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HEALTH & SAFETY LABORATORY

Guidance for HSE Inspectors: Smoke movement in complex enclosed spaces - Assessment of Computational Fluid Dynamics

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FOREWORD

The content of this guidance has been peer-reviewed by Pr Geoff Cox and Dr Suresh Kumar, Fire Research Station, Building Research Establishment.

Summary

Objective

The guidance is aimed principally at HSE Inspectors to aid them in their assessment of Computaional Fluid Dynamics (CFD) modelling of the movement of smoke (taken to mean in this report all products of combustion - particulates and hot gases) in complex spaces, that may be presented in a safety case, or written safety assessment. The advice is intended to enable the non-CFD expert to make a basic judgement on the adequacy of the modelling and to help decide when a fuller expert assessment is required.

Main Findings

The important issues that need to be assessed in order to determine the quality of a CFD simulation of the transport of smoke in complex spaces are highlighted.

This guidance does not however include all the existing modelling approaches but it concentrates on those most commonly employed, and thus the most likely to be encountered by HSE Inspectors.

Main Recommendations

If in doubt about the quality of a CFD simulation, it is strongly suggested that HSE Inspectors contact recognised experts for an in-depth assessment.

Note that as CFD is rapidly evolving, new models, not covered by this guidance, might appear.

Contents

1. INTRODUCTION

1.1. Objective

This guidance is aimed at HSE Inspectors or any other person who may have to assess safety cases in which Computational Fluid Dynamics (CFD) modelling has been used to predict smoke movement.

Its intention is to raise awareness of the capabilities and limitations of CFD, particularly as applied to smoke movement in complex geometries, which in this report are taken to mean structures containing interconnected rooms, corridors and other enclosed spaces; for example, underground stations, large warehouses storing dangerous substances, offshore accommodation and large, complex buildings under construction or undergoing refurbishment.

The guidance will allow Inspectors to make a basic assessment of the quality of the CFD modelling they may be asked to judge, and to help them decide when a fuller, expert assessment is required.

1.2. Need for this guidance

For predicting smoke movement, CFD has a number of benefits compared to other, simpler, techniques which have been developed in the past:

Empirical models are based on experiments. However they are typically limited to geometrically very simple situations. They cannot readily be used to extrapolate beyond the configuration in which the experiments were carried out, and may have the additional weakness of dependence on the fuels used for those underlying experiments.

Zone models are simpler mathematical models which divide the problem into a small number of “zones” - such as the fire plume, a hot layer and cold air. Typically empirical models are used to model some of these zones. They are applicable to simple spaces, such as regular-shaped rooms. For this application they are a good compromise between speed and accuracy. However, if used in the context of complex enclosed spaces, or even certain large regular spaces, i.e. modern warehousing, then the basic assumption that the flow can be divided, a priori a small number of distinct zones, breaks down. In this case other techniques should be employed.

Ideally assessment would be via actual fire tests, or other hot smoke experiments. But safety, cost and/or political considerations often make these impractical or limited in extent. Experiments may be carried out using “cold” smoke - from smoke bombs or theatrical smoke generators. Thyer (1999) described such tests, but highlighted the potential differences in behaviour between cold and hot smoke. These make extrapolation of the findings of cold smoke tests to a hot smoke (fire) scenario difficult - particularly when the flows are dominated by buoyancy.

In principle, CFD modelling provides a means to predict smoke movement without the constraints imposed by the above simpler modelling techniques. In particular it can be used to represent complex geometries.

CFD is a predictive tool which can be applied at the design stage as well as in assessing a finished structure. It can potentially be used to evaluate the effects of changes in structural design and ventilation, and to assess performance of safety measures over a range of fires; differing size, duration and locations. CFD results contain a wealth of information about the predicted flows; which may include velocity, temperature, smoke and gas concentrations at tens or even hundreds of thousands - possibly even up to a million- of points within the space.

However, the technique does have limitations and, unfortunately, these have yet to be fully investigated for its application to the movement of smoke in complex, enclosed spaces. In addition, CFD is a complex technique to apply and requires a knowledgeable approach to produce reliable results. It should be remembered that any modelling technique is, at best, an approximation to reality: inexpert or ill-considered application of CFD can produce predictions that may differ greatly from the true situation.

The potential usefulness of CFD is substantial, hence its growing use in fire safety engineering. However, results of CFD predictions need to be considered with care to ensure that they are not misleading.

1.3. Scope of this guidance

This guidance outlines the capabilities and limitations of CFD applied to prediction of smoke movement in complex enclosed spaces. The focus is on the transport of smoke, not its production by the fire. Issues relating to the consequences; such as visibility or toxicity, are not addressed in any detail.

The modelling approaches are not covered exhaustively, but are limited to those models that are practically applicable and commonly seen used in this type of problem. Other more sophisticated CFD modelling approaches do exist, but these are often too expensive in computational resource to be used commercially in this type of work.

Section 2 gives an introduction to CFD modelling, presenting the range of techniques that might be encountered. The process of setting up a CFD model is explained, presenting the assumptions that need to be made at each stage and the issues that need to be addressed.

Section 3 discusses the specific issues that need to be considered when assessing CFD predictions of smoke movement inside complex spaces. This section presents the information that an Inspector should consider when assessing such CFD results.

Readers may also benefit from consulting the glossary document by De Souza (2003), for the meaning of CFD-specific terms.

1.4. Methodology for producing this guidance

The advice presented in this guidance arises from a number of sources:

- the expertise in CFD that resides within the Computational Modelling Section of HSL - with experience of a wide range of different flow problems
- information presented in other publications, such as Cox (1995) and Grant & Lea (2001).
- the findings of the HSE-funded research project R04.080 (Gobeau and Zhou, 2002; Ledin et al., 2002).

This latter project was aimed specifically at addressing the worrying lack of validation for CFD predictions of smoke movement in complex spaces, and was jointly funded by HSE's Railway Inspectorate, HID Offshore, and Technology, Divisions.

The project examined the capabilities and limitations of CFD when used to predict such flows.

2. INTRODUCTION TO CFD

Computational Fluid Dynamics (CFD) is a powerful, rapidly evolving tool used for the prediction and analysis of fluid flows. The technique is able to provide a time-dependent three-dimensional approximate solution to the highly coupled differential equations that govern fluid flows. Its key benefits are: an ability to represent the effects of very complex geometries coupled with a means to solve complex flow problems based on a more fundamental modelling of the physics involved.

The technique originated in the aerospace sciences in the 1960's. It has since been developed and applied to an increasingly diverse range of problems, including automotive, nuclear engineering, biomedical field, environment and fire safety engineering.

However, a number of assumptions and approximations are made throughout: both in formulating and constructing a CFD tool, as well as in its application to a particular flow problem. Also, compromises are often required in order to achieve reasonable run-times. These all ultimately influence the reliance which can be placed on results of CFD simulations.

This section explains the basics of CFD as applied in fire safety engineering and presents the compromises that a CFD user often has to make. More information can be found in general books on CFD, for instance Ferziger and Peric (1996), Veersteg and Malalasekera (1995), Anderson (1995).

2.1. Overview

When applying a CFD package to undertake a flow analysis, there is a number of steps that the CFD user has to go through:

- Defining the geometry and domain (Section 2.2).
- Selecting physical sub-models (Section 2.3).
- Specifying boundary conditions (Section 2.4) at the frontiers of the domains - including walls, inlets, outlets and openings.
- Discretising the mathematical equations (Section 2.5), which includes creating a mesh (which sub-divides the space into small volumes), setting time steps (which divides the time into discrete steps) and selecting numerical sub-models.
- Monitoring the iterative solution process (Section 2.6).
- Analysing the solution obtained (Section 2.7).

Uncertainties that may arise at each of these steps are highlighted. Additional sources of uncertainties are presented in Section 2.8. Finally, Section 2.9 provides a summary.

2.2. Creation of a geometrical model

The starting point when applying a CFD package is to create a geometrical model of the scenario to be investigated. Basically, this means to represent by a set of surfaces the confines of the space, i.e. the walls of rooms, corridors, staircases, fixtures and fittings, furniture, etc...

Increasing the scope and complexity of this representation adds to the cost of the CFD modelling, both in extra effort during setting-up of the problem within the computer environment and in the amount of computer resources (processor power and time) needed to produce an answer. Resources will not permit everything to be included, and there are usually time and financial pressures to make the CFD model as simple as reasonably possible.

First, the limits of the region that will be modelled have to be set. This is called the ‘computational domain’. They are chosen according to the objective of the CFD simulation, focusing on the area of interest. They must also be located where the flow conditions are known. This is to be able to take into account the influence of the external flow by specifying its characteristics at the boundaries of the domain (see Section 2.3). This condition means that in some cases, the computational domain has to be extended beyond the area of interest. For example, surrounding buildings might need to be included when interested in computing the internal flow of a naturally-ventilated building. Examples of a computational domain are a room, a floor or an entire building.

Then the CFD practitioner has to balance up the need to include or simplify fine details, such as furniture in the model. If fixtures and fittings would only have marginal influence on the flow behaviour, then it is probably not necessary to include these in the domain. For example, in the underground station modelled as part of JR04.080, no furniture was included and staircases were represented by inclined planes.

There are no hard and fast rules saying what to include and what not to include in the model. It is for the modeller to make a judgement on a case-by-case basis, but equally also to justify the decisions made.

2.3. Selection of physical sub-models

The fluid flow equations solved in industrial CFD codes are not the exact governing Navier-Stokes equations. This is because the exact equations either cannot be solved for practical flows of interest, as is the case with turbulent flow, or because the exact governing equations are not completely known, as in the case of combustion.

Simplified physical sub-models are thus employed. They consist of a set of approximate equations, in-part derived from empiricism and physical reasoning. Examples of sub-models embodied in CFD codes amongst the most relevant to fire applications are presented below. They include a range of turbulence models, radiation models and combustion models.

The CFD user has to select the sub-models to implement in the simulation. Usually, the more physics is embodied in a model, the more equations must be solved and hence the longer the simulation will take. The CFD user therefore often has to make a compromise and implement the minimum physics required to obtain an acceptable solution. That is why it is crucial that the user has a good understanding of the physical mechanisms that govern the flow being modelled, as well as a good knowledge of the limitations of the sub-models.

2.3.1. Combustion models

The simplest approach to represent a fire is generally referred to as a volumetric heat source model. This approach does not predict the combustion process but instead accounts for its resulting effect - production of heat (and smoke), by imposing a typically uniform distribution of heat (and smoke) over a prescribed volume. The characteristics of the volume; its size and shape, have to be specified by the user. These should correspond to the expected characteristics of the flaming region in which combustion occurs. They can be deduced, for example, from experimental observations or well-established correlations.

In reality though, the distribution of heat and smoke produced by combustion is not uniform, and, importantly, the shape and extent of the volume is often unknown. Heat and smoke result from chemical reactions between the fuel and air. The chemical reactions are influenced by the respective quantities of fuel and air available. These depend on the quantities already consumed by the chemical reactions, as well as on the flow characteristics, including turbulence, which drive the fuel-air mixing. Imposed or induced ventilation flows will affect mixing in the combustion zone and the trajectory of the fire plume. The latter is also affected by the presence of surfaces such as walls.

A range of combustion models have therefore been developed to address these difficulties by <u>predicting</u> - as opposed to prescribing - the distribution of heat in the flame from the flow conditions and the shortage of one or another reactant. Most models assume that the combustion process can be represented as a single, one-step reaction of the form: fuel + air ---> product. Usually an instantaneous reaction is assumed between any fuel and oxidant contained within a cell in specific proportions. More elaborate schemes can accommodate chemical kinetics effects (Drysdale, 1998) and some formulation describing turbulence interactions. Contrary to the volumetric heat source approach, these models can be used to predict the volume in which the combustion and heat release take place.

One such approach, the most likely to be encountered, is the ‘eddy-break-up’ (Spalding, 1971) which assumes an instantaneous reaction - the rate of which is proportional to a computed turbulent time-scale. This model when used with a one-step reaction, however, does not address the numerous competing chemical reactions occurring in reality and when combustion does occur it assumes that the fuel is completely oxidised. Thus, it does not provide an accurate prediction of rates of products including smoke. More sophisticated models are under development to address these issues. However, they are unlikely, at the time of writing, to be routinely applied in fire safety engineered approaches.

2.3.2. Turbulence models

Turbulent flows contain a wide range of length and time scales. For enclosed fires, the scales will depend on the fire characteristics and the dimensions of the enclosure but typically length scales can vary from less than a millimetre to a few metres (Cox, 1995).

This makes the modelling of turbulent flows very challenging. Several approaches have been proposed. They can be broadly classified into three categories:

- Direct Numerical Simulation (DNS):

  All the turbulent motions are resolved by solving directly the Navier-Stokes equations that govern fluid flows, without additional modelling.

  This approach requires a very large number of grid cells and is thus impractical for industrial applications. It will not be seen in fire safety engineering.

- Large Eddy Simulation (LES):

  All but the smallest turbulent motions are resolved by the Navier-Stokes equations. The finest eddies are either ignored or modelled.

  Although this approach allows one to employ fewer grid cells than DNS it is still impractical for fires and smoke movement in complex spaces. It has only recently been applied to fires but is limited for the moment to simple scenarios - typically a single room.

- Reynolds-Averaged Navier-Stokes (RANS) Models:

  The Navier-Stokes equations are time-averaged and thus the equations so obtained do not aim to resolve the turbulent motions but to provide the time-averaged characteristic quantities of the flow.

  Since a RANS model is not trying to resolve the turbulent motions, the grid needs only to be fine enough to capture the important time-averaged features of the flow. Far less expensive than the two other categories, they are thus widely employed in Fire Safety Engineering - as well as many other engineering applications

The turbulence models most likely to be employed for fire and smoke movement in complex spaces are therefore of RANS type. Amongst these, the so-called k-ε model is used near-exclusively.

The limitation of RANS models lies in the modelling of the turbulent Reynolds stresses: unknown terms appearing in the equations as a result of the time-averaging process. The k-ε model is based on the assumption that the Reynolds stresses are linearly related to the local mean strain rate. This assumption is, however, not strictly valid for the following situations: buoyancy, streamline curvature, acceleration/deceleration, impingement and three-dimensionality (Leschziner, 1992) - which are obviously all features of fires in enclosed spaces.

Modifications to the k-ε model have been proposed to account for some of the gross effects of buoyancy on turbulence, for example by Markatos et al. (1982) and Viollet et al. (1983). They consist of adding a buoyancy-related term in the equations of the model so that the resulting computed Reynolds stresses behave more as expected in the presence of buoyant forces. The contribution of the added buoyancy-related term is proportional to a constant which is specified by the user.

Of note, the equations employed in a k-ε model make use of a set of constants which have now well-established values. Although these have been determined empirically by tuning against experimental data in simple specific configurations, they have often proven acceptable for a wide range of flows.

More sophisticated RANS models exist and aim to address by a more fundamental approach the shortcomings of the k-ε model. They consist of deriving a transport equation to predict the Reynolds stresses. However, the equation obtained contains unknown terms which again need either to be modelled or to be predicted by another transport equation. Unfortunately, other unknown terms appear in this additional transport equation and so at some stage make modelling necessary. The higher the order modelling is applied to, the lesser the effect on the results it is expected to have. However, modelling leads unavoidably to inaccuracies. The drawbacks of these more sophisticated models are that not only do they involve solving more equations but due to the mathematical nature of the equations they are also more numerically unstable, and thus require much more effort to obtain a ‘converged’ solution and sometimes this may not be achieved. The commercial CFD codes are usally offering up to second-order closures but not yet third or higher order closures - these can only be found in academic research codes at the present.

2.3.3. Radiation models

Radiation can play a very important role in the overall heat transfer in combusting flows, typically when temperatures are above 600K. The main sources of radiation are CO_2 and H_2O, which both emit energy in discrete bands, and soot, which emits radiation at all wavelengths. Radiative heat transfer occurs between the emitters and receivers, i.e. between solid surfaces, soot/gas phase mixtures of flames and smoke aerosols.

There are a number of different modelling approaches available. Those more likely to be encountered, in order of increasing complexity, are:

- Fractional heat loss due to radiative heat transfer to the surroundings
- Six flux modelling
- Discrete Transfer modelling
- Monte Carlo simulations

Unless otherwise stated, the models provide a prediction of the radiative heat transfer, which for the most sophisticated models, will mean solving a set of differential equations. The value obtained is then set as a source term in the transport equation for temperature, more precisely the enthalpy and energy equation.

- Fractional heat loss

  This method crudely accounts for radiation by simply ignoring in the simulation the percentage of the heat release from a fire due to radiation - values of 25 % are not uncommon. This means that the heat output of the fire in the model is set as the remaining (convective) percentage of heat.

  Most often, the radiated heat is completely ignored and not transmitted to the receivers. Glynn et al. (1996) have tried to account for the radiative exchanges between the fire and the walls by distributing the percentage of radiated heat ignored in the fire source to the air in the cells next to the walls opposite to the fire. In this method, the transfer of radiative heat is not predicted but has to be set in advance by the CFD user in the form of a prescribed wall area where radiation exchange takes place and in the form of a pre-defined heat distribution across this area. The uncertainties come from the specification of these prescribed values characterising radiative transfer.

- Radiative heat transfer at the walls

  This method aims to account for the radiative heat transfer between the smoke and the walls. This transfer is expressed as a function of the temperature of the wall and smoke and the emissivity of the smoke. It is applied between the wall and the fluid cell next to the wall. This approach can be used in combination with the previous fractional heat loss.

- Six flux modelling

  This method, only applicable to structured meshes - see Section 2.5.1, assumes that the radiant flux across each of the six faces of the grid cells is uniform. This simplifies greatly the set of equations to be solved to calculate the radiative source term. The accuracy of six flux models is highly directionally dependent; the radiation is assumed to be transmitted along the co-ordinate axis only. Snegirev, Makhviladze and Talalov (2001) point out that the six flux model approach is not a good choice for calculation of wall heat transfer in flames. Nevertheless it is commonly used.

- Discrete transfer modelling

  The model is very different from the previous approaches in that it aims to solve the discrete radiative rays. Only representative rays are solved. The directions of the rays are specified a priori. The solution for any particular ray is restricted to the path between two boundary walls rather than being partially reflected at walls and being tracked to extinction. The accuracy of the discrete transfer model is dependent on the ray directions chosen as well as the number of rays. The model has been used extensively in its original form (Lockwood and Shah, 1981) and a number of modified versions also exist, Docherty and Fairweather (1988), who included non-gray effects, Cumber (1995), who proposed a quadrature formulation and an improved integration procedure of the radiation energy equation, and Cumber et al. (1998), who proposed a more accurate and more computationally efficient discrete transfer model. The discrete transfer method is not ideally suited to the body fitted grids likely to be seen in fire and smoke movement applications in complex spaces. This is because it is computationally expensive, especially for situations where a large number of rays are required to obtain an accurate solution.

- Monte Carlo simulations

  A number of rays are "emitted" in (pseudo-)random directions. The rays are then traced until they either; hit an obstacle, hit a wall, or, disappear out of the computational domain. The quality of the heat transfer calculations is dependent on the number of rays. This is a costly approach, but offers potentially the most accurate solution and flexibility for complex geometries in different co-ordinate systems. Snegirev et al. (2001) claimed that it was now feasible, from a computational overhead point of view, to use the Monte Carlo method. However, the computational cost will remain high for flows where a large number of rays -typically thousands- are required in order to obtain accurate solutions. It is therefore fairly unlikely that such a method will often be seen applied to fires and smoke movement in large complex spaces.

The last three modelling approaches require the calculation of local emissive powers and absorptivities - which depend on the composition of the soot/gas mixture.

The most important species from a radiation point of view are CO, CO_2, CH_4 and H_20. These species radiate energy in discrete bands, at quire distinct wave numbers. Soot on the other hand radiates energy at all wave numbers. Soot absorption and emission is proportional to the soot volume fraction, provided that the radiation wavelength is greater than the soot particle diameter, de Ris (1979).

The simplest method by which to calculate local absorption coefficients is to assume that the smoke layer is a grey, isothermal gas of prescribed absorption coefficients. The grey, isothermal gas approach is based on a single radiative temperature and a single grey absorption coefficient. The model is a poor approximation for molecular emitters (CO, CO_2, CH_4 and H_2O). This simple, physically unrealistic model has nevertheless yielded accurate predictions of heat flux and burning rates in small to medium size fires (Modak, 1979). However, use of this simple method can lead to considerable errors in large scale fires (de Ris, 1979). It can not predict the distribution of radiant energy along a furnace wall or the effect of a cool absorbing layer on the local heat flux (Grosshandler, 1980).

Cumber et al. (1998) showed that specification of a mean absorption coefficient for each control volume, in the computational mesh, based on a curve fit to total emissivity, Modak (1979), is not a suitable approach - as the path length decreases, the absorption coefficient increases. The implication of this is that mesh refinement leads to an increased sensitivity of the predicted intensity field to the local path length.

Other, more realistic, techniques of varying complexity attempt to express the local properties as a function of gas and soot concentrations and on temperature. However, such methods do not account for the turbulent effects: the flame envelope is often essentially black due to heavy soot particle loading, but turbulent eddies occasionally will cause the envelope to expose a cleaner flame which yields bursts of radiation of high intensity. As a result, the radiative transfer tends to be under-predicted in the flaming region by the 'grey gas assumption'. These techniques are described briefly in the following paragraphs. Since they are however in less common use in complex enclosed spaces than the previous techniques, this part of the report can be skipped.

Grosshandler (1980) presented a methodology called Total Transmittance NonHomogeneous, TTNH, which calculates the absorption coefficient based on the composition of the mixture of air - combustion products. It is a much simpler method than either narrow band or wide band models presented below. Grosshandler and Modak (1981) found that fire and furnace calculations with TTNH yielded results which differed by 8 % from the results obtained with more complex models, but with a saving of two orders of magnitude in computational cost.

Statistical narrow band models, Grosshandler (1980), approximate the average behaviour of the absorption coefficient in a small spectral interval. Each of the intervals contains hundreds of lines; the mean line strength is arrived at by summation of contributions from all the lines. The width of the narrow bands, in wave number, must be of the order of 25 cm^{-1} for accurate predictions. Thus a total intensity calculation from a gas mixture involving CO, CO_2, H_2O and CH_4 involves scanning more than 300 narrow band regions. The Curtis-Godson approximation (Goody, 1964) is suitable for modelling non-isothermal behaviour by averaging the mean line intensity and line spacing over the non-homogeneous path. The complexity and computational cost of narrow band modelling has precluded the extensive use of these models for engineering calculations (Grosshandler, 1980). The advent of faster computer processors should alleviate some of the concerns over long computer run times, but this model is unlikely to be seen in widespread use in fire safety applications.

Edwards and Balakrishnan (1973) formulated an exponential wide band model, which is described in detail in Edwards (1976). In an exponential wide band model rotational lines in a band can be reordered in wave number space with exponentially decreasing line intensities moving away from the band centre (Cumber et al., 1998), The number of bands to be scanned, when applying a wide band model, are far fewer than in the case of narrow band models, typically of the order of six to eight bands as compared to 300-odd (Grosshandler, 1980). Cumber et al. (1998) concluded that an exponential wide band model, with no lower bound limitation on the band absorptivity, can yield accurate results with arbitrarily small numerical error.

2.4. Boundary conditions

Any mechanism which is external to the computational domain, but which influences the behaviour of the flow that is being calculated, must be represented. That includes:

- The flow that enters or leaves the domain, at openings such as doors, windows or vents;

- The transfer of mass, momentum and heat at walls;

- The source or sink of mass, momentum or heat due to an external event, for instance a fire or the release of a suppressant.

Boundary conditions can be of several types:

- Prescribed variable values, known as Dirichlet boundary conditions. Used, for instance, to specify velocity and temperature as flow enters the computational domain;

- Prescribed gradients of variables, known as Neumann boundary conditions and used, for instance, to set a plane of symmetry in the domain by specifying that gradients of all flow variables normal to the plane are zero;

- A mixture of both previous methods;

- Volumetric sources or sinks of heat, mass and momentum. For instance, to represent a fire via the prescribed volumetric heat source approach; to include space or solar heating, forced ventilation flows, etc...

The results of CFD simulations are determined by the boundary conditions. It is thus essential that the user specifies boundary conditions correctly and understands the key role they play.

However, usually not all of the required boundary conditions will be well-defined. For instance: turbulence parameters as flow enters the computational domain are typically unknown; there may be uncertainty in wall heat transfer coefficients; fire sources and fire growth rates, or heat loading, may be ill-defined; events external to the selected computational domain, such as pressure distributions arising from natural or forced ventilation, may in reality affect flow inside the domain - these couplings should ideally be encompassed. If doubt remains, the CFD user should ideally carry out a sensitivity test; to evaluate the influence of a range of plausible values for boundary conditions on the predictions.

2.5. Discretisation of the mathematical equations

The set of equations obtained cannot be solved analytically except in special, highly simplified cases. The equations are indeed highly non-linear and strongly coupled. It is the task of CFD to generate approximate solutions to these equations by numerical means. This is achieved by a discretisation method: the differential equations are applied to small domains in space, i.e. grid or mesh cells, and time, i.e. time steps. Hence a large system of algebraic equations is obtained. A solution algorithm is used to solve this system and an iterative procedure, consisting of guessing a solution and then correcting it, is often applied to overcome the coupling between the equations.

2.5.1. Creation of a computational mesh

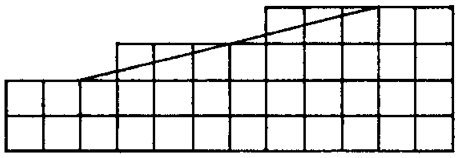
The volume of the computational domain has to be divided into small domains called grid or mesh cells over which the differential equations will be discretised. The mesh has to represent the geometrical shape of the domain, and be constructed to allow adequate resolution of the key flow features. The process of creating a suitable mesh involves both experience of fluid flow behaviour, trial and error. It is not uncommon to have to make a number of attempts at creating an acceptable mesh and then make further improvements as the calculations progress.

Grids can be broadly divided into three categories:

- Structured Cartesian grids (Figure 1.I): grid lines are continuous across the domain and grid cells are hexahedral; curved boundaries are simplistically represented by staircase-like steps in the mesh.

- Structured Curvilinear or Body-Fitted grids (Figure 1.II): the grid lines follow the

(I)



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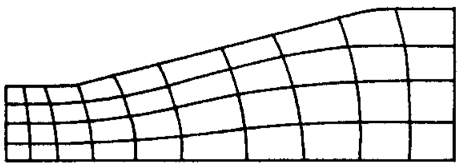

Figure 1 - Comparison of structured cartesian (I) and curvilinear (II) two-dimensional grids (from Tucker and Mosquera, 2000)

computational domain boundary.

- Unstructured mesh (Figure 2): constructed from tetrahedral or more complex-shaped cells. There are no clearly defined grid lines which are discontinuous across the domain

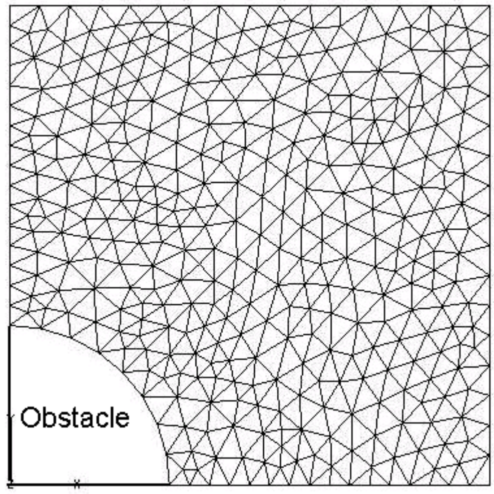

Figure 2 - Example of an unstructured two-dimensional grid

Unstructured meshes are more suited for highly complex geometries since they can be adapted to any shape. Relatively they are also easier to generate. Creating a geometry and a grid for a complex space is however, by and large, the most time-consuming task for the CFD practitioner. Unstructured meshes nevertheless have several disadvantages. Their associated discretised equations are more complicated than is the case with structured grids. As a result, the system of equations can be more difficult to solve and the solution obtained less accurate.

As a compromise, hybrid meshes, combining structured and unstructured cells, can be employed. An example is shown in Figure 3 where structured grid cells are used near a wall boundary. It can be compared with Figure 2 where the same domain was divided into unstructured grids only. This allows one to capture more accurately the transfer of heat and momentum at walls and is advised when these significantly affect the bulk flow. An

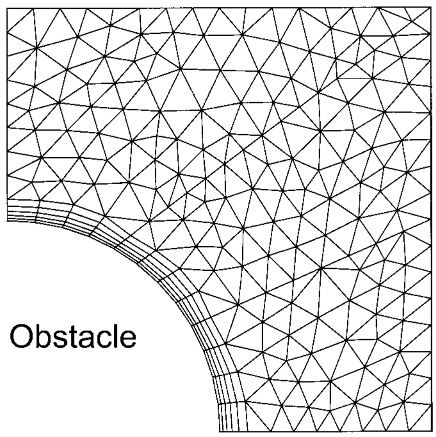

Figure 3 - An example of a hybrid two-dimensional mesh

alternative is to inflate unstructured cells, i.e. to create thin cells with surfaces parallel to a geometry (see Figure 4 at the walls).

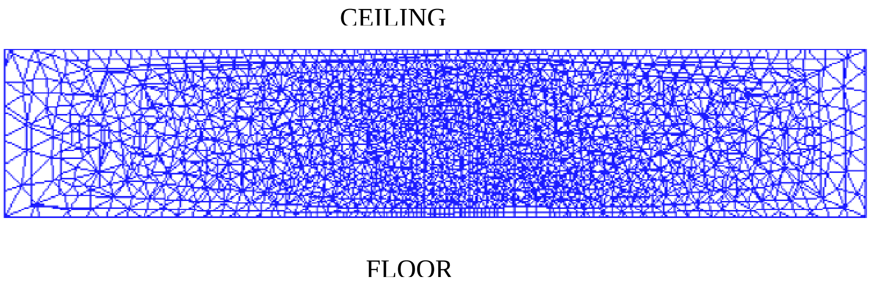

Figure 4 - Example of a compressed (centre) and inflated (wall boundaries) Three-dimensional unstructured mesh (from Gobeau and Zhou., 2001)

Many variations are possible, but the above approaches are the most commonly used and are the ones embodied in most commercial CFD codes.

An important mesh parameter is the size of the cells. It needs to be chosen with great care since it can significantly influence the solution. It should ideally be smaller than the length scale of key flow features. However, in a complex geometry, a wide range of length scales exist at different locations. Choosing a grid of the size of the smallest length scale, then applying this uniformly over the overall geometry would lead to a large number of grid cells and result in prohibitive computing times. To overcome this problem, it is possible to cluster cells at specific locations determined by the user. For example in Figure 5, the grid is compressed where the flow changes rapidly, i.e. where large gradients occur. Figure 4 shows compression of an unstructured mesh where a source representing a fire is located. Basically, when creating a mesh, the CFD practitioner must have an intuitive idea of the flow behaviour prior to the simulation. In some situations, this can prove difficult and the only way to achieve a good mesh may be by successive trials and corrections.

The grid size has also to be consistent with the modelling approach chosen. For example, pre-defined functions are often employed in combination with a k-ε turbulence model to calculate the velocity profiles near walls. These functions model the very small scale mechanisms of heat and momentum transfers occurring in a very thin region close to solid boundaries. They make it possible, and even necessary, to set the size of the cells next to walls larger than this region.

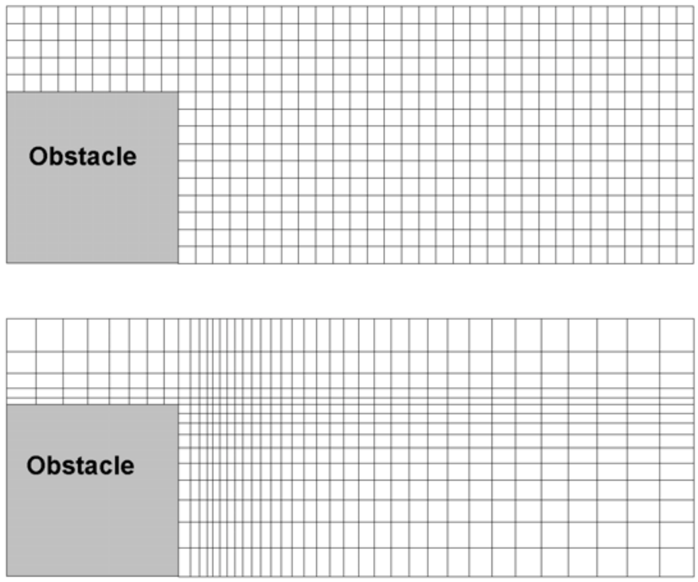

Figure 5 - Comparison of uniform (top) and compressed (top) structured two-dimensional grids.

2.5.2. Division of time

When things change over time, a transient simulation - as opposed to a steady-state simulation (where the transient terms are ignored), is needed.

In the same way as the space is sub-divided into small volumes, time is divided into discrete steps. These need to be small enough to reproduce the important transient features of the flow. The time steps also need to be consistent with the mesh; the smaller the size of the cells, the smaller the time step, to help in the solution of the set of algebraic discretised equations and to obtain reliable results.

2.5.3. Discretisation

This section may seem highly technical, since it focuses on mathematical techniques employed to transform the set of continuous differential equations describing the physics of the problem, for which an analytic solution cannot be found, into a system of (approximate) discretised equations for which a numerical solution can be obtained. However, the choice of numerical schemes used to perform this discretisation can be as important as the appropriate selection of physical sub-models and the specification of realistic physical parameters or boundary conditions.

Each continuous differential conservation equation is translated into an algebraic equation, where the unknowns are the flow variables, such as velocity or temperature, at discrete locations in space and in time. The spatial locations are linked to the computational grid, either the grid cell centres or corners. The temporal locations correspond to the boundaries of the time steps which subdivide the continuous time into intervals; in the same way as the grid breaks down the whole volume into smaller domains. There are various methods to approximate the differential equations by algebraic equations. The most common ones are the finite difference, finite volume and finite element methods. Most of the commercial CFD codes are based on the finite volume method, for example CFX4, CFX5, PHOENICS, FLUENT, JASMINE, STAR-CD. An example of a commercial code based on the finite element method is the general purpose code FIDAP. It has, however, apparently not been applied to the prediction of smoke movement (Grant and Lea, 2001).

The discretisation of the differential conservation equations involves relating the values of quantities such as fluxes across the faces of the cells, to the unknowns of the problem, which are typically the variable values at the centres of the cells. CFD codes offer the user a choice of numerical schemes that express the convective terms and transient terms of the conservation equations as a function of the unknowns. They all incur numerical errors as they include approximations.

The most frequently encountered error due to the discretisation of the convective terms is known as 'numerical diffusion'. Its effect is to increase rates of diffusion of heat, mass and momentum, generally leading to an over-prediction of mixing. In some circumstances, this error can be so large as to completely swamp the real effects of mixing due to turbulence! Numerical diffusion is most severe from use of discretisation schemes which are referred to as 'first-order accurate'. 'Higher-order accurate' schemes are likely to provide better results, but they tend to give more difficulty in obtaining a solution. First-order accurate schemes include those known as 'upwind', 'hybrid', 'exponential' and 'power law'. Higher-order accurate schemes include those known as 'QUICK', 'CCCT', 'TVD' and second order upwind. More details can be found in Patankar (1980) and Versteeg and Malalasekera (1995).

Time discretisation schemes will also be of different orders of accuracy and either implicit or explicit; depending respectively on whether the results at previous time steps are used in the solution of the current time step, or not. It is likely that the lower order schemes will tend to smear temporal variations in the same way as the spatial discretisation schemes.

2.6. Solution of the system of discretised equations

By this stage, a set of linear, highly coupled algebraic equations has been obtained. An approximate solution is now achieved by iterative algorithms (Patankar, 1980). These start by an approximation to the flow solution. They gradually iterate to a final result which satisfies the imposed boundary conditions, whilst ideally ensuring that mass, momentum and energy are conserved both locally for each grid cell and thus globally over the whole computational domain, a 'converged' solution. For unsteady problems this process is repeated at each of many time steps until the total time required has been covered. Exceptionally, there may be circumstances where the initial guess set by the user influences the final solution computed.

These iterative solution algorithms can be inherently unstable. They require careful selection and optimisation of control parameters if a converged solution is to be found.

Since the process of solving the algebraic equations is iterative, it is ‘important to know when to quit’ (Ferziger and Peric, 1996). The CFD code user has thus has to specify convergence criteria, which, when met, stop the solution algorithm. If the criteria are not appropriate to the flow problem, the errors introduced at each iteration, even though small, are likely to add up and could result in an erroneous final solution.

2.7. Analysis of the CFD results

The approximate solution obtained consists of the values of the variables of interest at all the grid cells and at the time steps chosen by the user. The data generated by a CFD simulation can thus be huge, typically hundred of thousands of values for each time step recorded. It can be quite challenging to then extract the information required, for instance the hot layer interface (Hadjisophocleous et al., 1999) or smoke detectors response (Klote, 1998).

The CFD practitioner really has to make use of a ‘post-processor’ to analyse this large amount of data. A post-processor is a piece of software that can read a file containing the data from a CFD simulation and translate it into visualisations: for example, contours of temperature or smoke concentrations; three-dimensional iso-surfaces; plots of velocity vectors. It is also possible to extract information from the data, such as interpolated values of variables at a given location; the transported quantity of a variable across a surface defined by the user. The information provided by a post-processor results from interpolation methods, and thus additional, although usually small, numerical errors are also introduced at this stage.

Considering the wealth of data provided by a CFD simulation, results presented to support a safety case are often, of necessity, limited in extent. The range of illustrations selected by the CFD practitioner should nevertheless provide a comprehensive ‘picture’ of the transport of smoke across the whole domain. This means, for example, that several, rather than a single, smoke iso-surfaces may need to be presented

To evaluate the reliance that can be placed in the results, the CFD user should wherever possible check the predictions against spot measurements. When these are not available then well established empirical correlations can sometimes be used in limited parts of the domain - for example the fire plume.

The accuracy required from a CFD simulation depends, however, on the purpose of the simulation. For some fire safety applications, it may be sufficient just to know the direction of smoke movement from a fire. Alternatively it can be to obtain quantitative data, such as heat flux or time available for evacuation. When uncertainties in a CFD methodology preclude ‘accurate predictions’, it may be adequate to ensure conservatism. That is, that each aspect of the modelling is weighted such that the overall result is likely to err on the side of caution.

2.8. Additional sources of uncertainties in CFD

CFD is a powerful technique since it can provide an approximate solution of the three-dimensional equations that govern fluid flows. However, it remains an approximation and in no circumstances is the solution obtained exact.

Numerical and physical errors are introduced at virtually all the stages of a CFD simulation described in the previous sections, since assumptions and approximations are made. However, it is possible to control these errors with a good understanding of both fire science and CFD, i.e. a thorough knowledge of the capabilities and limitations of the physical and numerical sub-models as applied to fires and smoke movement.

Unfortunately, errors are also possible as a result of faults in the software, i.e. ‘bugs’ (Beard, 1996). Commercial CFD codes are highly complex, typically in excess of one hundred thousand lines of code, and so mistakes exist. ‘Bugs’ are outside the control of the CFD code user and they are often difficult to identify. Unfortunately, mistakes do happen and are a ‘feature’ of complex engineering software. The CFD user thus needs to be vigilant. Careful analysis of the results obtained can help pinpoint potential problems.

Mistakes are more often made by the user, who can, for instance, enter a wrong value for a fire heat output simply by pressing the wrong key. Another possible source of error, especially when using a commercial CFD code, is to misunderstand the equations and parameters included in the selected sub-models. The users do not generally have access to the coded equations. Even if they did, it would be a tremendous task to read and understand them. The code manual aims to explain which equations are included in a sub-model, how to ‘turn them on’ and what parameters need to be specified. If the user fails to set a parameter, a default value will be used. This value can be inappropriate to the problem at hand. For example, HSL have compared the predicted rate of smoke propagation for two different values of a buoyancy-related constant in the k-ε model. They have found that setting this constant equal to zero, its default value in most commercial CFD codes, does not properly take into account buoyancy effects and thus significantly over-predicts the rate of smoke propagation. This is adequate for most flows, but not for fire safety engoneering applications !

However, perhaps the main source of uncertainty in the output of a CFD simulation is that resulting from the actions of the user. Commercial CFD packages are highly complex pieces of engineering software. To use them reliably, the user must have a good understanding of fluid flow, in particular of the application, in this case fires and smoke movement, as well as all aspects of CFD methodology relevant to the application. The user should also preferably have a track record of applying CFD to this class of flow problem.

2.9. Summary

To summarise, uncertainties in a CFD simulation may arise from:

- Level of detail represented by the geometry
- Mesh resolution
- Selection of physical sub-models
- Selection of spatial and temporal discretisation schemes
- Specification of the boundary conditions
- Selection of convergence criteria
- User errors
- Cursory analysis of results
- Software errors
- Experience of CFD user

3. ASSESSMENT OF CFD PREDICTIONS OF SMOKE MOVEMENT

CFD is a powerful technique that can provide a time-dependent, three-dimensional, solution of the equations that govern fluid flows, in highly complex geometries; for which simpler models would be inadequate. CFD has, therefore, been extensively employed to evaluate smoke transport issues in modern complex buildings: for example in the Millenium Dome (Hiorns and Sinai, 1999); the Coventry Library (Mills, 2001); office building atria (Sinclair, 2001). CFD is also being used to investigate different generic ventilation configurations and provide guidance on smoke management issues (Hadjisophocleous et al., 1999; Klote, 1999).

However, the solution obtained by CFD is not exact. A number of assumptions and approximations are made throughout the whole process and some of them can have a significant influence on the results (Gobeau and Zhou, 2002; Ledin et al., 2002). If the decisions made by the CFD practitioner are not based on a sound judgement, the results can be significantly affected, and, for example, worringly lead to overestimates of available time for evacuation.

This section provides HSE Inspectors with the issues that should be considered when assessing CFD simulations of smoke movement submitted in a safety case and help them determine their accuracy. A summary of the main points that should be scrutinised is provided in Appendix A.

If, as a result of the Inspector’s assessment, doubt remains about the reliability of the results, a more in-depth examination by HSL CFD and Fire Safety Engineering experts is strongly recommended.

3.1. Expertise of the CFD user

The creation of the geometrical model, the selection of appropriate physical and numerical sub-models, specification of boundary conditions and assessment of solution convergence all require a thorough knowledge of both CFD and fire and smoke movement dynamics. If the user is a well established practitioner for fire engineering applications - evidenced for example by a track record of applications, possibly supplemented by publications in peer-reviewed journals or proceedings, this should give confidence that the capabilities and limitations of the technique have been fully understood and the choices have been made on a sound basis.

Someone who is only a CFD expert, with no or little understanding of fire and smoke movement dynamics, will be aware of the general limitations of CFD, such as the need to create a computational grid of a size appropriate to the scales of the physical mechanisms. However, if they lack an understanding of fire dynamics, then even armed with the above knowledge they may find it difficult to design a grid which is appropriate to the problem.

On the other hand, an expert in fire dynamics who has no grounding in CFD and is new to its application might be aware of some key aspects of the physical sub-models required in this application area, but may not realise that the results could significantly depend on specific numerical issues such as the discretisation schemes.

In any case, the reliability of the results cannot be based solely on the expertise of the user. Thus even a CFD expert in fire safety engineering might, due to budget and time constraints, have to make drastic assumptions - such as reducing the number of equations solved or using a coarse grid. This is especially attractive for simulations of large complex spaces which are intrinsically demanding in computing resources. Although the assumptions might be based on sound judgement - for instance large grid cells away from the fire and small cells in the fire which is driving the flow, they can potentially lead to non-conservative results.

Summary - <u>CFD user expertise</u>:

- ***The practitioner must have an in-depth understanding of both CFD and fire and smoke movement dynamics.***

3.2. CFD code

Commercial CFD packages consist of hundreds of thousands of lines of code which embody the physical and numerical sub-models, and in some cases provide a sophisticated interface to help the user create the geometry and define the problem.

Uncertainty in CFD solutions, as seen in the previous section, can arise from many sources: inappropriate physical or numerical sub-models, along with errors or bugs in the coding. It is important that any CFD code is validated against test cases for the range of applications the code claims to cover. It is especially important to be aware of the extent to which the code has been validated for the application of smoke movement.

The number of users employing the code in general and specifically to predict smoke movement can also give an indication of how likely the code is free of bugs. With such complex pieces of software, mistakes are unavoidable. However, the more people use the code, the more likely the mistakes are to be found out and corrected.

Commercial codes are to some extent validated by their developers and user base, although these tests are generally not well documented or readily available (Casey and Wintergerste, 1999).

However, there is no well established benchmark set of data from large-scale tests in complex spaces available for extensive validation. Data has recently been generated at lab-scale (Ledin et al., 2002) but there is still a need for specific large-scale data. This being the case, the best that can usually be expected in the way of validation for fire and smoke movement is evaluation of the underlying physical and numerical sub-models by comparison to experimental data for relatively simple fire problems; such as diffusion flame, plume, simple compartment fire, ceiling layer, etc... In some cases it may be possible to compare CFD results to limited measurements made during commissioning trials.

The most well known commercial codes that have been widely applied to fire safety problems in the United-Kingdom are: FLUENT, CFX4, CFX5, PHOENICS and STAR-CD which are all general purpose codes; JASMINE and SOFIE, which are fire specific. CFD results presented in safety cases are very likely to come from one of those codes. These should not raise any specific concern and acceptable results can often be obtained provided the problem has been properly specified by the CFD practitioner, as described in the next sections.

CFD simulations could also have been undertaken with an in-house code. If this is the case, it is advisable to seek information on the level of validation undertaken, especially in the area of fire and smoke movement, and on the number of users both as a whole and for the simulation of fires. Ideally, an independent assessment of the code should have been carried out (Beard, 1996).

Summary - <u>CFD code</u>:

- ***The CFD code employed should ideally be validated for application to fire and smoke movement.***

3.3. Computational domain

3.3.1. Two- or three-dimensional domain

The geometry represented in the model must be three-dimensional. Complex geometries rule out the use of a two-dimensional simulation. Indeed, even in simple geometries such as tunnels, the flows induced by fires are three-dimensional. Serious errors can occur by assuming that the flow can be treated by a two-dimensional representation.

3.3.2. Definition of the domain

The user has to fix the boundaries of the computational domain. This can seem quite straightforward for stand-alone scenarios, for example the external walls and roof of a building. In reality, representing the whole building or indoor space could lead to unreasonable run-times. Therefore the domain may have to be restricted to a manageable size. This, however, must not jeopardise the realism of the scenario modelled. For example, Gobeau and Zhou (2002) have represented only three floors out of eighteen when simulating fire and smoke movement in a building under construction. The first three floors and the top floor were modelled. The other floors were excluded, since at this stage of the construction their access from the atrium was through a door. All the doors of the intermediate floors were assumed to be closed as this was identified as the worst case scenario for which the smoke could rise more rapidly in the atrium and reach the top floor.

Another possibility to reduce the computational domain is to exploit any axis of symmetry. In such a situation, only a proportion of the volume of interest is represented: half for one axis of symmetry; a quarter for two axis, etc... A symmetric boundary condition is applied on the symmetry plane. In real complex scenarios, it is quite unlikely that there will be any axis of symmetry at all. However, if this happens, Cox and Kumar (2002) recommend that the validity of the approach is checked by comparing it with a simulation in the full domain, potentially using the reduced domain results as the initial conditions for economy. This can, however, require a significant computing run-times and may not be always practical.

There are situations for which choosing the domain boundaries can be difficult because the volume of interest is connected and influenced by areas that are not part of the CFD analysis. For example, an underground station is connected to other stations by tunnels. Since the entire underground complex cannot be modelled using CFD, boundaries have to be set at locations where a flow exists. This flow can be obtained via measurement, or use of additional predictive tools such as network models to cover the entire complex.

As an example, Gobeau and Zhou (2002) have defined the boundaries of an underground station at the exits at street levels and across a horizontal plane between the ticket hall and the platforms. Since the fire was assumed to be in the ticket hall, the levels below were of no special interest and were not included. Information about the flow at these boundaries must then be specified by the user - see Section 3.7 on boundary conditions. This includes setting up appropriate boundary conditions so that smoke which is likely to leave the domain can do so and fresh air can enter at lower level if the smoke flow is stratified - as through the exits of the underground station (Gobeau and Zhou, 2002). Locating a boundary where the smoke may re-enter the domain should however be avoided, since CFD will not be able to predict the amount re-entrained inside the domain by what happens outside nor will the CFD user be able to specify it in advance. A necessary condition is thus to place the boundaries away from the fire. For ‘pressure’ boundaries (see Section 3.7 - Boundary conditions), it is possible to check once the simulation is completed that the predicted velocities for air flow and smoke movement cannot cause smoke once it has left the domain to re-enter.

3.3.3. Details represented in the computational domain

Any object which may have a significant impact on smoke movement must be accounted for in the model. This includes any significant heat source other than that generated by the fire itself, for example powerful spot lights or significant solar gain, since these may create a natural convection flow which can interfere with the fire plume. Significant obstacles to smoke transport must also be represented such as deep ceiling beams. However, it may not be practical for large spaces to include all the details. Simplifications have to be made. For example, Gobeau and Zhou (2002) ignored fixtures and fittings in all three real scenarios. Staircases were represented simply as inclined planes rather than individual steps in the underground station and offshore accommodation module. For the building under construction, the stairwells were more simply represented by empty towers, as this was thought as being the worst-case scenario for which smoke can be transported freely and quickly to the upper floors without having to travel around the staircases.

Similarly, geometrical shapes can be slightly modified if this is not likely to influence the flow to any great extent. The advantages of such simplification are that it is possible to generate a less distorted grid - a step which tends to produce less numerical error, and, grid cells can instead be employed to capture more important flow features. Overall, these advantages can outweigh the loss of details in the geometry specification. This is especially true for structured grids.

Summary - <u>Computational domain</u>:

- ***The domain must be three-dimensional.***
- ***The domain boundaries should be located such that they do not adversely affect simulated smoke movement: for instance, open boundaries should not be located close to the fire source.***
- ***The level of geometric detail represented inside the domain should include anything that might significantly affect the flow, for instance potential obstacles, heat sources other than the fire, etc...***
- ***Ensure that geometric simplifications are justified and unlikely to significantly affect the flow.***

3.4. Computational grid

Once the domain has been created, it must be sub-divided into much smaller domains, i.e. grid cells. The size of the grid should be chosen so that all the important geometric details and flow phenomena that drive smoke movement can be resolved. Also, that it is consistent with requirements imposed by the modelling approaches chosen.

For fire applications, it is important to capture correctly the rise of the plume and the formation of a hot gas layer near ceilings. This requires a division of the plan area where the fire is specified into a significant number of cells, typically at least 4 x 4. For structured grids, it is recommended to set a significant number of cell layers in the vertical direction possibly refined near the ceiling - so as to capture ceiling layer flows. However, this might result in highly distorted cells if their lengths in the lateral directions are relatively long. Cox and Kumar (2001) recommend that cell aspect ratios (defined as the ratio height to length) are kept below 50. Ideally, the ratio should be of the order of one near the fire. For unstructured grids, it is recommended that the first few layers of grid cells next to the ceiling are parallel to the ceiling. This again helps capture steep gradients which may occur in ceiling layer flows.

The use of turbulent wall functions (see Section 3.7 - Boundary conditions) imposes conditions on allowable sizes of the grid cells at walls. This depends on the local turbulent properties of the flow, and, since these are unknown at the start of a simulation, may require the user to go back and modify the grid.

Quite often, some of the requirements outlined above are contradictory. For example, refining the grid in the region of the fire might lead to overly small cells at the ceiling - such that turbulent wall functions then become used outside their range of validity.

Designing a grid is therefore not an easy task since it requires some prior knowledge of what governs the flow and its likely form. Past experience of simulations of similar flows is therefore helpful. Ideally, a sensitivity test to the disposition and number of grid cells should be undertaken. Such a test consists of carrying out simulations with increasingly decreasing size of grid cell until no significant differences in the predictions are found. The CFD solution is then said to be grid-independent. The size must be reduced by a significant factor in each co-ordinate direction, ideally two. However, for large and complex spaces, such a test might not be practical.In this case it may be possible to limit it to a region close to the fire or to refine the grid in one co-ordinate direction, such as the vertical, by a factor two. Thus whilst both Gobeau and Zhou (2002), and Ledin et al (2002), have undertaken a grid sensitivity test for one of the scenarios they modelled, to save computing time, Gobeau and Zhou (2002) reduced the size of the grid cells only on the floor where the fire was assumed to occur. If in doubt of the quality of the grid, the assessment by a CFD expert is recommended.

Summary - Computational grid:

- ***The design of the computational grid - the disposition of grid cells and their size, should be based on an understanding of the key flow phenomena and preferably experience of a similar case;***

- ***The plan area of the fire source should be divided into several grid cells - typically at least 4x4 cells;***

- ***For unstructured meshes, use of 'inflated grid cells' is recommended next to ceilings;***

- ***For structured meshes, a significant number of cell layers should be employed in the vertical direction - particularly in ceiling layer flows;***

- ***The cells should not be too distorted - particularly near the fire; Kumar and Cox (2001) recommend that the cell aspect ratio does not exceed 50. Ideally it should be of the order of one close to the fire.***

- ***A test of sensitivity of the results to the grid size should preferably be undertaken.***

3.5. Physical sub-models

The CFD user has to select appropriate physical sub-models. This effectively decides the modelled equations that will be solved, including their parameters. The first step in this process is identify the important physical mechanisms that govern the flow.

For fire applications, the mechanisms involved are:

- Combustion processes that are responsible for the production of heat and smoke.

- Buoyancy: the heat released by the fire results in natural convection due to buoyancy effects; buoyancy also affects turbulence.

- Turbulence: the fire induces a turbulent flow that influences the heat exchange with the ambient air and that has a reciprocal action on the fire by affecting the fuel-air mixing. It also subsequently affects smoke transport and dilution through mixing;

- Heat transfer at walls: fire-generated flows will lose some of their heat at the walls;

- Radiation: part of the heat produced by the fire and transported in the smoke is exchanged with the surroundings by radiation.

To take into account these effects, the CFD user has a choice of modelling approaches. The approaches employed in Fire Safety Engineering, their advantages and limitations, as well as the effects they may have on the results, are outlined in this section. The issues of interpreting the CFD smoke-related data, usually smoke concentration or mass fraction, in terms of safety hazard quantities - visibility and toxicity - are raised briefly.

3.5.1. Combustion models

There are basically two types of modelling approaches to account for combustion:

- A volumetric heat source model which does not predict the release of heat and smoke in the flame but only their transport away from it. The quantities of heat and smoke released by the fire and the volume of flame where the releases occur have to be specified by the user. The distributions of heat and smoke released are assumed uniform over the flame volume.

- A combustion model which aims to predict, although simply, the chemical reactions that happen in the flame. The overall quantity of heat released and the area of the fire have still to be specified. However, the non-uniform distribution of heat in the flame region is predicted and aims to take into account the influence of the local flow.

The first approach is the most economic and therefore widely employed to investigate fire consequences in large spaces (Klote, 1999; Hadjisophocleous et al., 1999; Sinclair, 2001)

Both approaches were compared by Gobeau and Zhou (2002) for a fire which started in a large open area in a building under construction. The predicted transport of smoke was similar. This is in agreement with the findings of Xue et al. (2001), but not with those of Kumar and Cox (2001). This is believed to be due to the different characteristics of the fires investigated: Kumar and Cox modelled a fire located in a doorway - the plume of which was deflected by the jet of air going through the doorway. The combustion model successfully reproduced the tilted fire plume whilst the volumetric heat source approach imposed a straight plume and as a result failed to predict the distribution of temperature and air entrainment rates into the plume.

Whilst the volumetric heat source model is apparently able to provide results comparable to use of a combustion model in some circumstances, the need to prescribe the volume of the flaming region is clearly a limitation of this approach and it makes it suited only for situations where the shape and volume of the flaming region is known in advance, i.e. is not overly dependent on the local flow conditions. These situations include those in which the fire source is remote from walls or openings. For any other situations, the use of a combustion model should be preferred over a volumetric heat source model. Examples include under-ventilated fires, fires subject to forced ventilation, fires located near walls or where supply of air is not symmetrical.

Gobeau and Zhou (2002) investigated the sensitivity of the volumetric heat source model to the specification of the plume volume, namely its height and shape. Predictions were found different near the fire source although the differences were no longer significant further away. Hadjisophocleous (1999) found a sensitivity of the results to the height and area of the prescribed volume over the whole domain. Kumar and Cox (2001) also stress the importance of defining an appropriate fire area in the case of a combustion model. Indeed, failing to set properly the input parameters for both models will lead to inaccurate results - although the level of inaccuracy will depend on the scenario.

To summarise, the model employed must be able to adequately represent the behaviour of the flaming region and consequent fire plume, since this will ultimately affect smoke transport further away from the fire. This means that the values set for the input parameters must be chosen carefully, based on experimental data or well-established correlations. There are circumstances, i.e. when the fire plume is influenced by the local air flow, for which the prescription of realistic input parameters for a volumetric heat source model will be difficult. In such cases, use of a combustion model requiring fewer parameters, is preferred.

3.5.2. Buoyancy

In flows accompanied by heat transfer, the fluid properties, in particular density, are functions of temperature. The Boussinesq approximation, however, assumes a constant density in the most of the terms of the momentum equations, and treats it as a variable only in the gravitational term - and then usually linearly dependent on the temperature. This approach is valid for very small temperature gradients, of the order of a few degrees or a maximum few tens of degrees Celsius. Despite this limitation, this model is sometimes used to predict the transport of smoke from a fire in large volume spaces. The argument presented is that the model assumption will be valid in most parts of the domain with the exception of the immediate vicinity of the fire and that the difference in the end result will therefore be small. The benefit is the relatively modest need in computing resources.

However, Gobeau and Zhou (2002) compared this approach with a more realistic compressible model which calculates air density using the perfect gas law. The simulations were undertaken for a modest fire size (the burning of a passenger suitcase, circa 200kW heat output) in the large ticket hall of an underground station. Significant differences were found in the predicted temperatures reached near the fire and ultimately in the transport of smoke.

Therefore, the Boussinesq approximation cannot be recommended for modelling the effects of buoyancy in fire and smoke movement simulations unless it can be demonstrated that the impact of this simplification is negligible. Instead, an equation of state should be solved.

3.5.3. Turbulence models

At the time of writing, the turbulence models most likely to be employed for fires in complex spaces are of RANS type - see Section 2.3.2. If Inspectors encounter CFD results obtained with other models, such as LES and DNS, they are advised to contact HSL CFD experts for advice.

In principle, amongst the RANS models, the second moment closure models are better suited to predict flows dominated by buoyancy forces. However, the computing time is drastically increased compared to eddy viscosity models, not only because of the larger number of equations to be solved, but principally because these models are unstable and less robust (Grotjans et al., 1999). Indeed, Ledin et al. (2002) tried to employ a Reynolds stress model for the scenario in a straight corridor. Convergence could not be achieved. This was thought to be due to the somewhat deformed grid that was designed to match the cylindrical source. Results could however be obtained relatively easily with a k-ε model. This demonstrates that the application of a high order turbulence model is likely to be difficult, if not impossible, for complex geometries for which the shapes of the computational grid cells are necessarily distorted.

As an alternative to second moment turbulence models, modifications have been suggested to eddy viscosity models in order to improve their performance. In particular, gross modifications have been proposed to the k-ε model to crudely take into account the buoyancy effects on turbulent mixing, for example Rodi (1978) or Viollet et al. (1983). The models are not identical, but they are based on the same principle: additional terms related to the buoyancy forces are added to the k and to the ε equations to correct the behaviour of the model. Some argue that the term in the ε equation can be neglected. However, this can have a severe effect on the results (Gobeau and Zhou, 2002). So for fire applications, a k-ε turbulence model is appropriate only if both turbulence equations are modified to account of buoyancy effects.

Simpler eddy viscosity models that solve none or only one of the transport equations to characterise the turbulence must not be used since they are unable to cope with buoyancy effects, nor can they be modified to account for these.

3.5.4. Radiation models

When employing a volumetric heat source model, the simplest method of accounting for radiation loss, by removing an appropriate proportion (fractional heat loss), is adequate. This approach however only accounts for the radiative loss of the flaming region and ignores other radiative heat transfer, in particular the transfer from hot smoke to walls and the transfer within the smoke. Woodburn (1995), who simulated a fire in a tunnel, found that including radiative heat transfer at the walls improved the agreement between the predicted temperatures with the measurements in the hot gas layer, although the model still ignored the radiative transfer within the gas. However, employing more sophisticated approaches to account for radiation in combination with a volumetric heat source model is unlikely to increase the accuracy of the results due to the limitation of this model which assumes a uniform heat distribution in the flaming region.

Any radiation model can be combined with a combustion model. Kumar and Cox (2001) compared an eddy-break-up model with and without radiation. The radiation model used was a simple, yet commonplace, six-flux model with a grey gas assumption to calculate the emissive power of hot gases - see Section 2.3.3. This model takes into account the radiative heat transfer within the gas. Its inclusion generated a redistribution of the heat energy within the gas and consequently the radiation model gave better agreement with experimental data although the model is nevertheless quite a crude representation of reality.

More sophisticated models, based on the calculations of a significant number of representative rays - see Section 2.3.3, are unlikely to be routinely applied to large complex spaces due to their prohibitive computing cost.

It is believed that, in the absence of more ‘fundamental’ models, even simple models such as the fractional heat loss approach are appropriate. Appropriate modelling of other aspects than radiation, such as turbulence and control of numerical error, are believed to be a necessary condition to obtain reliable CFD results. Indeed, since the mixing of combustion products and air ultimately plays a significant role in determining radiative heat transfer, sophisticated radiation models can only be expected to add value if models of other physical mechanisms, such as turbulence, adequately capture the flow behaviour.

Summary - Physical sub-models:

- ***The Boussinesq approximation should not be used for modelling the effect of buoyancy, unless it can be demonstrated that the impact of this simplification is negligible.***

- ***If, as is common, a k-ε turbulence model is used, it must include modifications for buoyancy effects in both k and ε equations.***

- ***Simpler, zero- or one-equation, turbulence models should not be used.***

- ***A volumetric heat source or combustion model can be used when the fire is not influenced by proximate walls or ambient air flows and providing the fire source is well specified: heat output and heat release volume for a volumetric heat source model; heat output and heat release area for a combustion model: see Section 3.6.***

- ***Where the fire plume might be affected by proximate walls or local flow conditions which cannot be adequately determined in advance, a combustion model is preferred to a volumetric heat source model.***

- ***Whichever means is used to model the fire, the resulting plume and flaming region temperatures should be checked to ensure they are representative.***

- ***Radiation should be taken into account, at least by reducing the fire heat output to account for the radiative loss - failure to do that is expected to lead to conservative predictions in the near-field in some cases (for example when the predictions are employed to evaluate the time available for evacuation) but could provide misleading information for other applications (for example when the predictions are used to advise on the positions of heat detectors). The radiative loss has to be soundly based.***
  In the far-field, more sophisticated radiation models than a reduction of the fire heat output may need to be included for large fires in constrained spaces; it is less critical for modest fires or fires in large spaces.

3.6. Fire source specification

3.6.1. Selection of fire scenarios

Fires have to be specified in the CFD model, i.e. at least their location and heat output and possibly other parameters depending on the modelling approaches chosen by the CFD user. Selection of fire scenarios is not trivial and is obviously an important pre-cursor to CFD modelling. It is however outside the scope of this document. Experience in identifying fire hazards is required. Heat release rates from potential combustible materials can then be found in the SFPE Handbook.

3.6.2. Prescription of heat release

An unwanted fire is essentially a natural combustion: the rate of supply of fuel is determined by the fire itself. The fundamental mechanisms of a fire (including its ignition) that lead to the production of heat and smoke cannot at present be predicted for practical fire scenarios and for the complex nature of combustible materials commonly encountered. CFD is thus not yet able to predict the intrinsic release of heat caused by the burning of materials. This has to be specified in the CFD model by the user.

When employing a volumetric heat source model, the volume over which the heat is released has to be specified. The area depends on the shape of the goods that are burning. The height of the flame can be estimated by empirical correlations (Drysdale, 1998). The shape of the volume can be made conic in order to crudely match the shape of a flame. The volume can also be time-dependent and grow at a rate determined by the heat release. Results are however dependent on the prescribed volume (Hadjisophecleous, 1999; Gobeau and Zhou, 2002). The choice of the volume must therefore be justified and the predicted temperatures inside and near this volume should be compared with those expected. This can be done by using experimental data or well-accepted values from the literature.

A combustion model does predict the heat distribution in the flaming region and the influences of the local fluid mechanics on it. However, parameters characterising the fire still need to be specified; for example, the area over which the heat is released or the rate at which the fuel is introduced. Again, the value of the parameters should be chosen carefully and its choice justified.

3.6.3. Prescription of smoke production

As for the production of heat, the intrinsic process leading to smoke generation from a fire can not be predicted and so the smoke production rate has to be specified.

Production of smoke depends on the properties of the burning materials, the quantities available, the physical state of the materials (for example stacked or piled goods) and the air flow conditions. The smoke production rate can however be crudely linked to the heat release rate by a yield factor that has been determined experimentally for a wide range of materials and conditions. The CFD user needs to select the one closest to the scenario under investigation, or alternatively the one that is likely to lead to the worst case. This yield factor represents only the production of aerosols from combustion; it does not include the gaseous products.

Depending on the model employed, the smoke produced is then either uniformly distributed over a volume (volumetric heat source models) or over an area (combustion models).

Although this approach is quite crude, it is fairly commonplace as it is the most practical approach. It should yield adequate results, except maybe if there is a change in the ventilation regime, for example from an under-ventilated to an over-ventilated fire, which in practice will modify the rate of smoke production whilst the CFD model will assume it is constant.

Summary - <u>Fire source specification</u>

- ***CFD cannot predict the intrinsic heat release from a fire and so the user has to specify input parameters characterising the fire; the parameters needed depend on the modelling approach chosen but in any case, they have to be specified so as to lead to realistic temperatures. This can be ensured by comparing the predicted temperatures near the fire source with measurements or well-accepted correlations***.

- ***A constant smoke yield rate (of particulate and aerosol fractions) to model the production of smoke is a crude approach but it is acceptable in most cases, providing its value is based on sound data - for example Table 3-4.11 of the SFPE Handbook, 1995.***

3.7. Boundary conditions

The boundary conditions have to be defined by the user. They represent the effect of conditions external to the computational domain on flow inside the domain. These include friction at walls, the influence of a flow entering or leaving the computational domain, ventilation conditions, space heating, etc... They can, justifiably, be said to determine the CFD solutions.

3.7.1. Inlets and outlets

At a free boundary where the flow will be mainly influenced by what happens inside the computational domain, a constant pressure boundary - which implicitly assumes that the flow is fully developed - is applicable. Such boundaries have to be placed where the 'fully developed' assumption is either valid or has little impact on flow inside the domain. That means away from the fire and at locations where the flow is not expected to experience strong spatial variations. For example, this type of boundary condition was applied to the exits of the underground station (Gobeau and Zhou, 2002) since they were located far from the fire and since their areas were relatively small compared to the dimensions of the station.

The other boundaries - where flow is driven principally by mechanisms external to the computational domain, such as forced ventilation, must be located where the flow conditions are known and can be specified.

Specification of the flow at the boundaries might require further analysis which can be provided either by measurements or additional modelling - including CFD. Detailed analysis is necessary when the flow across the boundary is expected to be complex. This could be the case for a space partially open to the atmosphere and for which the surroundings influence the direction and velocity of the incoming wind. As an example from another application area, Saunders and Ivings (2002) were interested in determining the dispersion of flammable gas inside a naturally-ventilated offshore module under different wind conditions. They first created a CFD model of the exterior of the module and the surrounding platforms to calculate the pressure distribution over the openings to the module. They then used these predictions as boundary conditions for a separate detailed CFD model of the inside of the module. Other fire-related examples where such a situation could occur are railway stations and buildings at an early stage of construction.

In the case of nominally well-sealed spaces, it can be very important to represent leakage flows into or from the domain. Even small leakages can have a dramatic impact on the distribution of smoke. It can then become crucial to model these leakages (Ivings, 1999; Sinai, 2000).

3.7.2. Walls

In order to save computing times, universal wall laws are often applied as wall boundary conditions. These functions preclude the need to resolve in detail the large gradients of temperature and velocity near walls, which would necessitate a large number of grid cells.

Instead, momentum and convective heat fluxes between the near-wall nodes of the computational grid and the wall itself are assumed to be described by universal laws of the wall.

These laws include parameters that acount for the roughness of the walls and lead to lower velocities in the case of rough walls. Kumar and Cox (1988) investigated the sensitivity of the results to these parameters for a fire in a railway tunnel. They found a difference in the predicted temperature of up to 30^{o}C. Although there are recommended values for these parameters for smooth surfaces and a variety of rough surfaces in industrial engineering, there are only very few for practical building materials (Chapter 6 - Cox, 1995).

Also, for these laws to be valid, the near-wall cell grid size must be chosen such that the first grid nodes must lie within and above certain distances from the wall, based on the local turbulent Reynolds number.

Uncertainties associated with the use of wall laws are of two types: the difficulty in complying with restrictions on the location of the near-wall nodes across the whole domain, and because they are strictly only valid for rather idealised situations - such as no flow acceleration or deceleration. Nevertheless they are in common use and are often the only practical means of modelling the near wall region.

The CFD user has to specify how heat transfer is to be modelled at the walls. One possibility is to assume nil heat transfer, i.e. an adiabatic wall. The other extreme is to assume a constant wall temperature - leading to maximum rates of heat transfer. The heating of the wall can also be modelled, by solving for thermal conduction within the wall. However, this requires a much finer grid resolution near the wall and specification of the properties of the wall - and these may not be fully known.

Whilst it is possible in a CFD model to allow for wall heating - by defining a time-dependent boundary condition based on local predictions of temperatures (Ivings, 1999), simpler approaches can also be useful. Thus Gobeau and Zhou (2002) and Ledin et al. (2002) applied steady wall boundary conditions to investigate the two extreme situations: no heat transfer (adiabatic walls) ; maximum heat transfer (walls fixed at ambient temperature). The results were found sensitive to these boundary conditions in all but one out of four scenarios. The isolated scenario comprised a relatively small fire in a large open area with background ventilation, i.e. where wall heat transfer is less of an issue. For the other scenarios, smoke propagation was faster in the case of adiabatic walls, with the smoke more concentrated in the hot gas layer near the ceiling. However, less smoke was however predicted at lower levels than with a fixed wall temperature.

Radiation adds further complications, which are not dealt with here.

It is therefore recommended that close attention be paid to wall heat transfer conditions. The adiabatic wall condition, which generally leads to the most rapid rate of lateral smoke propagation, can be used as a conservative estimate. One must bear in mind, though, that smoke concentrations at lower levels are then likely to be under-estimated.

3.7.3. Fire-dependent conditions

As the fire is growing, it may change the conditions inside the computational domain. For example, windows can break causing the fire to spread more rapidly and possibly letting fresh air from outside enter and smoke escape. Structures can also fail and collapse. Theoretically, it is possible to include these in a CFD simulation, employing the predicted temperatures to determine when the events happen. It is also possible to combine CFD with a computational finite structure analysis to predict the effect of fire on structures. Guidance on the assessment of such models is, however, out-of-the-scope of this guidance.

An example of an analysis by a computational technique of the structural response of an industrial portal frame to fires can be found in Wong, 2001.

When these phenomena are not included in the model, it is acceptable if it is accounted for in the use made of the results. For example, if near a material, the predicted temperatures reach a value above the one causing its liquefaction or destruction, one must bear in mind that the results at a later stage are no longer strictly valid. This should be reflected in the analysis of the results.

Summary - <u>Boundary conditions</u>:

- ***If forced ventilation exists then this is usually prescribed as a boundary condition. It is recommended that the location of these boundaries be remote from the fire source and that the specified values are justified by the CFD user.***

- ***The presence of leakage flows to other parts beyond the computational domain, or the outside atmosphere, can have a significant effect on the flow inside the domain - particularly when that flow is governed by convection generated by the fire, rather than forced ventilation. The possibility of leakage flows should therefore be considered.***

- ***When flow through a boundary is governed by fire-generated convection, it is commonplace to use a prescribed pressure boundary condition. Pressure boundaries should however be located remote from the fire.***

- ***Heat loss to the walls can have important knock-on effects on smoke movement. This is particularly the case when the fire products are in close and immediate proximity with walls. In general it can be considered that a conservative approach as regards rates of lateral smoke propagation is to assume no heat loss at walls, i.e. an adiabatic condition. Note, however, that this approach may then under-estimate smoke concentrations at low levels.***

3.8. Smoke transport

3.8.1. Characterisation of smoke movement

Sometimes, temperature is used to illustrate the transport of smoke. However, this can be misleading since unlike smoke mass, temperature is not a conserved variable (Grant and Lea, 2001).

A transport equation for smoke mass concentration must be solved.

The simplest approach consists of assuming that smoke production is proportional to the heat output, with a constant conversion factor used to relate the two. The value of the factor is determined experimentally and has been tabulated for a wide variety of flammables (The SFPE Handbook, 1995; Table 3-4.11). The smoke is then assumed to follow the motions of the air and its mass concentration is obtained by solving a transport equation for a passive scalar. This approach can be used in combination with either a volumetric heat source or combustion model. If used with a volumetric heat source approach, the smoke released by the fire is uniformly distributed over the prescribed flaming volume. If used with a combustion model, the quantity of smoke released is distributed over the region or area in which fuel is introduced in the domain.

One problem with this approach is that rates of smoke propagation are actually strongly determined by ventilation conditions. However, this modelling approach would not generally be able to distinguish when predicted conditions change from over- to under-ventilated. Hence this should be monitored by the user.

More complex soot formation models do exist. They are used with combustion models which aim to take into account the fire chemistry. The smoke produced is released over the fire area and its distribution in the flaming region is predicted by the model based on the influence of chemical reactions and local properties flow conditions. However, the combustion model most widely employed for smoke movement in large and complex spaces is the eddy-break-up model. This assumes complete combustion where the oxidant is in sufficient supply. However, smoke is a product of incomplete combustion. The eddy-break-up approach is therefore not well-suited for coupling with soot formation models.

More sophisticated models are under constant development in academia. At the moment, however, the simple approach of assuming a constant smoke conversion factor is probably the most practical approach for investigating the transport of smoke.

3.8.2. Smoke toxicity

A large proportion of fatal and non-fatal fire casualties are in fact caused by the smoke generated by the fire rather than directly by the fire itself (The SFPE Handbook, 1995; p. 2-85).

The health effects of smoke are numerous: they can cause severe eye irritation - which will further reduce a person's ability to see exit signs etc... They can also lead to asphyxiation and inflammation of lung tissue when inhaled. The parts of the airways reached by the smoke particulates will depend on their sizes. Soot particles with a diameter of 5 μm or less reach deep into the lungs, thus leading to inflammation of tissue, while larger particles are deposited in the nasal passages, Jagger (1991). Carbon monoxide and other toxic gases contained in smoke and the hot fire gases can also have debilitating and deadly effects.

Quantification of exposure to smoke will depend on factors such as its composition, the rate of uptake of toxic products in the target organ of the body, and the time period over which exposure occurs. This means that modelling the detailed effects of exposure is difficult: quantification of the toxic constituents of smoke and hot fire gases is necessary and the exposure will depend on the escape route followed by an individual.

Nevertheless, smoke concentrations and temperatures obtained by CFD can provide an insight into the risk to occupants within the enclosed space. In particular, an indication of the risk of exposure along emergency routes can be obtained.

3.8.3. Smoke visibility

Visibility though smoke is an important characteristic to consider when assessing the risks to occupants in the event of a fire, as this can have a significant impact on their decision whether to try and use an excape route or not; e.g. smoke can easily obscure exit routes and signs even at quite low concentrations, Jagger (1991).

There are a number of factors that visibility depends upon: smoke concentration obviously, but also brightness or luminance of objects, daylight or electric lighting conditions, distance of an individual to an object, as well as visual acuity of an individual.

Representing smoke visibility by simply post-processing CFD results to give iso-surfaces of smoke concentration can however be misleading. Instead, integration of the cumulative effects along lines of sight is ideally required. Such 'line of sight' visibility predictions are being seen in CFD applications.

Experimental data on visibility have been gathered by tests with humans viewing objects through smoke, Jagger (1991), Ouelette (1993). Correlations have been established from these experiments. Once coupled with smoke concentrations predicted by CFD they an be used to simulate smoke visibility - for example, see illustration Figure 6.

The correlations are at present quite simple, typically deducing a local transmittance from the smoke concentration and an extinction coefficient. This last coefficient depends on the smoke properties and is likely to vary in space and time. It is however considered constant in the correlations and its value is based on a single specific experiment (see the SFPE Handbook, 1995 pages 4-253 and 4-254 for more details). Visibility is obtained by integrating the transmittance over the distance between the individual and the point considered. This approach does not take into account all the complex factors that influence visibility and more research work is needed to validate it and if necessary suggest improvements. However, it is a first step towards extracting from CFD simulations data that are more appropriate to assess risks.

Unfortunately such approaches are not well-validated. If they are used to demonstrate that despite the presence of smoke on an escape route the level of predicted visibility is acceptable, such a finding should be viewed with great caution and ideally supported by practical tests.

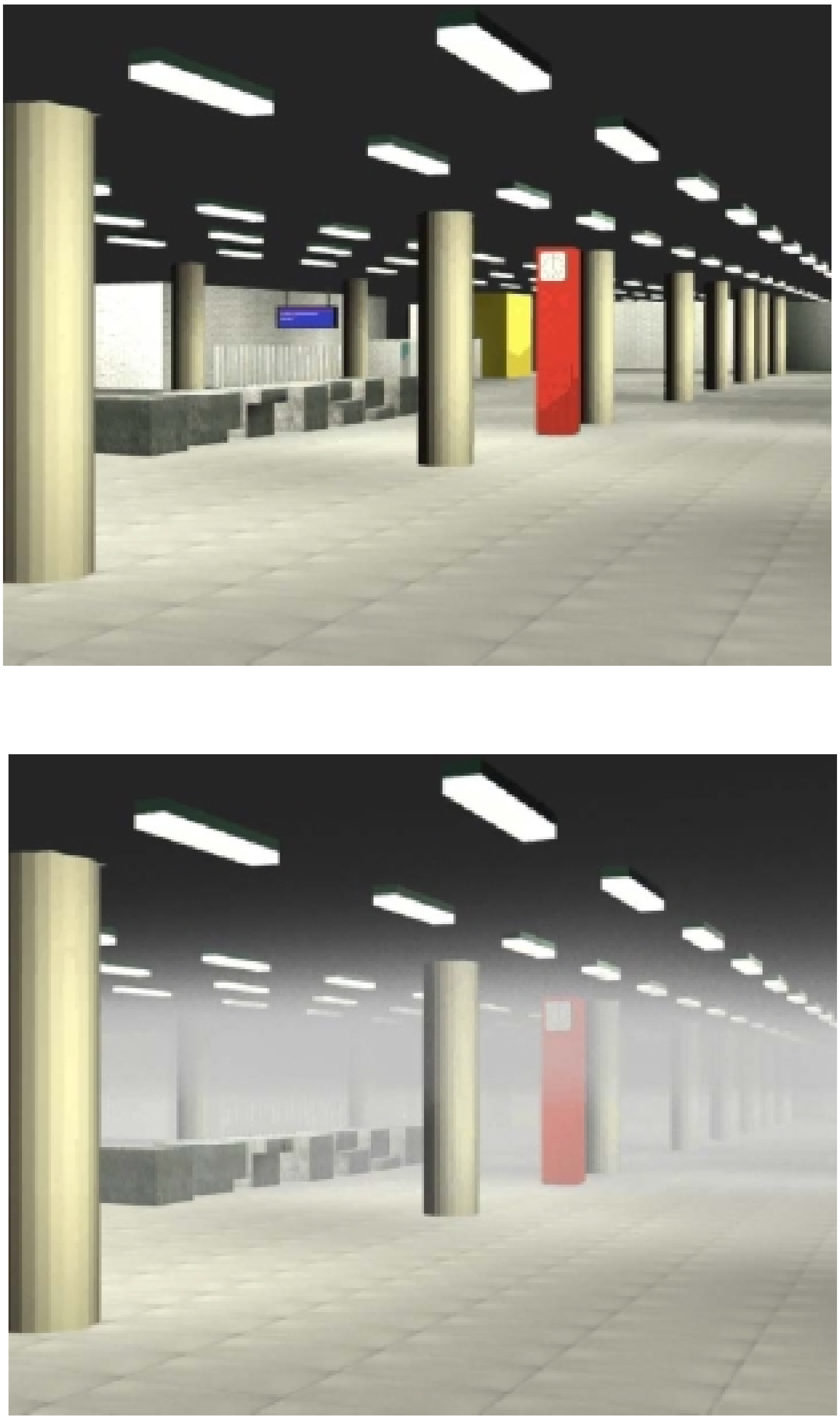

Figure 6 - Illustration of smoke visibility obtained from CFD predictions on an underground station concourse - top: no smoke; bottom: visibility through smoke
(courtesy of Mott MacDonald Limited)

Summary - <u>Smoke transport</u>

- ***The temperature field should not be used as a means to illustrate smoke movement, since unlike smoke mass, temperature is not a conserved variable. Instead a transport equation for smoke mass concentration should be solved.***

- ***Use of a constant smoke conversion factor, to link smoke production with fire heat output, is a commonplace practical approach. However, the CFD solution should be checked to ensure that the fire does not move from over- to under-ventilated, since the conversion factor will then change significantly.***

- ***Any prediction of visibility through smoke should be treated with great caution: presentations of visibility based on iso-surfaces of smoke concentration can be misleading; A more soundly-based approach - using line-of-sight integration is emerging, but is not well validated. It is recommended that predictions of visibility are supported by practical tests or reference data.***

3.9. Numerical sub-models

3.9.1. Temporal discretisation

CFD simulations can be steady or transient. Steady simulations are less time consuming since they aim to calculate directly the steady solution whilst ignoring the transient period that led to the steady state. They can only be applied to steady fires and ventilation systems that do not change with time. They, however, do not provide any information on the time it takes to reach the predicted flow pattern. They are beneficial for predicting the final height of a smoke layer or identifying the regions logged with smoke. They cannot be employed to predict the rate of smoke propagation nor to evaluate evacuation time.

Transient simulations can account for the period of fire growth and any resulting or imposed changes in airflow patterns with time. Such a simulation is particularly useful for investigating effectiveness of emergency ventilation, which will typically only be activated several minutes after ignition. For example, the scenario modelled in the underground station by Gobeau and Zhou (2002). The spread of smoke with time is predicted and thus the results can be used for instance to evaluate the evacuation time.

However, the time step has to be chosen carefully: according to the physics of the flow and to be consistent with the grid - the finer the grid is, the smaller the time step must be. Thus a rapidly-propagating smoke layer modelled on a fine grid would need a far smaller time step than slowly evolving smoke logging on a coarse grid. It is sometimes possible for the CFD practitioner to select an automatic time-stepping algorithm which corrects the values of the time steps as the iterative process progresses to the final solution. The correction is based on the intermediate predictions. However, the user still needs to enter a number of parameters which are based on the physics of the flow to be able to employ such an algorithm.

The best, although most time-consuming, way to ensure that the value chosen for the time steps is appropriate, is to undertake a sensitivity test similar to that for the grid. An appropriate value is found when there is no significant difference in results with a smaller time step. It may also be the case that different time step size can be used at different times, i.e. initially a small step size, increasing if the flow tends towards a steady-state.

3.9.2. Spatial discretisation schemes

A range of numerical schemes is typically offered in commercial CFD codes for the discretisation of the convection terms. The first order schemes are prone to what is called 'numerical diffusion'. The ultimate effect is to increase the mixing thus leading to more uniform distributions of heat and smoke than those obtained with higher order schemes (Gobeau and Zhou, 2002; Ledin et al., 2002). The effect is particularly pronounced on coarse grids.

Ideally second- or higher-order discretisation schemes should be used. Unfortunately in some instances these can be unstable and a solution cannot be obtained. In these circumstances, it may be acceptable to use first order schemes, provided that the grid is not coarse and that the resulting error can be shown to be conservative.

3.9.3. Convergence criteria

The equations are solved iteratively: that is, the solution gradually converges on a single set of values which locally and globally satisfy mass, momentum and energy conservation. A convergence criterion, which determines when the iterative process stops for a steady state simulation, or goes on to the next time step for a transient simulation, must be set in advance by the CFD user. The criterion can be based on 'residual' measures of the imbalance in mass, momentum and energy compared to appropriate reference values. However, the latter are not always easy to define. The change in these 'residuals', from one iteration to the next, could also be used. A small change from one iteration to the next, usually indicates that the solution may be converged. However, this criterion alone is not sufficient, since the error could still be significant (Lea, 1997; Kumar and Cox, 2001). It should be combined with monitoring all the variable values at key locations, i.e. near the fire, and checking they are steady.

The error resulting from an inappropriate convergence criterion can be significant as an error will be introduced at every time-step and is likely to be cumulative. Kumar and Cox (2001) illustrated this point and compared a fully converged solution with a 'badly converged' solution. The velocities in the fire plume were different by a factor of three.

Summary - <u>Numerical sub-models</u>

- ***An appropriate time step, consistent with the physics of the flow and the grid, must be employed. Ideally, a sensitivity test of the results to the time step should be undertaken to demonstrate the time step is adequate.***

- ***Ideally second- or higher-order discretisation schemes should be employed. First-order schemes may be acceptable providing the grid is not coarse and the resulting error can be shown to be conservative.***

- ***The criteria employed to ensure the convergence of the solution should be presented in order to ensure a sufficient number of iterations has been undertaken.***

3.10. Validation and verification

As seen in Section 2, there are a number of uncertainties linked to CFD simulations. Mis-representation of the problem by employing an inappropriate numerical or physical sub-model or by wrongly defining the parameters of a model is one potential source of error, and possibly the easiest one to pinpoint. However, other uncertainties come from ‘bugs’ in the code or physical/numerical sub-models that are too simplistic. The former error can be checked by code ‘verification’, the latter by code ‘validation’.

Thus, the CFD code employed should have been verified -i.e. ensure there is no significant mistakes in the coding of the equations or any problem with the numerical behaviour of the code- and ideally validated for fire applications; i.e. model well-documented fire experiments and assess the accuracy of the CFD predictions against experimental data.

Commercial codes are usually verified by their developers. Since these codes are usually employed by a wide range of people, the likelihood of any mistake being identified and corrected is increased. However, bugs nearly always exist in these complex pieces of software. Verification seeks to minimise these bugs and reduce their impact to relatively unimportant processes. Examples of well-established commercial codes widely employed for fire safety applications are: FLUENT, CFX4, CFX5, PHOENICS, STAR-CD, JASMINE and to a lesser extent SOFIE. These have all, to a greater or lesser extent, been subject to verification or validation for fire safety applications.

If a non-commercial code is employed, the extent to which the code has been verified and validated for fires should be sought. HSL can help Inspectors establish whether such a code has been sufficiently validated for the application that is presented.

Then, for each CFD simulation, the CFD user should check that the results are sensible. Ideally, predictions would be compared with good quality measurements, but these are usually not available and often impractical to obtain. As an alternative, well-established correlations can be employed, especially to check that predicted temperatures and velocities in the vicinity of the fire are credible.

The verification and validation of CFD is an essential part of the process to establish the reliability, capabilities and limitations of the code. Ideally, the outcomes of code verification and validation tests should be readily available.

Even a well-validated code cannot produce a perfect match with reality. There will always be errors. Unfortunately, code verification and validation tests may ultimately not provide the quantification of error which is sought: for example, the scenarios under investigation may be far removed from validation cases. In these circumstances validation may, however, be useful for indicating whether results err on the side of safety.

Summary - <u>Validation and verification</u>

- ***The CFD code employed should have been verified and validated, especially for the transport of smoke movement in complex spaces. This will reduce but not eliminate the uncertainty of CFD.***

- ***Ideally, validation should be presented to indicate whether the results err on the side of safety.***

4. CONCLUSIONS AND RECOMMENDATIONS

4.1. Conclusions

This report highlights the issues that need to be considered when assessing CFD simulations of smoke movement in complex enclosed spaces submitted in safety cases. It does not include all the existing modelling approaches but it encompasses those most commonly employed by the Fire Safety Engineering community.

4.2. Recommendations

If in doubt, contact recognised experts to aid assessment of CFD modelling of smoke movement.

Note that CFD is rapidly evolving. For example, new models, not covered by this guidance note, might appear. In addition, the continued rapid growth in computer power continually extends the range of possibilities.

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APPENDIX A

Summary of the key points for assessing CFD results of smoke transport in complex enclosed spaces

<u>CFD user expertise</u> - Section 3.1

- ***The practitioner must have an in-depth understanding of both CFD and fire and smoke movement dynamics***

<u>CFD code</u> - Section 3.2

- ***The CFD code employed should ideally be validated for application to fire and smoke movement.***

<u>Computational domain</u> - Section 3.3

- ***The domain must be three-dimensional.***

- ***The domain boundaries should be located such that they do not adversely affect simulated smoke movement: for instance, open boundaries should not be located close to the fire source.***

- ***The level of geometric detail represented inside the domain should include anything that might significantly affect the flow, for instance potential obstacles, heat sources other than the fire, etc...***

- ***Ensure that geometric simplifications are justified and unlikely to significantly affect the flow.***

<u>Computational grid</u> - Section 3.4

- ***The design of the computational grid - the disposition of grid cells and their size, should be based on an understanding of the key flow phenomena and preferably experience of a similar case;***

- ***The plan area of the fire source should be divided into several grid cells - typically at least 4x4 cells;***

- ***For unstructured meshes, use of 'inflated grid cells' is recommended next to ceilings;***

- ***For structured meshes, a significant number of cell layers should be employed in the vertical direction - particularly in ceiling layer flows;***

- ***The cells should not be too distorted - particularly near the fire; Kumar and Cox (2001) recommend that the cell aspect ratio does not exceed 50. Ideally it should be of order one close to the fire.***

- ***A test of sensitivity of the results to the grid size should preferably be undertaken.***

<u>Physical sub-models</u> - Section 3.5

- ***The Boussinesq approximation should not be used for modelling the effect of buoyancy, unless it can be demonstrated that the impact of this simplication is negligible.***

- ***If, as is common, a k-ε turbulence model is used, it must include modifications for buoyancy effects in both k and ε equations.***

- ***Simpler, zero- or one-equation, turbulence models should not be used.***

- ***A volumetric heat source or combustion model can be used providing the fire source is well specified - heat output and heat release volume for a volumetric heat source model; heat output and heat release area for a combustion model: see Section 3.6.***

- ***Where the fire plume might be affected by local flow conditions which cannot be adequately determined in advance, a combustion model is preferred to a volumetric heat source model.***

- ***Whichever means is used to model the fire, the resulting plume and flaming region temperatures should be checked to ensure they are representative.***

- ***Radiation should be taken into account, at least by reducing the fire heat output to account for the radiative loss - failure to do that is expected however to lead to conservative predictions in the near-field. The radiative loss has to be soundly based.***
  In the far-field, more sophisticated radiation models than a reduction of the fire heat output may need to be included for large fires in constrained spaces; it is less critical for modest fires or fires in large spaces.

<u>Fire source specification</u> - Section 3.6

- ***CFD cannot predict the intrinsic heat release from a fire and so the user has to specify input parameters characterising the fire; the parameters needed depend on the modelling approach chosen but in any case, they have to be specified so as to lead to realistic temperatures. This can be ensured by comparing the predicted temperatures near the fire source with measurements or well-accepted correlations***.

- ***A constant smoke yield rate (of particulate and aerosol fractions) to model the production of smoke is a crude approach but it is acceptable in most cases, providing its value is based on sound data - for example Table 3-4.11 of the SFPE***

Handbook, 1995.

Boundary conditions - Section 3.7

- *If forced ventilation exists then this is usually prescribed as a boundary condition. It is recommended that the location of these boundaries be remote from the fire source and that the specified values are justified by the CFD user.*

- *The presence of leakage flows to other parts beyond the computational domain, or the outside atmosphere, can have a significant effect on the flow inside the domain - particularly when that flow is governed by convection generated by the fire, rather than forced ventilation. The possibility of leakage flows should therefore be considered.*

- *When flow through a boundary is governed by fire-generated convection, it is commonplace to use a prescribed pressure boundary condition. Pressure boundaries should however be located remote from the fire.*

- *Heat loss to the walls can have important knock-on effects on smoke movement. This is particularly the case when the fire products are in close and immediate proximity with walls. In general it can be considered that a conservative approach as regards rates of lateral smoke propagation is to assume no heat loss at walls, i.e. an adiabatic condition. Note, however, that this approach may then under-estimate smoke concentrations at low levels.*

Smoke transport - Section 3.8

- *The temperature field should not be used as a means to illustrate smoke movement, since unlike smoke mass, temperature is not a conserved variable. Instead a transport equation for smoke mass concentration should be solved.*

- *Use of a constant smoke conversion factor, to link smoke production with fire heat output, is a commonplace practical approach. However, the CFD solution should be checked to ensure that the fire does not move from over- to under-ventilated, since the conversion factor will then change significantly.*

- *Any prediction of visibility through smoke should be treated with great caution: presentations of visibility based on iso-surfaces of smoke concentration can be misleading; A more soundly-based approach - using line-of-sight integration is emerging, but is not well validated. It is recommended that predictions of visibility are supported by practical tests or reference data.*

Numerical sub-models - Section 3.9

- *An appropriate time step, consistent with the physics of the flow and the grid, must be employed. Ideally, a sensitivity test of the results to the time step should be undertaken to demonstrate the time step is adequate.*

- ***Ideally second- or higher-order discretisation schemes should be employed. First-order schemes may be acceptable providing the grid is not coarse and the resulting error can be shown to be conservative.***

- ***The criteria employed to ensure the convergence of the solution should be presented in order to ensure a sufficient number of iterations has been undertaken.***

Validation and verification - Section 3.10

- ***The CFD code employed should have been verified and validated, especially for the transport of smoke movement in complex spaces. This will reduce but not eliminate the uncertainty of CFD.***

- ***Ideally, validation should be presented to indicate whether the results err on the side of safety.***