	October 2003
FLACS-99	Flacs2.2.5	October 2001
	Flacs2.2.4	January 2001
	Flacs2.2.3	February 2000
FLACS-98	Flacs2.2.2	June 1999
	Flacs2.2.1	December 1998
FLACS-97	Flacs2.1.2	October 1998
	Flacs2.1.1	December 1997
FLACS-96	Flacs2.0.2	June 1997
	Flacs2.0.1	March 1997
	Flacs1.1.1	February 1997
	Flacs1.0.2	February 1997
	Flacs1.0.1	December 1996

Once the geometry has been created or imported, a computational mesh must be constructed. In FLACS, the grid is composed of cubic or rectangular cells with grid lines arranged in vertical or horizontal directions, i.e. a single-block Cartesian grid. It is possible to vary the mesh resolution in any of the Cartesian directions. However, it is not possible to fit the mesh to curved or angled

[5] N.B. When a version has several release dates, this is either due to bug fixes or a functionality update that was not significant enough to warrant a new version number

walls. Instead, these are modelled approximately using stepped walls and cells with a predefined porosity (see, for example, Figure 1). Refining the grid in one region of the flow necessarily leads to refinement elsewhere within the fluid domain, where perhaps it is not needed.

Most general-purpose CFD codes, such as ANSYS-CFX, Fluent, Star-CCM+ and OpenFOAM, use unstructured grids that are able to contour around complex curved or angled walls. Grid refinement can be focused in selected areas and there is considerable flexibility in the shape of cells (e.g. tetrahedra, hexahedra, polyhedra). Such approaches are likely to provide more accurate solutions of flows featuring complex geometry than the Cartesian approach used in FLACS.

Some of the shortcomings of the Cartesian grid approach used in FLACS were mentioned briefly by Hansen *et al*. (2007), who performed simulations of dense gas dispersion over sloping terrain. Modelling the angled surface as a series of steps in the Cartesian grid was reported to produce overly high momentum losses and poor predictions of the hazard distance. It was recommended that to improve predictions, a fine vertical grid resolution should be used to minimize the height of each step in the surface.

For atmospheric buoyant gas releases, the use of a Cartesian grid in FLACS is likely to be less of a limiting factor since any inaccuracies in the predicted flow behaviour near the sloping or undulating ground should have less influence on the mixing processes at higher elevations, where the gas is diluting. An exception to this, however, is where the buoyant gas is released downstream from curved or slanted bluff bodies (for example, a large storage tank or hill), where dilution of the gas is affected by the pattern of flow separation and recirculation produced by the slanted or curved surface. A Cartesian grid with a stepped surface is unlikely to produce reliable predictions of separation and reattachment from curved or slanted surfaces.

It was recently reported by Melheim (2008) that GexCon are planning to implement a more sophisticated Ghost Cell Immersed Boundary Method (GCIBM) to improve the treatment of grid cells bisected by a wall boundary. The merits of GCIBM approaches are discussed by Tseng & Ferziger (2003) and Mittal & Iaccarino (2005).

3.4 DISTRIBUTED POROSITY CONCEPT

The standard method of including solid objects in CFD models is to resolve them using the mesh and to apply appropriate boundary conditions on the surfaces of the objects, such as no-slip conditions. FLACS is commonly used for modelling very complex geometries, such as process plant, which often involve complex arrangements of pipes and ducts that are too small to resolve with the mesh. To resolve such small-scale structures would produce a very fine mesh, which would lead to very long computing times. FLACS therefore uses a distributed porosity approach to model small obstacles. This approach is also employed to model curved or angled surfaces, as illustrated for the case of a cylinder in Figure 1.

The distributed porosity approach involves assigning porosities to the individual mesh cells containing small "sub-grid" obstacles. A volume porosity value of zero corresponds to a completely solid obstruction whilst a volume porosity value of one corresponds to free space. Additionally, FLACS calculates area porosities on each of the control volume faces. These area porosities play an important role in determining the local fluid flow (MEQ, 2008).

The implementation of the distributed porosity concept is outlined briefly in the FLACSv9 Draft User's Manual (2009) and was reviewed by Deevy & Ledin (2004). The approach specifies a source term in the fluid momentum equations which applies a resistance to fluid flow according to the porosity values of the control volumes. Additional production terms are included in the transport equations for the turbulent kinetic energy and dissipation rate to account for the generation of turbulence by sub-grid obstacles. Some further details of the distributed porosity model are given by Arntzen (1998), although there are significant differences between the models described by Arntzen (1998) and the standard implementation in FLACS (Hansen, 2009). This is discussed further in the next section.

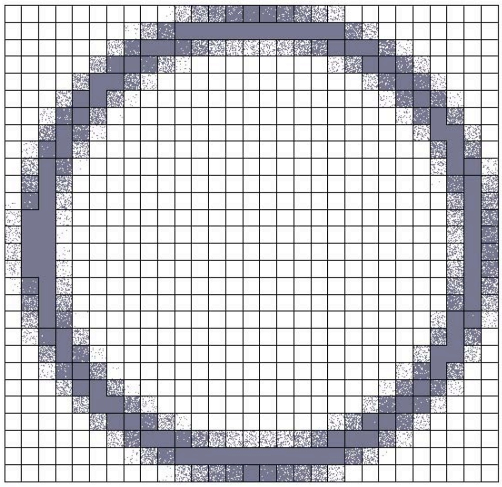

Figure 1 A mesh used to model a cylindrical geometry in FLACS (reproduced from Deevy & Ledin, 2004).

3.5 TURBULENCE

FLACS models turbulence using a Reynolds-Averaged Navier-Stokes (RANS) approach. This is based on the concept of separating the fluid velocity components and scalar quantities such as pressure, temperature and gas concentrations into mean and fluctuating components. Transport equations are solved for the mean values and a model is used to account for the effect of the fluctuating components on the mean values. The mean velocity, pressure, temperature and concentrations calculated by FLACS can be considered as either long time-averaged values (in statistically steady flows) or as ensemble-averaged values. The RANS approach is widely accepted and documented (e.g. Pope, 2000), and is commonly used in engineering CFD studies.

There are a large number of different RANS models which range in terms of complexity and computational cost. FLACS uses a model based on the standard k-ε model of Launder & Spalding (1974). This has been widely used for 30 years in engineering studies and the performance of the model is well-documented in the literature. There are, however, a number of particular features of its implementation in FLACS that differ from the standard approach. These modifications have not been verified by the wider research community.

In the response to the Model Evaluation Questionnaire, GexCon stated that there were two different turbulence models in FLACS version 9.0, both based on the Launder & Spalding (1974) model. The default model, K-EPS-1, was reported to have fixed model constants and the K-EPS-2 model was used for testing purposes only (MEQ, 2008). However, in more recent communications from GexCon it was stated that there is just one k-ε turbulence model in FLACS version 9.0 (Melheim, 2009).

The turbulence model equations used in FLACS are documented in the FLACS version 9.0 User's Manual. However, some details, such as the coefficients used to account for sub-grid obstacles, are not described in the open literature. It is unclear whether the approach used to model sub-grid obstacles, which was derived initially by considering explosion-driven flows, has been recalibrated to model dispersion.

There are differences between the turbulence model equations solved in FLACS version 9.0 and in earlier versions of the software. Some of these differences are discussed in Appendix A. It is unclear whether FLACS version 9.0 would therefore return the same results as earlier versions of the software, although GexCon state that they perform benchmark tests whenever a new version of FLACS is released in order to ensure consistency between the different releases (see Section 4).

The basic turbulence model used in FLACS developed by Launder & Spalding (1974) has a number of known weaknesses which have been documented by, for example, Casey & Wintergerste (2000) and Pope (2000). The model overpredicts turbulence intensities in the stagnation region of impinging jets, which leads to wall heat transfer rates being overpredicted by a factor of two or more (Kato & Launder, 1993, Durbin, 1996). Developing boundary layers around bluff bodies are also poorly predicted as a consequence of the overly high turbulence levels predicted in the upstream stagnation zone. In flows featuring boundary layer separation due to adverse pressure gradients, such as in expanding duct flows, the extent of the separated region is often significantly underpredicted. Secondary swirling flows produced naturally in non-circular ducts are not predicted at all. The spreading rate of round jets is overpredicted by around 40% and the model predicts that plane two-dimensional jets spread 15% faster than round jets, whereas in fact they spread 15% slower (Pope, 1978). There are further issues for jets parallel to walls, as discussed by Etheridge & Sandberg (1996) and Nielsen (2004). Despite these limitations, however, the k-ε model is still very widely used in industrial CFD studies.

Most general-purpose CFD codes offer alternative turbulence models that have been designed to overcome some of the limitations of the standard k-ε model. For example, the industrial codes, Star-CCM+ and OpenFOAM, offer "realizable" k-ε models that limit the production of turbulence energy at stagnation points, which significantly improves the prediction of impinging jets and bluff-body flows. Commercial CFD codes commonly offer ten or more different turbulence model variants. One of the skills of the CFD practitioner is to select an appropriate turbulence model for a given flow. Guidance on the factors that should be considered in selecting a turbulence models are discussed by Casey & Wintergerste (2000). In complex flows, where it is difficult to identify the optimum model, it is recommended to assess the sensitivity of the CFD predictions to the choice of turbulence model by running simulations with more than one model. Such sensitivity analyses are not possible in FLACS, which only offers one model.

3.6 HEAT TRANSFER

Temperature variations can have a significant influence on fluid density and hence dispersion and it is important therefore that it is modelled accurately. FLACS version 9.0 determines fluid temperatures by solving a transport equation for the fluid enthalpy. Details of the thermal boundary conditions are not provided in the FLACSv9 Draft User's Manual (2009).

Radiation is typically less important in most dispersion scenarios. However, it can be modelled in FLACS version 9.0 in two ways. Firstly, using a simple model which accounts only for the heat loss due to radiation inside a rectangular region, and secondly, using a 6-flux model calculating radiation heat fluxes (MEQ, 2008). A more advanced radiation model that uses a ray-tracing approach is under development for the FLACS-Fire model (MEQ, 2008).

FLACS cannot currently model heat conduction in solids, unlike many other industrial CFD codes which can model so-called conjugate-gradient heat transfer. However, this is not critical in most dispersion calculations.

3.7 DENSITY VARIATIONS

FLACS version 9.0 employs a non-Boussinesq approach to model density variations due to differences in fluid temperature and composition (FLACS RTC, 2008). In the non-Boussinesq approach, variations in fluid density are accounted for throughout the governing equations. This is suitable for modelling a wide range of density variations.

Many CFD models also provide the option to use a Boussinesq approach, in which the variations in fluid density are only accounted for in a buoyancy term in the momentum equations and in a buoyancy production term in the turbulence model equations. The advantage of the Boussinesq approach is that it is typically less computationally expensive and numerically more robust than the non-Boussinesq approach. However, the Boussinesq approach is only valid when density variations are small (typically less than five percent). FLACS version 9.0 does not offer a Boussinesq approach.

Density variations can have a significant effect on dispersion through its effect on turbulence. A stably stratified density field (with density decreasing with height) acts to damp turbulence and thus reduce mixing, whilst an unstably stratified density field can act to generate turbulence and increase mixing. FLACS uses the simple gradient diffusion model to account for the effect of buoyancy on turbulence (FLACSv9 Draft User's Manual, 2009). This is widely used in engineering studies but is known to produce too little turbulent mixing in vertical buoyant plumes. As a consequence, spreading rates are underpredicted and mean centreline values of velocity and temperature or concentration are overpredicted (see for example Van Maele & Merci, 2006).

3.8 MULTI-COMPONENT AND MULTIPHASE FLOWS

In multi-component flows, for example the dispersion of hydrogen in air, two or more components are mixed at a molecular level and share the same velocity, pressure and temperature. Multiphase flows, on the other hand, involve distinct interfaces between the different phases and the two phases may not necessarily share the same velocity or temperature. Examples of multiphase flows include the transport of coal dust in air or the dispersion of a spray of petrol droplets.

For modelling multi-component or multiphase flows, FLACS version 9.0 employs a single set of Navier-Stokes equations to model a homogeneous velocity field and a scalar transport equation to model the volume fraction (or concentration) of the different fluid components (FLACS RTC, 2008). The two or more components or phases share the same velocity and temperature field. This approach is commonly used in CFD models to simulate multi-component flows.

Details of the transport equations employed in FLACS98 are documented in the FLACS version 8 User's Guide (1998) and a similar approach is employed in FLACS version 9.0 (FLACS RTC, 2008). Turbulent mixing is accounted for via an effective viscosity term (FLACS version 8 User's Guide, 1998).

Most general-purpose CFD codes feature two alternative models for multiphase flows: Eulerian and Lagrangian. In the Eulerian approach, the dispersed phase (e.g. coal dust, petrol droplets) is modelled as a continuous fluid, which in some cases may have a different velocity to that of the surrounding fluid. In the Lagrangian approach, the paths of individual particles are tracked through the fluid. Usually several thousand particles are modelled and each computational particle represents a statistical sample of many droplets or solid particles. FLACS does not currently feature either of these models for multiphase flows.

FLACS version 9.0 cannot model the dispersion of aerosol particles (FLACS RTC, 2008). However, a utility program called FLASH can be applied to define the release source at a distance where aerosol particles have been vaporised (MEQ, 2008).

A module called FLACS-DESC is included in FLACS version 9.0 to model dust explosions. Whilst this may be used to model certain scenarios involving the dispersion of particles, it was not specifically designed for this purpose. According to Skjold (2007) particles are modelled as a continuous phase with variable concentration. This model has been reviewed by Deevy and Ledin (2004).

A beta version of the FLACS-Pool model was released as part of FLACS version 9.0 to simulate the spreading of liquid pools. The model uses a shallow-water approach (FLACS RTC, 2008). A brief description of the model's application to simulate LNG releases is given by Hansen *et al*. (2007) and Hansen *et al*. (2008). Although the model is demonstrated in these papers, there does not appear to exist yet any validation of the model in the open literature.

3.9 BOUNDARY CONDITIONS

3.9.1 Inlet Conditions

In FLACS version 9.0, either constant speed or fluctuating velocities can be applied with specified direction at inlets. Fluctuating velocities are defined using sine and cosine waves, where the user specifies the amplitude and frequency (FLACS RTC, 2008). Alternatively, an arbitrary velocity distribution can be specified through an ASCII data file (Hansen *et al*., 2005). There are three set levels of turbulence intensity in the inlet flow that can be selected: low, medium or high, but details of these conditions are not provided in the FLACSv9 Draft User's Manual (2009).

For atmospheric dispersion simulations, FLACS version 9.0 includes some specific models to provide inlet velocity profiles for the wind which take into account the atmospheric stability (classified in terms of Pasquill classes A to E), upstream surface roughness and the velocity at a reference height.

Hanna *et al*. (2004) reported that standard engineering approaches for specifying inlet boundary conditions based on logarithmic velocity profiles and specified turbulence intensity and length scale typically lead to over-prediction of the gas concentrations in gas dispersion simulations, due to under-prediction of atmospheric boundary layer turbulence (see also Hanna *et al*., 2002, and Riddle *et al*., 2004). To improve predictions, FLACS version 9.0 uses an approach devised by Han *et al*. (2000) and Arya (2001) in which the turbulence characteristics are modified, based on the Pasquill stability class or Monin-Obukhov length. Details are provided in the FLACSv9 Draft User's Manual (2009).

In atmospheric dispersion simulations, large-scale turbulence or meandering flow is accounted for in FLACS version 9.0 by imposing a sinusoidal fluctuation in the mean velocity. In the case study of Hanna *et al*. (2004), they chose harmonic waves with periods 10-15 seconds and 60-70 seconds. Slightly different frequencies were chosen for the fluctuations in the three coordinate directions to avoid producing repeated flow patterns. The fluctuations had magnitudes of 2.4, 1.9 and 1.3 times the friction velocity in the streamwise, spanwise and vertical directions respectively, which were selected based on observations of near-neutral stability conditions reported by Arya (2001). It is unclear whether the period of the wind fluctuations in the Hanna *et al*. (2004) study were chosen based on measured meteorological conditions, and whether the default values for the fluctuating wind boundary conditions in FLACS version 9.0 are appropriate for a wide range of atmospheric flows.

3.9.2 Wall Functions

In turbulent flows, the velocity, temperature and turbulence parameters vary rapidly in a thin region close to solid boundaries. In most engineering studies, rather than try to resolve these rapid changes, which would require a very fine grid and prolonged computing times, simplifying assumptions are used. The velocity and temperature are usually assumed to vary logarithmically with distance from the wall within the wall-adjacent grid cell and certain simplifying assumptions are used to modify the turbulence transport equations (for details, see for example Versteeg & Malasekera, 1995). The assumed profiles and modified terms are commonly referred to as “wall functions”.

FLACS uses the standard approach of applying wall functions, where the velocity within the near wall grid cell is assumed to vary linearly or logarithmically, depending upon the height of the cell. From the description given in the FLACS version 9.0 Draft User’s Manual (2009), the wall function does not appear to be able to account for wall roughness. Details of the thermal boundary conditions at walls are also not provided in the FLACS version 9.0 Draft User’s Manual (2009).

3.10 SOURCE MODELS

3.10.1 High Momentum Jets

FLACS version 9.0 features a separate sub-model for high momentum gas jets (FLACS RTC, 2008; MEQ, 2008). Rather than attempt to model the complex arrangement of shock structures in the region immediately adjacent to the jet release location, the sub-model calculates pseudo-source conditions which approximate flow conditions a short distance downstream from the release point, where the jet has expanded to atmospheric conditions. This approach is commonly used in CFD simulations of high-pressure jets (e.g. Ivings *et al*., 2008). The sub-model assumes that there is no air entrainment from the gas source to the point where the jet has expanded to atmospheric conditions. The area that is modelled in FLACS is the area of the expanded jet and the velocity at the pseudo-source is the subsonic velocity after expansion.

Once the conditions have been calculated using the separate sub-model they are entered manually into FLACS (FLACS RTC, 2008). The sub-model uses an Abel-Noble equation of state, which makes it suitable for modelling hydrogen releases (MEQ, 2008). Details of the sub-model for FLACS98 are provided in the FLACS version 8 User’s Guide (1998).

Unlike most general-purpose CFD codes, in FLACS version 9.0 the jet must be aligned to one of the Cartesian axes (FLACS RTC, 2008). Since FLACS is limited to using Cartesian meshes, the circular pseudo-source jet exit must also be approximated using staggered cells with an equivalent surface area. In jet simulations, it is important to ensure that the grid is sufficiently fine in the shear layers around the jet to avoid numerical diffusion artificially increasing the spreading rate of the jet. Designing a mesh in FLACS to resolve these shear layers leads to cells being clustered together needlessly elsewhere in other regions of the flow, due to the limitations of the single-block Cartesian grid used in FLACS.

In the FLACS version 9.0 User's Manual, it is warned that in simulations of dispersion from gas jets in large domains, where relatively coarse grids are normally used, the production of turbulence may be underestimated and the simulation may be influenced by numerical diffusion so that "one might expect that the turbulent (or effective) mixing process is not represented with high accuracy". This issue was also raised in the recent work by Middha *et al*. (2007b) on hydrogen jets.

3.10.2 Evaporating Liquid Pools

The capability to model evaporation from a steady-state liquid pool source was introduced in FLACS version 8.1 and some details of this function are documented in the FLACS version 8.1 Release Notes (Hansen *et al*., 2005) and by Kim & Salvesen (2002). Only circular shaped pools can be modelled and it is necessary to specify the evaporation rate of the liquid fuel (Hansen *et al*., 2005).

Evaporation from transient liquid pool sources cannot be modelled in FLACS version 9.0. However, GexCon are developing a sub-model for the spreading of a liquid pool (FLACS RTC, 2008, Hansen *et al*., 2007; 2008).

3.10.3 Flashing Releases

FLACS contains a utility program called "FLASH" that calculates the location and characteristics of a pseudo-source for a flashing release to input as boundary conditions into FLACS. The model accounts for air entrainment, droplet rain-out and evaporation and provides source conditions at the position downstream from the release where the conditions are purely gas phase and the liquid fraction has either rained-out or evaporated. FLASH was used in the study of chlorine gas release by Hanna *et al*. (2009) and its development is described in the report by Salvesen (1995).

Recently, GexCon has developed a new source model for flashing releases and tested a homogeneous equilibrium model to simulate the vaporisation of droplets. The model development and its validation for the recent Ineris tests on propane and butane releases is presented by Ichard *et al*. (2009). These models are not available in the standard FLACS version 9.0 release.

3.11 NUMERICAL METHODS

In contrast to many CFD models, FLACS does not have the option to operate as a steady-state solver (FLACS RTC, 2008). For statistically steady flows, which remain unchanged over time, a transient calculation is performed until a quasi-steady solution is reached.

Details of the spatial or temporal discretization schemes are not provided in the FLACSv8 User's Guide (1998) or FLACSv9 Draft User's Manual (2009). According to Middha *et al*. (2007b), second-order spatial discretization schemes are used to solve the conservation equations for mass, impulse, enthalpy, turbulence and species/combustion consisting of Kappa schemes with weighting between second-order upwind and second-order central difference, with delimiters for some equations.

FLACS version 8.1 employed a first-order backward Euler time differencing scheme (Skjold, 2007), while version 9.0 uses a combination of first- and second-order accurate temporal discretization schemes (FLACS RTC, 2008).

The SIMPLE pressure-correction algorithm of Patankar & Spalding (1972) is used to ensure mass continuity (FLACSv8 User's Guide, 1998).

3.12 GRID DEPENDENCE

One of the challenges in modelling atmospheric dispersion using CFD is the physical scale of the problem. The distance over which a gas cloud travels in many cases is of the order of a kilometre and the computational domain can therefore be very large. In the case of dense gas dispersion, the cloud thickness may only be a few metres deep, and for reliable simulations it may also be necessary to account for obstacles that can be of the scale of a metre or less. To resolve these small flow features, the grid must therefore be reasonably fine. This means that the total number of grid cells can be very high. Moreover, since for starting plumes or "puff" releases the flow is inherently transient, the computing time required for these CFD calculations can be very long (days or weeks for a single run). To undertake practical dispersion simulations using desktop computers within a reasonable length of time necessitates the use of relatively coarse grids. Results are therefore more likely to be grid dependent, i.e. if a finer mesh is used the predictions may change. Whilst it may be impractical to achieve fully grid-independent results, it is critically important that the sensitivity of the results to the grid resolution is assessed by obtaining predictions with coarser or finer grids. This is standard practice (Casey & Wintergerste, 2000).

This issue of grid dependence is compounded in FLACS due to two features of the code. Firstly, FLACS is constrained to use a Cartesian grid. This means that sloping ground has to be modelled as a series of steps, and circular objects (such as jet orifices) have to be approximated as an equivalent square or stepped circle (see Section 3.3). As the grid is refined, the shape of the topography or orifice changes. Secondly, objects that are too small to be resolved by the grid are accounted for by assigning cells a certain porosity (see Section 3.4). Using a finer grid may result in some of the objects being modelled explicitly, as blocked regions with walls on the surfaces, rather than cell porosities. These features of the code mean that for complex geometries it is even more important to undertake tests to examine the grid dependence of the results. Even if the grid cannot be refined significantly throughout the domain, small-scale tests should be undertaken in certain critical regions of the flow domain.

The FLACSv9 Draft User's Manual (2009) contains some guidance on the appropriate design of grids. It suggests that users should consider the location of the grid lines when constructing the geometry to ensure that walls and decks are placed at the nearest grid cell interface, to avoid the porosity pre-processor automatically moving the geometry in unwanted directions. For jet releases, it recommends that the area of the source, once expanded to ambient pressure, should be resolved by one grid cell. It also suggests that the grid be refined in directions normal to the axis of the jet, but not in the direction parallel to the jet axis. For dense gas releases, the manual recommends refining the grid in the vertical direction near the ground. Further advice is provided for the design of grids used to model gas explosions and the propagation of blast waves. With a few exceptions, such as the resolution of sloping terrain, Gexcon consider that these guidelines produce simulations that do not exhibit significant grid dependency (Olav Hansen, Private Communication, August 2009).

Research undertaken as part of a joint industry funded project on modelling dispersion in gas turbine enclosures (Ivings *et al*., 2004) found that to obtain accurate predictions it was advisable to resolve the leak source with at least 10 cells, or more in the case of sub-sonic releases. Furthermore, it recommended the grid be refined along the length of jet, where high flow-variable gradients exist. The difficulty in applying such recommendations to FLACS simulations, is that they will lead to grid cells being clustered together needlessly in other regions of the flow, far from the jet source, due to the limitations of the single-block Cartesian grid arrangement. To run simulations using this type of grid is likely to result in very lengthy computing times. Such difficulties were not encountered in the study by Ivings *et al*. (2004), since the commercial CFD codes employed in their study used unstructured grids, which offered more flexibility in terms of the grid design, and meant that grids could be refined solely in the region near the jet.

The FLACSv9 Draft User's Manual (2009) contains quite specific guidance on the size of cells for modelling gas explosions and blast wave propagation. For example, it recommends use of purely cubic cells within the combustion zone and a maximum control volume size of 10% of the gas cloud diameter. However, these guidelines were developed following extensive validation in explosion-driven flows and tuning of model parameters, such as the turbulence generation terms described in Appendix A. Such validation is not directly relevant to the application of FLACS to modelling dispersion.

The issue of grid dependence of CFD results is well known and recommendations are provided in most CFD best practice guides, such as those produced by Casey & Wintergerste (2000) and Franke *et al*. (2004). The latter guide recommends that for validation of CFD models of flows in the urban environment, a systematic grid convergence study should be undertaken using at least three different grids. For microscale obstacle-resolving meteorological models, it states that results obtained using two different grids should agree within allowed discrepancies, such as those published by VDI (2005). Publications such as the well-respected ASME Journal of Fluids Engineering will not accept articles for publication unless CFD results have been shown to be grid-independent[6].

[6] *http://journaltool.asme.org/Templates/JFENumAccuracy.pdf, accessed September 2009.*

4 VERIFICATION

Verification is the process of checking that the computer implementation of a model accurately represents its mathematical basis, i.e. that the model equations have been coded correctly. It can be undertaken following a number of different approaches. One approach is to compute problems for which there are known analytic solutions. In the case of CFD models, an alternative approach is the method of manufactured solutions (Roache, 1998).

Model verification is essential and it should be assessed as a part of any model evaluation process. In the MEP described by Ivings *et al.* (2007) verification is treated passively as part of the scientific assessment rather than as an exercise in its own right. The same approach has been adopted here and evidence for the verification of FLACS has been sought from GexCon. This information is recorded and assessed.

Some details of verification activities undertaken by GexCon have been provided in the MEQ (2008). GexCon report that benchmark simulations are performed for cases with analytical solutions, such as a shock-tube flow.

FLACS is supported on different operating systems and GexCon state that identical calculations are undertaken on each operating system in order to ensure that the different versions produce the same results. Similar tests are also performed with different compilers to discover any optimisation errors. GexCon state that they perform benchmark tests whenever a new version of FLACS is released in order to ensure consistency between the different releases. Only minor adjustments or improvements were made between FLACS versions 8.1 and 9.0, so the results should only differ slightly (MEQ, 2008).

In addition to computing benchmark scenarios, GexCon state that whenever a new numerical scheme is implemented, they undertake tests to ensure that the model remains internally consistent. This includes checking that where the initial and boundary conditions are symmetrical, the model produces symmetrical results and also that the model remains directionally independent.

The GexCon programmers use version control systems when writing source code, but different releases of FLACS have the same version number. For example, FLACS version 9.0 was first released on 24/04/08 and an updated version also called FLACS version 9.0 was subsequently released on 04/06/08 (MEQ, 2008).

Unfortunately, detailed information on the verification of FLACS is not available publicly. Hence, the model verification described here is reliant on the claims made by the model developer and cannot be substantiated. Based on what GexCon state, good verification is undertaken for FLACS. Clearly, it would be better if this information were available in the public domain. However, it is not unusual that such information is not publicly available.

5 VALIDATION

5.1 INTRODUCTION

Validation consists of comparing a model's predictions against measurements to determine whether the underlying physics has been well approximated. Ideally, validation should be undertaken over the range of applications for which the model is intended to be used.

Validation of atmospheric dispersion models is not straightforward. Difficulties relate to the need to ensure the quality of measurement data used to evaluate model performance, and to understand the general behaviour of the models, instead of relying on a few limited statistical metrics. In some cases, it may be incorrect to assume that a perfectly-accurate model will reproduce measured values. For instance, models based on RANS turbulence closures should not be expected to predict the instantaneous maximum concentrations in field experiments, since they inherently solve for mean values. It is also important to understand how certain parameters have been determined in the experiments. For example, in the Kit Fox trials (WRI, 1998), discussed later, the reported cloud speed was averaged over the entire trajectory of the cloud, determined by dividing its downwind distance by the time from the release (Hanna & Chang, 2001). This is not necessarily the same as the local cloud speed predicted by a dispersion model. It is also necessary to understand the physical basis of models to ensure that good predictions are obtained for the "right reasons", not a fortunate coincidence of several errors cancelling each other.

Compared to many fields of engineering, especially aeronautics, the acceptance standards for validation of atmospheric dispersion models are relaxed. Commonly, a model is considered to provide acceptable performance if predictions are within a factor of two of the measurement data for half of the time (CCPS, 1996). This in part reflects the level of uncertainty in many of the sets of measurement data. It was shown by Davies (1987) that multiple repeats of an instantaneous release of a dense gas under nominally identical conditions in a wind tunnel can produce concentrations at downstream locations which vary by roughly a factor of two. Ensemble-averaged mean data sets are rarely available, especially for field trials.

In some of the validation studies discussed below, the grid dependence of the FLACS results has not been presented. Consequently, there is some uncertainty in what can be concluded from these validation exercises. Whilst in some cases good predictions have been obtained, it is difficult to know whether different results would be obtained if a finer, or coarser, grid was used. Most of the validation studies also do not report which version of FLACS was used.

5.2 DENSE GAS DISPERSION

5.2.1 Open Terrain

Hansen *et al*. (2007) and Hansen *et al*. (2008) used FLACS to simulate the dispersion of LNG, produced by spills on water, over open terrain. Simulations were compared to data from the Burro, Coyote and Maplin Sand experiments (Koopman *et al*., 1982; Puttock *et al*., 1982). The source term of vapour from the LNG vaporisation was not predicted or modelled in the simulations. Instead, a low-momentum source of vapour was specified based on the evaporation rate reported in the experiments. The area over which the vapour was released was also fixed.

In addition to the dispersion simulations, Hansen *et al*. (2007) and Hansen *et al*. (2008) presented a shallow-water model for LNG pool spread and evaporation. However, neither this model nor the LNG pool source model of Kim & Salvesen (2002), which was also mentioned in the papers, were used to provide the vaporization rates for the Burro, Coyote and Maplin Sand trials (Hansen, 2009).

A grid-dependency study involving two grids comprising either $4 \times 4 \times 0.5$ or $2 \times 2 \times 0.25$ metre cells was performed. Gas concentrations were up to one-and-a-half to two times higher on the fine grid than the coarse grid in the important region between 100 and 400 metres from the source. In the Burro and Coyote simulations, two buildings used for instrumentation and gas storage were included in the modelled geometry.

Details of the boundary conditions used were limited. It was stated only that the "proper" wind direction was simulated with some assumed meandering of the wind.

As mentioned above, FLACS uses a RANS turbulence model which provides values of the mean gas concentrations. To compare its predictions of the maximum gas concentration to the measured values, Hansen *et al*. (2007) and Hansen *et al*. (2008) averaged the experimental gas concentrations over a period of 10 seconds. Although different averaging periods were said to have been tested (0, 10, 30 and 60 seconds), only the results using an averaging time of 10 seconds were presented. It was considered that an averaging period longer than 10 seconds was not appropriate since in some cases the measurements only recorded a finite gas concentration for a short period of time (of the order 20 s) and so averaging over a longer period would have artificially decreased the peak concentration (Hansen, 2009). Ivings *et al*. (2007) have shown that averaging times can have a significant effect on the mean value, producing differences of a factor of two or more for short averaging times of around a second compared to an averaging time lasting the duration of the release. This issue is also discussed with respect to the Thorney Island dense gas dispersion trials by Webber (2002).

In general, the FLACS results reported by Hansen *et al*. (2007) and Hansen *et al*. (2008) were in reasonably good agreement with the averaged data. The results are compared to the predictions of various other dispersion models, taken from Hanna *et al*. (1993), see Figure 2. The geometric mean (MG) and geometric variance (VG) shown in Figure 2 are parameters commonly used for dispersion model validation, definitions can be found in CCPS (1996). A "perfect" model has MG and VG values of 1.0, and the parabola marked in the graph represents the minimum value of geometric variance for a given value of the geometric mean. A value of geometric mean of 0.5 and 2.0 can be considered as "factor of two" over- and under-predictions of the mean, respectively. A geometric variance of around 1.6 represents a typical factor of two scatter between individual pairs of observed and predicted values. The Hansen *et al*. (2007), Hansen *et al*. (2008) and Hanna *et al*. (1993) results shown in Figure 2 are not directly comparable, since the latter includes validation from a wider set of experiments, but the comparison provides an indication of the general level of accuracy obtained using various dispersion models. The models: HGSYSTEM, DEGADIS, GASTAR, B&M and SLAB, show roughly similar levels of performance to FLACS in terms of VG and MG.

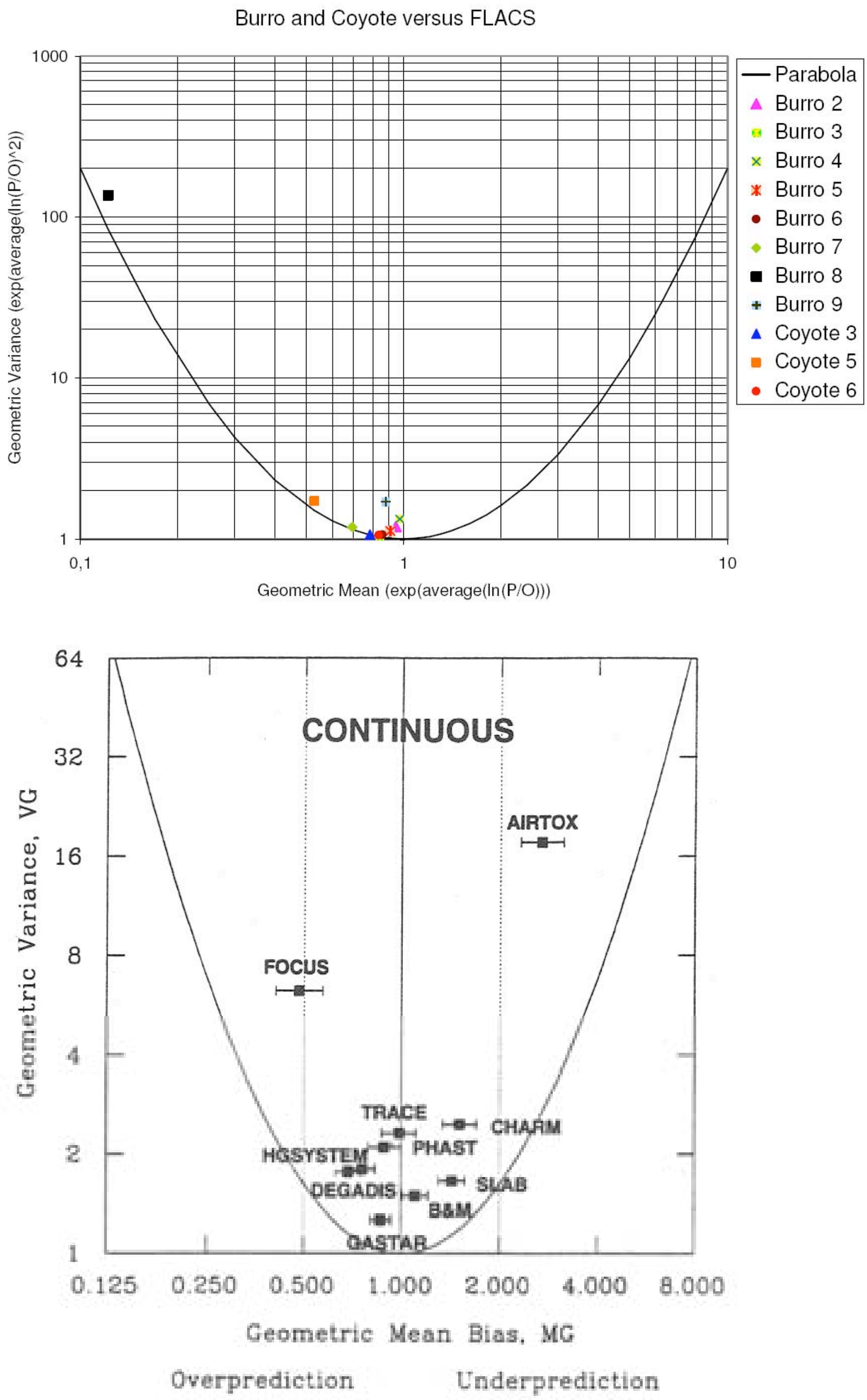

Figure 2 Comparison of geometric variance versus geometric mean for the Burro and Coyote tests using FLACS from Hansen et al. (2007) (top), and for ten other dispersion models compared to the Burro, Coyote, Desert Tortoise, Goldfish, Maplin Sands and Thorney Island tests from Hanna et al. (1993) (bottom), reprinted with permission from Elsevier. Note: vertical scales are different.

All of the FLACS results were within a factor of two with the exception of the Burro 8 test, for which the gas concentrations were underpredicted by a factor of ten. The poor prediction for this case was attributed to the fact that the gas cloud was mainly below the lowest measurement sensors in the simulations, whereas in the experiments the more chaotic wind field led to the gas cloud sporadically reaching the sensors. The Burro 8 trial was notable in that it was conducted under very low wind speed conditions and the spread of the gas cloud was therefore affected more by the site topography than the other tests. The terrain rose to a height of around 7 metres above the pool level at a downwind distance of 80 metres and thereafter remained relatively level. In the FLACS model, however, the terrain was treated as flat. This limitation was acknowledged by Hansen *et al*. (2007), who reported that some simulations had been performed using sloping terrain with FLACS. However, the stepped geometry gave an overly high momentum loss, which adversely influenced the spreading rate of the cloud. Hansen *et al*. (2007) commented that dense gas dispersion simulations over sloping terrain should use a fine vertical grid resolution to minimise this effect and that future development of FLACS will investigate different approaches to minimize the momentum loss.

Further details of the validation study by Hansen *et al*. (2007) and Hansen *et al*. (2008), such as a description of the assumed LNG pool evaporation rate and fixed pool size, the boundary conditions and the mesh[7] may be provided in a more comprehensive 140-page confidential report on the work which was written for the project sponsors (Hansen, 2009).

5.2.2 Obstructed Terrain

Kit Fox Trials

A validation study for dense gas dispersion over obstructed terrain was reported by Hanna *et al*. (2004). FLACS predictions were compared to measurements for the Kit Fox trials (WRI, 1998) which involved carbon dioxide releases across a Nevada test site fitted with thousands of flat billboard obstacles 0.2 and 2.4 metres high, installed across a 123 × 314 m area. Tests were undertaken with different combinations of obstacles with both short “puff” releases lasting 20 seconds and long duration “plume” releases lasting 2 to 5 minutes. All of the experiments took place in the evening when the atmosphere was neutral or stable and the average wind speed was 2.5 m/s. The lowest atmospheric wind speed in the tests was 1.8 m/s.

FLACS simulations were performed using a mesh comprising 33,000 cells with some checks performed using a finer mesh with 308,000 cells. The size of the cells was not given, although it was stated that the source of the gas release, with dimensions 1.5 × 1.5 metres was resolved with at least one cell. The size of the computational domain was also not given. Assuming the domain extended across the test site to a height of around 8 metres, the average cell dimension for the coarse mesh would be around 3 metres. It is not clear whether the mesh resolved any of the billboard obstacles, or whether these were all treated using the distributed porosity model. It was mentioned that the model needed to be modified as too little turbulence was generated behind obstacles with size equal to one grid cell. This modification may have been that described in Appendix A of Arntzen (1998). No results were presented or discussed for the finer mesh.

Details of the boundary conditions used were limited. The wind inflow boundary condition was based on the assumed roughness upstream of the experiment. The meandering flow conditions mentioned in Section 3.9.1 were used with periods of 10 to 15 s and 60 to 70 s, and amplitudes

[7] *It is not clear from Hansen et al. (2007) and Hansen et al. (2008) whether the coarse or fine grid was used to generate the majority of the results for the Burro, Coyote and Maplin Sand tests.*

3.4, 1.9 and 1.3 times the friction velocity in the streamwise, spanwise and vertical directions respectively. It is unclear how these related to the conditions present in the Kit Fox trials or whether they are default values in FLACS.

The FLACS predictions for the Kit Fox trials were found to be in fairly good agreement with the experiments. The relative mean bias was ±20%, and over 90% of the model predictions were within a factor of two of the observations. The results tended to overpredict the maximum concentration when taller obstacles were present and underpredict concentrations when lower obstacles were present (in each case by 30 – 40%). There were no general trends to over- or under-predict maximum concentrations with wind speed, stability or downwind distance.

To assess to the quality of these predictions, the results can be compared to the earlier study of Hanna & Chang (2001), who performed simulations of the Kit Fox trials using standard and modified variants of HEGADAS, an integral model for dense gas dispersion that uses assumed profiles and empirical relations for air entrainment. The modified model, HEGADAS 3+, was found to give predictions of the Kit Fox trials with a mean bias of about 5% and with approximately 90% of the predictions within a factor of two of the observations, in a similar overall level of agreement to the FLACS results. CFD results for the Kit Fox trials are also reported by Mazzoldi *et al*. (2008).

Chlorine Releases

A second and more recent study of dense gas dispersion over complex terrain using FLACS was reported by Hanna *et al*. (2009). Simulations were performed of an incident at Festus, Missouri, in 2002, in which chlorine was released from a railcar following an accident. Nearly 22 tonnes of chlorine was released from a pressurized vessel at a constant rate for over 3 hours. Videos and photos showed a large visible gas cloud extending about 20 or 30 metres around the railcar to a depth of around 1 metre. No information exists on the arrival times of the visible gas cloud. The weather conditions were overcast with some drizzle and the wind speed at the nearest airport 60 km away was 3 m/s.

The release was modelled in FLACS as a 2.02 kg/s flashing jet. Pseudo-source conditions were calculated using the FLASH utility in FLACS (see Section 3.10.3). The jet pseudo-source had a temperature of -71ºC and a velocity of 76 m/s, and due to air entrainment, a total mass flow rate of 6.83 kg/s. The diameter of the pseudo-source was not stated. The conditions were applied 1 metre from the actual source and the jet impinged on the nearby cylindrical body of the railcar. Although the wind speed was measured at the nearby airport to be 3 m/s, a lower velocity of 2 m/s at a reference height of 10 metres was used to account for the effect of local obstructions on the wind field.

The geometry of the domain was typical of a medium sized industrial site, including numerous obstacles such as buildings, tanks, railcars and trees. The grid was refined near the source of the release with cubic cells of side 0.2 m. In the region where the gas cloud was observed, within 50 metres of the source, cells of size 1 × 1 × 0.2 m were used. Further away from the release a coarser mesh was used. The total size of the domain and the number of grid cells was not stated. No grid sensitivity tests were reported.

The upstream boundary conditions were specified using the wind speed at a reference height, the Pasquill stability, and the default FLACS models for the velocity, temperature, turbulence profiles, and wind meandering effects. A no-slip condition was used on the ground and passive, ambient pressure conditions were used at outflow boundaries. The conditions used on the upper surface of the domain were not described.

Results were presented comparing the extent of the visible gas cloud from the FLACS predictions to images from video footage of the incident. The concentration of chlorine gas that gives rise to a visible cloud was uncertain. Hanna *et al*. (2009) noted that it was likely to comprise condensed water droplets (mist) in addition to chlorine, and that a report by the agency WorkSafeBC had stated that chlorine was not visible as a greenish-yellow cloud at concentrations below 1000 ppm. Hanna *et al*. (2009) presented the cloud as an iso-contour at a concentration of 2000 ppm as this best matched the observed cloud extent. The effect of changing the selected chlorine concentration level used in the comparison was not discussed. Overall, the predicted shape and depth of the cloud appeared to be in reasonably good agreement with the video footage. In the incident, the cloud appeared to have been blocked from dispersing on one side by a thick hedgerow. This appeared to be represented in the FLACS model as a row of circular cross-section obstacles. It is unclear how these obstacles were designed or whether the sensitivity of the model predictions to the choice of obstacles was explored.

Further simulations of chlorine dispersion were presented by Hanna *et al.* (2009) for a hypothetical release occurring at a railroad junction near downtown Chicago. The FLACS model included realistic city geometry. No data were available for model validation but results were compared to several, more simple dense gas dispersion models: SCIPUFF, ALOHA, SLAB HGSYSTEM and PHAST. Results were compared for the predicted 10-minute average maximum concentrations at several distances up to 2 km from the source. There was a factor of approximately 8 to 10 difference between the minimum and the maximum predicted concentrations with the different models at any distance, with FLACS results near the middle of the range of predictions. It was concluded that the FLACS results were not inconsistent with the predictions of other dispersion models.

5.3 PASSIVE DISPERSION

5.3.1 Open Terrain

Prairie Grass Experiments

Hanna *et al*. (2004) presented FLACS simulations of passive (neutrally-buoyant) tracer gas dispersion over open terrain and compared results to the Prairie Grass field experiments of Barad (1958). In the experiments, a tracer gas was released continuously from a small tube at a height of 0.46 metres over an open agricultural field which at the time contained short dry stubble. The atmospheric conditions were neutral or unstable.

The grid used in the FLACS simulations comprised 50,000 cells. No sensitivity tests to the grid resolution were reported, although it was noted that the gas concentration near the source would probably be underpredicted because the mesh was too coarse to resolve the small source diameter. Details of the boundary conditions used to model the Prairie Grass tests were also not described.

Modifications to FLACS to enhance the turbulence intensity behind obstacles as described above for the Kit Fox trials were reported to have been used for the Prairie Grass simulations, despite the fact that there were no obstacles present.

FLACS simulations were performed for both unstable and neutral conditions. Taking the median over all five measurement arcs, just under half of the predictions were within a factor of two of the measurements. The model was found to overpredict gas concentrations at the measurement positions furthest from the source in unstable conditions. This was attributed to unstable buoyant plumes (thermals) lifting the plume off the ground, a phenomena previously noted by Weil *et al*. (1992) and also reported in the CFD simulations of the Prairie Grass experiments by Mazzoldi *et al*. (2008). It was also found that simulations took longer for FLACS to converge for the unstable cases (Pasquill classes A – C).

5.3.2 Obstructed Terrain

EMU Building

Hanna *et al*. (2004) presented results from two sets of tests involving dispersion of a passive tracer gas over obstructed terrain. The first study involved flow over an L-shaped building which had been studied previously as part of the EU-sponsored Evaluation of Model Uncertainty (EMU) project (Hall, 1997). Wind-tunnel experiments were performed in which neutrally-buoyant gas was released from the inside corner of the L-shaped building and gas concentrations were monitored at various downstream positions.

To model this scenario using FLACS, no meandering of the wind was assumed as it was considered less likely to have occurred in the wind tunnel. The wind inflow conditions were calculated using a surface roughness height which was assumed based on the upstream conditions in the experiment. No further details of the boundary conditions were described by Hanna *et al*. (2004), nor was there a description of the grid or the computational domain. It is unclear whether a grid dependency study was carried out.

To assess the model performance, Hanna *et al*. (2004) presented the FLACS predictions and wind tunnel measurements of gas concentrations as numeric values in a large table. These values are plotted as six profiles in Figure 3. The y/H values shown refer to spanwise positions, where y is the distance and H is the building height (10 m), with the source location at y = 0. The results shown are for an array of points one building height downstream of the EMU building. Concentrations are generally slightly overpredicted in the recirculation region downstream of the building and underpredicted (by up to a factor of three) elsewhere. In a related validation study of dispersion over an array of building-shaped obstacles, Chang & Meroney (2003) also found that the k-ε turbulence model overpredicted gas concentrations in the wakes of buildings. This was attributed to the model's lack of ability to capture the intermittent nature of the turbulence in the recirculation zone. In the Hanna *et al*. (2004) study, the length of the recirculation zone was reported to be underpredicted (a length of 1.0 – 1.5 H, compared to the measured value of 1.5 – 2.0 H). This may have been a consequence of the k-ε model's known tendency to overpredict the turbulent kinetic energy in bluff body flows. Overall, 72% of the FLACS predictions of gas concentration in the EMU experiments were within a factor of two of the measurements.

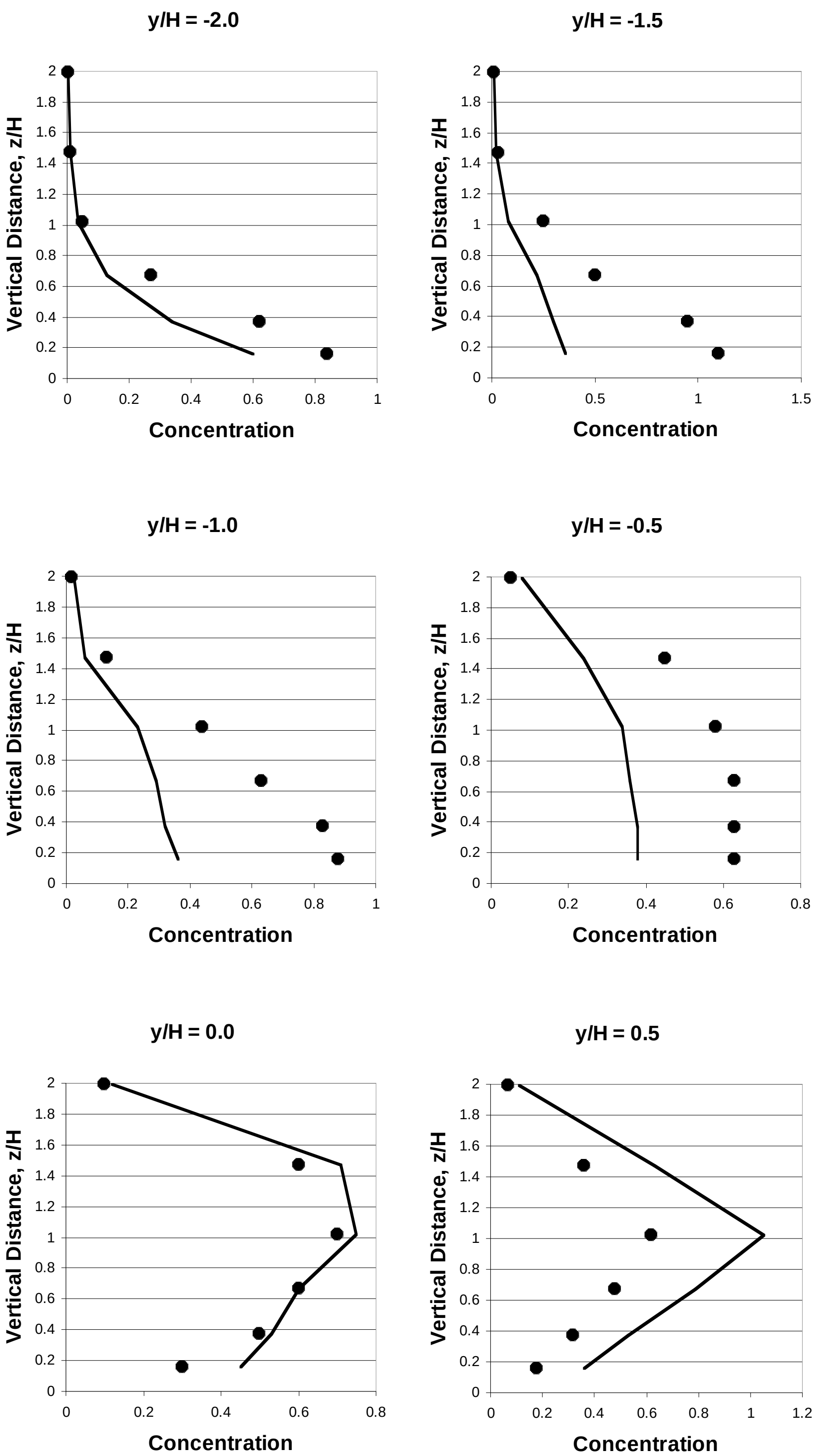

Figure 3 Comparisons of FLACS predicted concentrations (solid line) versus observed concentrations (from wind tunnel measurements) for EMU L-shaped building. Data is taken from Hanna et al. (2004).

MUST Experiments

Hanna *et al*. (2004) also studied passive dispersion over obstructed terrain using the Mock Urban Setting Test (MUST) experiments of Biltoft (2001). These involved 37 releases of propylene tracer gas in a regular array of 120 obstacles across one of the U.S. Army's desert test sites. The obstacles comprised shipping containers 12.2 m long, 2.42 m wide and 2.54 m high. Releases took place below the height of the shipping containers on the upwind side of the array and measurement positions started a few rows of obstacles further downwind, within the array of containers.

Obstacles were introduced into the FLACS model to account for sagebrush and other bushes present on the desert floor. It is unclear what proportion of either the shipping containers or the vegetation was modelled explicitly as blocked regions or as cell porosities. Since the sagebrush was only 0.4 m tall, it would seem likely that this was modelled as cell porosities.

Although the source of the gas was not described fully by Hanna *et al*. (2004) it was mentioned that the orifice was too small to resolve by the grid and therefore it was expected that gas concentrations would be underpredicted in the immediate vicinity of the release. The grid comprised between 55,000 and 75,000 cells and it was reported that it took up to 15 hours of computing time to simulate a single release duration of 500 seconds. Computing times were longer for cases involving unstable atmospheric conditions.

The wind inflow conditions were derived based on a reference velocity which was calculated by averaging measured conditions near the four corners of the array, and a surface roughness that was assumed based on the upwind conditions in the experiments. The average wind speed in the tests was around 3 m/s.

It was mentioned that the k-ε model was modified to increase the turbulence generated behind obstacles with size equal to around one grid cell (see Appendix A and Arntzen, 1998).

No further details were provided of the domain size, the results from any grid sensitivity tests or the remaining boundary conditions.

The FLACS model was found to under-predict both the maximum and the average concentrations by a factor of two and 36%, respectively. The relative scatter was approximately 1.5 times the mean and 65% of the predictions were within a factor of two of the measurements.

5.3.3 Urban Dispersion

Manhattan Tests

Hanna *et al*. (2006), Flaherty *et al*. (2007) and Allwine *et al*. (2007) discuss a model validation exercise involving urban dispersion field tests undertaken in Manhattan in 2005, sponsored primarily by the U.S. Department of Homeland Security. Two sets of experiments were undertaken, in Madison Square Garden and Midtown Manhattan, just south of Central Park in New York, known respectively as MSG05 and MID05. In both experiments, a tracer gas was released and air velocity and gas concentration measurements were made over a 1 × 1 km and a 2 × 2 km area, respectively. The sites were highly built up with some buildings taller than 150 m.

Hanna *et al*. (2006) presented results for the MSG05 case in which five different dispersion models were tested, namely: FLACS, Fluent-EPA, CFD-Urban, FEM3MP and FEFLO-Urban.

The models used a realistic flow geometry taken from a three-dimensional building database. Meteorological conditions were neutral with a steady wind and temperatures of around 0˚C. Although slightly different inflow conditions were used in the different models, the results were expected to be relatively unaffected due to the strong effect of the buildings on the flow behaviour. Predictions from the five different models were presented for the horizontal and vertical wind vectors and a small set of the experimental measured velocities were also shown. However, Hanna *et al*. (2006) did not present any direct cross-comparisons and the model results were each presented in a slightly different format, making direct comparisons difficult. For the gas concentrations, only the model results were presented (again in different formats) and no measurement data were given due to "security reasons". Overall, the work provided limited validation of the model.

A similar set of models, including FLACS, were used to study the MID05 case, as reported by Flaherty *et al*. (2007). Some blind model predictions were made without prior access to the measurement data. An independent team evaluated the results from the simulations. No direct model versus measurement comparisons were given by Flaherty *et al*. (2007) and only general comments were provided, without distinguishing the relative merits of different models. Slightly more information was provided in the WebEx presentation given by Flaherty which is available from the American Meteorological Society[8].

Currently, there do not appear to be any further freely-available reports on the Manhattan tests which document the performance of FLACS against the measurement data, or compare quantitative statistical indicators of performance for FLACS against the other four or five models tested.

5.4 BUOYANT GAS DISPERSION

5.4.1 Confined Spaces

Gas Build-up Experiments

Savvides *et al*. (2001a) presented a comparison of FLACS predictions with large-scale gas build-up experiments in offshore modules. Details of the computational model were only briefly mentioned: large, medium and small gas releases were simulated from three locations and directions within the module. In some cases, the gas jets impinged on adjacent equipment or module walls, while in other cases the jet was aligned or opposed to the ventilation flow. There was no mention of the computational grids used, or whether any grid-sensitivity tests were undertaken. Some results were reported for the sensitivity of the model predictions to variations in the wind speed and direction. The methodology used in undertaking the simulations was said to have followed guidance specified in BP Internal Document (2001).

FLACS predictions were compared to experimental measurements in terms of the flammable gas cloud volume. Most of the predictions were within 30% of the observed data. The geometric mean and geometric variance were 1.25 and 1.16, respectively. Results for the same test cases were also reported by Savvides *et al*. (2001b) for the commercial CFD code, Fluent. These showed a similar degree of accuracy with a geometric mean and geometric variance of 0.98 and 1.20, respectively.

[8] *http://ams.confex.com/ams/7Coastal7Urban/techprogram/paper_127264.htm, accessed March 2009.*

Hydrogen Releases

An overview of the validation of FLACS for modelling hydrogen dispersion is provided by Middha *et al*. (2007a). Comparisons of model predictions against experimental measurements have been made for unobstructed subsonic jet releases using data from the INERIS tests (Venetsanos, 2005), small-scale GexCon tests (Hansen *et al*., 2005) and experiments by Swain *et al*. (2007); unobstructed sonic jets using the INERIS (Chaineaux, 1999) and HSL test data (Shirvill *et al*., 2006); and impinging jets, using the experimental data from FZK (Friedrich *et al*., 2007). Much of this work has been undertaken under the auspices of the EU HySafe Project[9].

Middha *et al*. (2007b) described in more detail the validation study using the FZK data for impinging sub-sonic hydrogen leaks in an enclosure (Friedrich *et al*., 2007). The modelled mass release rates ranged from 0.14 to 6.0 g/s with nozzle diameters from 4 to 100 mm and two flow configurations: the vertical gas jet impinging onto either a flat plate or a semi-enclosed inverted box. The study involved both dispersion and explosion modelling. For the dispersion results, gas concentrations were generally in reasonable agreement with the measurements, in many instances within 10%, although in some cases centreline values were under or over predicted by more than 30%. For the larger releases, gas concentrations tended to be underpredicted near the nozzle and overpredicted towards the impingement plate. The poor predictions appeared in part to be due to the use of coarse meshes, where in one case the plume width of 10 – 15 cm was resolved using cells 5 cm wide. The nozzle orifice was also resolved by between 1 and 4 cells in all of the simulations. No grid-dependence studies were reported. This approach was justified on the basis that a “typical risk assessment project setting” was taken whereby many CFD simulations were run over a 1-2 week period. Most of the simulations were carried out “blind”, prior to publication of the experimental data. These results are also summarised in Middha *et al* (2007a).

FLACS simulations of dispersion experiments carried out at INERIS (Venetsanos, 2005) are summarised by Middha *et al*. (2007a) and compared to other CFD model predictions by Venetsanos *et al*. (2009). The experiments involved a 1 g/s release of hydrogen into a 78.4 m^3 rectangular room through a 20 mm orifice for a period of four minutes. Following the release, the dispersion characteristics were studied over a 1 to 2 hour period. There was no ventilation in the room except for two small openings on one of the walls. As part of the HySafe project a number of different groups using a variety of different CFD codes produced blind predictions of the gas concentrations, prior to having access to the measurement data, and in some cases refined model predictions were submitted later, after the experimental data had been made available. The degree of scatter in the blind model predictions was significant (generally within a factor of two, from half to two-times the experimental values) although this degree of error was not unexpected. The gas concentrations predicted by GexCon using FLACS were amongst the best of models tested. DNV also used FLACS and produced results generally in good agreement with those of GexCon. Their success was attributed to the grid, the time step and convective schemes used. There were various discrepancies between different model predictions which were related to the choice of turbulence model, turbulent Schmidt number, source boundary conditions, grid, time-step and discretization scheme (Venetsanos *et al*., 2009).

[9] *http://www.hysafe.org, accessed January 2009.*

6 CONCLUSIONS

This report provides a review of the capabilities of FLACS version 9.0 for modelling dispersion. Its main strengths and weaknesses that have been identified are listed below:

6.1 STRENGTHS OF FLACS

1. FLACS has been tested for a wide range of different dispersion scenarios including releases of dense, passive and buoyant gases in open, obstructed and enclosed spaces. Results from these tests are available publicly, either from the GexCon website or from published conference proceedings and journals. In most of these tests, FLACS is shown to produce reasonably good predictions (within a factor of two for more than half of the time in nearly all cases).

2. FLACS features a distributed porosity model for small, sub-grid scale obstacles, a semi-automated process for creating complex flow geometry and a simple Cartesian grid that enables simulations to be produced more rapidly than for many other general-purpose CFD codes.

3. Source models for high-pressure gas releases, flashing releases and evaporating pools are provided with FLACS. These are not usually available in general-purpose CFD codes.

4. A reasonably sophisticated approach to model atmospheric conditions at inlet boundaries is provided with FLACS that takes into account upstream surface roughness and atmospheric stability. Such boundary conditions are not usually available in general-purpose CFD codes.

5. FLACS uses a well-established turbulence model and some proven solution methods, including wall functions, the SIMPLE pressure-correction algorithm and a second-order spatial discretization scheme.

6. Training courses and support are provided for the software by GexCon. The company has been helpful in freely providing additional information for this review when requested.

7. In addition to modelling dispersion, FLACS can be used to model vapour and dust explosions.

6.2 WEAKNESSES OF FLACS

1. Many of the validation studies reported for FLACS do not provide sufficient details to be confident that the results are repeatable if, for example, a finer grid is used. Often the results are shown for only one grid and no grid-sensitivity tests are reported, despite the solution being likely to be under-resolved. A different user repeating the simulations using a different mesh may obtain different results. The version of FLACS used in the validation tests is also rarely stated. In some cases, a fuller description of the tests may not have been possible within the short space provided in the conference or journal paper. More detailed descriptions may be available in confidential internal reports.

2. Documentation of FLACS version 9.0 is poor. Despite the new version having been released in April 2008, a draft version of the User's Manual was only provided to the authors of this report, following some discussion, in January 2009. A new user manual was released publicly in February 2009. Details of the underlying mathematical models are lacking in these manuals and in manuals for previous versions of the code. There is no mention of the spatial or temporal discretization schemes or thermal boundary conditions, for example, and it is unclear whether FLACS includes models for rough walls[10]. Some of the responses from GexCon have been contradictory, for example, with respect to the k-ε turbulence model (see Section 3.5).

3. From cross-referencing the FLACS manuals, it appears that some underlying mathematical models have changed between FLACS versions 8.1 and 9.0 (see Appendix A). It is unclear how this affects the model predictions. GexCon state that they undertake verification tests to ensure consistency between different releases and only minor adjustments or improvements have been made, so the results may differ slightly (MEQ, 2008).

4. FLACS uses a single-block Cartesian grid. This may lead to unreliable predictions of dense gas dispersion over sloping or undulating terrain due to the overly high dissipation of momentum from modelling a stepped surface. Grid-dependency issues in resolving circular orifices are also likely to be more acute. Nearly all commercial CFD codes now use body-fitted grids and do not suffer this problem. Fine grids are difficult to use in FLACS because the code is not parallelised. Gas jets have to be aligned with one of the Cartesian axes and care must be taken in using the geometry import tool geo2flacs (see Section 3.3).

5. FLACS lacks choice in its sub-models. Only one turbulence model is provided so the sensitivity of predictions to the turbulence model cannot be assessed. The code also lacks a Lagrangian model and an inhomogeneous Eulerian model for simulations of sprays or particles. These are all usually available in general-purpose industrial CFD codes.

6. The scientific basis of the wind meandering model for atmospheric dispersion simulations is unclear.

7. The application of the distributed porosity concept to dispersion modelling is gaining acceptance but is still not fully-established. Much of the development of the distributed porosity model was undertaken for explosion-driven flows. There is a lack of validation data examining the accuracy of dispersion predictions across a range of different grid resolutions, modelling obstacles as either solid obstructions or as sub-grid porosities.

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[10] *Although inlet conditions for the flow velocity can account for roughness upstream of the inlet, within the flow domain itself it does not appear that a surface roughness can be defined on walls.*

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APPENDIX A: DETAILS OF THE FLACS MODEL

Production of Turbulent Kinetic Energy

In the transport equation for the turbulent kinetic energy in FLACS version 9.0 there is a term which represents the production, or generation, of turbulence (Equation 8.28 in FALCSv9 Draft User's Manual, 2009):

$$\beta_v P_k \tag{1}$$

where β_v is the volume porosity and the term P_k split into four components:

$$P_k = G_s + G_w + G_b + G_o \tag{2}$$

These represent the production due to shear stresses (G_s), wall stresses (G_w), buoyancy (G_b) and sub-grid obstacles (G_o).

Turbulence Production due to Shear Stress, G_S

According to the FLACS version 8.0 User's Guide (1998) and Arntzen (1998), the generation of turbulence due to shear, G_s, is given by:

$$G_S = \max\left[\underbrace{\left(\beta_v \sigma_{ij} \frac{\partial U_i}{\partial x_j}\right)}, \underbrace{C_T \left(\Delta x_j^{2/3} \frac{\partial U_i}{\partial x_j}\right)^3}_{G_T}\right] \tag{3}$$

Presumably this is the same in FLACS version 8.1, since it is not mentioned in the release notes that it is changed from version 8.0 (Hansen *et al*., 2005).

The first underbraced term in Equation (3) is the standard shear-generated turbulence expression scaled by the volume porosity, β_v. The second underbraced term, G_T, involving the cell dimensions Δx_j and the velocity gradient $\partial U_i / \partial x_j$ is a special term introduced in FLACS to "secure a rapid buildup of the transient turbulence field" (FLACS version 8 theory manual, 1998). The standard *k*-*ε* model predicts a rate of increase of turbulent kinetic energy that is too slow in explosion-driven transient flows and this limiter is introduced to increase the rate. The term is derived by Arntzen (1998) based on the Prandtl mixing length model, empirical models for the thickness of the mixing length shear layers and the Kato & Launder (1993) modification that prevents overproduction of turbulence energy at stagnation points. The empirical models used in the derivation are based on a velocity deficit across the whole of a boundary layer, but the resulting expression takes the velocity gradient across one grid cell. Therefore, it appears that the limiter is aimed at relatively coarse-grid simulations where obstacles are around one grid cell across.

The limiter term, G_T, as written above, which is copied from the FLACSv8 User's Guide (1998) and Arntzen (1998) does not obey the standard rules for tensor algebra[11] and it appears that a density may be missing (the term is not dimensionally consistent).

The effect of the limiter was demonstrated by Arntzen (1998) for the case of an explosion-driven transient flow over a plate arranged at right-angles to the oncoming flame front. The limiter was demonstrated to produce a more rapid increase in the turbulent kinetic energy. Its effect is unclear in flows which feature less rapid transients or, for example, steady-state dispersion. Arntzen (1998) remarked that the limiter is "always smaller than the steady state production", but also claimed that the limiter was independent of grid resolution, despite it involving explicitly the cell size, Δx_j.

The numerical implementation of the production term and its limiter is described by Arntzen (1998). The velocity gradient is calculated using the mean of the absolute values of the velocity gradients on both sides of the cell centre. This is done to provide a more accurate representation of the velocity gradient and turbulence production in the wake of an obstacle that is only one cell wide. In the wake behind such an obstacle, the velocity gradients on either side of the centreline will often be equal and of opposite sign so pure summation of the velocity gradient would produce no gradient and no turbulence production. This modification to the calculation of velocity gradients is also mentioned in the dispersion modelling study of the Kit Fox, Prairie Grass and MUST by Hanna *et al*. (2004). It is unclear whether it is used in FLACS version 9.0, it is not mentioned in the FLACSv9 Draft User's Manual (2009).

When asked to confirm the details of the turbulence production terms in FLACS, Gexcon suggested that the authors refer to the FLACSv9 Draft User's Manual (2009) (Melheim, 2009). The limiter term, G_T, in Equation (3) is absent from the production term in FLACS version 9.0. The authors were also informed that FLACS does not contain any of the standard corrections for low Reynolds number flows, although it has been used to simulate laminar flows for the HySafe project and produced reasonable results (Middha *et al*., 2007a; 2007b). The authors were also warned that the thesis of Artnzen (1998) contained a number of significant differences compared to FLACS.

Turbulence Production due to Buoyancy, G_b

The generation of turbulence due to buoyancy is:

$$G_B = \frac{\overline{\rho' u_i}}{\rho}\left(\frac{\partial P}{\partial x_i} + \rho_\infty g_i\right) \qquad (4)$$

where ρ' is the density fluctuation, ρ the Reynolds-averaged density, and ρ_∞ a reference density, $\overline{\rho' u_i}$ is the density-velocity correlation, $\partial P/\partial x_i$ the pressure gradient and g_i the acceleration due to gravity (Wilcox, 2006; Van Maele & Merci, 2006). The generation of turbulence due to buoyancy is modelled in FLACS (FLACS version 8 User's Guide, 1998) as follows:

[11] *A scalar parameter such as G_s should comprise no free indices nor should indices be repeated more than once.*

$$G_B = -\frac{1}{\rho}\frac{\mu_{eff}}{\sigma_t}\frac{\partial \rho}{\partial x_i} g_i \qquad (5)$$

where μ_{eff} is the sum of the molecular and eddy viscosities $(\mu_{eff} = \mu + \mu_t)$, $\partial \rho / \partial x_i$ the density gradient and σ_t a turbulent Prandtl number, which Arntzen (1998) reported was set equal to 0.9. The approximation used for the density-velocity correlation, $\overline{\rho' u_i}$, is known as the Simple Gradient Diffusion Hypothesis (SGDH), although this should involve the eddy viscosity, μ_t, instead of the effective viscosity[12], μ_{eff}. The pressure gradient term has been neglected, presumably on the basis that it is small compared to the $\rho_\infty g_i$ term, and then the reference density has been taken to be equal the mean density ($\rho_\infty = \rho$). These are common assumptions. The production term is positive and turbulence kinetic energy is increased if the density increases with height (unstable stratification, where $\partial \rho / \partial z$ is positive) and conversely G is negative if density decreases with height.

The SGDH model predicts zero density-velocity correlation ($\overline{\rho' u_i} = 0$) in situations where the density gradients are zero. However, in a simple shear flow with only cross-stream temperature gradients, the turbulent heat flux in the streamwise direction actually exceeds that in the cross-stream direction (Ince & Launder, 1989). The model is known to significantly underestimate the magnitude of the heat flux in vertical buoyant plumes (Shabbir & Taulbee, 1990) and studies by Yan & Holmstedt (1999) and Van Maele & Merci (2006) have shown that the $k - \varepsilon$ model with SGDH produces buoyant plumes which are too narrow, with overly high temperatures and velocities in the core of the flow[13].

Turbulence Production due to Sub-Grid Obstructions, G_o

The turbulence production due to sub-grid obstructions, G_o, is given by Equation (8.35) in the FLACSv9 Draft User's Manual (2009):

$$G_o = C_o \beta_v \rho |\vec{u}| u_i^2 f_i \qquad (6)$$

where C_o is a model constant, ρ the density, $|\vec{u}|$ the magnitude of the velocity vector, u_i the velocity component and f_i is a dimensionless parameter depending upon sub-grid objects (which is undefined). Equation (6) does not follow the standard rules of tensor algebra, since the suffix i appears in effect three times, and its expansion is therefore unclear.

There is also a production term in the modelled dissipation rate equation that accounts for the effect of sub-grid obstacles. Rearranging Equations (8.36) and (8.37) in the FLACSv9 Draft User's Manual (2009), this production term can be written:

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[12] This possible mistake is likely to have only a minor effect as in most simulations, the eddy viscosity will be significantly larger than the molecular viscosity.

[13] There is some uncertainty in the experimental measurements used in these works, see for example Shabbir & George (1992, 1994), Dai et al. (1996) and Brescianini & Delichatsios (2003).

$$G_o^{\varepsilon} = C_{1\varepsilon} \frac{k}{\varepsilon} C_o \beta_v \rho |\vec{u}| u_i^2 f_i \qquad (7)$$

Equations (6) and (7) appear to be different to the equivalent terms presented in the manual for the previous version of FLACS. The source terms in the turbulent kinetic energy and dissipation rate equations are given by Equations (3.16) and (3.17) in FLACSv8 User's Manual:

$$P_{k,R} = \sqrt{\sum_{i=1}^{3} \left[u_i^3 T_i \left(\frac{a}{\Delta x_i} + \frac{b}{d_i} \beta_v \right) \right]^2} \qquad (8)$$

$$P_{\varepsilon,R} = \sqrt{\sum_{i=1}^{3} \left[\frac{b u_i^4 T_i}{\Delta x_i d_i} \left(1 + \frac{\beta_v}{a} \right) \right]^2} \qquad (9)$$

where T_i is a dimensionless constant dependent upon the type, blockage and orientation of the obstruction, d_i is the smallest of the two obstacle dimensions perpendicular to the flow direction, a and b are constants, and Δx_i is the cell width. The terminology used in the FLACS manuals has changed between versions 8.0 and 9.0, but term G_o in version 9.0 should be equivalent to $P_{k,R}$ in version 8.0, and G_o^{ε} equivalent to $P_{\varepsilon,R}$.

In FLACS version 9.0, the production terms are multiplied by the porosity, β_v, when they appear in the k and ε equations, whereas in FLACS version 8.0 they are not (see Equations 3.6 and 3.7 in the FLACSv8 User's Manual, 1998, and Equations 8.28 and 8.29 in the FLACSv9 User's Manual, 2009).

Since terms such as f_i, a, b d_i and T_i are not defined it is possible that the production term in the turbulent kinetic equation may be equivalent in FLACS versions 8.0 and 9.0, with the exception of an additional density term and a porosity that appears in the model equations in FLACS version 9.0. However, the production term in the dissipation rate equation in FLACS version 8.0 varies with velocity to the fourth power, whereas in FLACS version 9.0 it is only to the third power (compare Equations 7 and 9).

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Dispersion modelling capabilities

FLame ACceleration Simulator (FLACS) is a commercial Computational Fluid Dynamics (CFD) code developed and marketed by Global Explosion Consultants (GexCon), based in Bergen, Norway. The software has been developed to model the dispersion and combustion of flammable liquids, gases and dust clouds in open and bounded geometries.

The first version of FLACS, released in 1986, was developed by CMI (Christian Michelsen Research Institute). CMI continued the development of FLACS until 1992 at which time its development was passed to CMR (Christian Michelsen Research). GexCon was established in 1998 to manage the consultancy activities of CMR and in 2000 it took full responsibility for the development of FLACS. At present the company employs around 35 people, many of whom are involved in the development of the software. The present release of FLACS is Version 9.0, which forms the subject of the present review.

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