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HEALTH & SAFETY LABORATORY

Outstanding safety questions concerning the analysis of ventilation and gas dispersion in gas turbine enclosures:

Best Practice Guidelines for CFD

CM/03/12

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ACKNOWLEDGEMENTS

The authors gratefully acknowledge many helpful comments and suggestions made on this guidance by Yehuda Sinai (ANSYS CFX), Richard Underhill (Frazer-Nash), Chris Carey (FLUENT Europe), Peter Stephenson (RWE Innogy), Rob Brooks and Laurent Bonnet (GE), Ian Cowan and Steve Gilham (WS Atkins), Keith Littlebury and Elizabeth Garry (Mobius Dynamics) and Sverre Hansen (Dresser-Rand).

We also gratefully acknowledge the funding provided by the following organisations:
Alstom Power Generation Ltd
ANSYS CFX
Centro Elettrotecnico Sperimentale Italiano
Cullum Detuners
Darchem Flare
Derwent Cogeneration Ltd
Deeside Power
Dresser Rand (UK) Ltd
Flowsolve Ltd
Fluent Europe Ltd
Frazer Nash Consultancy Ltd
GE Power Systems
GHH Borsig
Groveley Detection Ltd
Health and Safety Executive
Hydrocarbon Resources Ltd
Information Search and Analysis Consultants
Killingholme Power Ltd
Mech-Tool Engineering Ltd
Mitsubishi Heavy Industries Europe Ltd
Mobius Dynamics Ltd
Powergen CHP Ltd
Rolls Royce Plc
RWE Innogy
Scottish Power
Siemens AG
Thames Power Services Ltd
Transco National Transmission System
WS Atkins

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EXECUTIVE SUMMARY

This document provides best practice guidance in the application of Computational Fluid Dynamics (CFD) to the design and assessment of ventilation and gas dispersion in gas turbine (GT) enclosures. The focus is from a safety perspective. Gas turbines located in spacious turbine halls are also considered briefly in this document. The technology may be relevant to similar process safety applications where dilution ventilation is the basis of safety against explosion hazards.

The guidance draws attention to the key modelling issues that need to be addressed, and, where appropriate, provides recommended approaches. A checklist is also provided. The guidance is not intended as a guide for non CFD-users but to provide a code of best practice for experienced CFD users.

The guidance has been produced with the assistance of substantial input from a number of CFD consultants and vendors active in this field of application. Their contribution is gratefully acknowledged, and detailed above.

1 INTRODUCTION - AIMS AND SCOPE OF THE GUIDANCE

The aim of this document is to provide best practice guidance in the application of Computational Fluid Dynamics (CFD) to the design and assessment of ventilation and gas dispersion in gas turbine (GT) enclosures. The focus is from a safety perspective. Gas turbines located in spacious turbine halls are also considered briefly in this document.

Best practice guidelines covering the general industrial application of CFD are also available (Casey and Wintergerste[(1)]; NAFEMS[(2)]) and these are recommended to the reader. They contain more specific guidance on physical and numerical sub-models than is addressed here.

The guidance has been produced with the assistance of substantial input from a number of CFD consultants and vendors active in this field of application; their contribution is gratefully acknowledged.

This guidance document starts with an introduction to CFD, mainly aimed at non CFD users. This is then put into the context of the current application in Section 3, where the safety criterion set out in HSE's guidance note PM84[(3)] is introduced. Section 4 describes in some detail best practice in CFD modelling for the assessment of ventilation and gas dispersion in GT enclosures. Further technical CFD modelling details are provided in Sections 5, 6, 7 and 8. Section 9 underlines the importance of the user in carrying out CFD simulations and Section 10 provides guidance on CFD model validation. A list of information that should be recorded to describe a CFD analysis is provided in Section 11 and a useful checklist for carrying out a CFD analysis is provided in Section 12.

2 OVERVIEW OF CFD METHODOLOGY

A brief introduction to CFD, and overview of the main elements of a CFD approach to the modelling of ventilation and gas dispersion, is given below. This is primarily for the benefit of non CFD-users.

CFD is a powerful tool for the analysis of fluid flows. It is a computer-based simulation technique providing an approximate three-dimensional solution to the equations governing fluid motion. The technique is characterised by a division of the region in which flow is to be computed - the computational domain, into a very large number of much smaller domains referred to as mesh, or, grid cells. Complex geometries, and time-dependent flows, are readily handled. The solution consists of values of flow parameters of interest, such as velocity or gas concentration, calculated at each of the grid cells. In essence it provides a complete three-dimensional, time-dependent picture of complex fluid flows.

CFD is used in the design process, with usage ranging from application as a numerical flow visualisation tool giving a crude indication of overall flow behaviour, to quantitatively accurate predictions of key performance parameters. CFD can be used to supplement and refine experimental studies, in some cases reducing the number of experiments required, or, allowing investigation of scenarios which are too costly, dangerous or impractical to undertake other than by computer simulation. CFD can also be used to undertake repetitive parameter and optimisation studies, usually at substantially lower cost than experiment.

Recently there has been very rapid growth in the uptake of CFD, such that SME’s can now afford to invest in the technique. This growth exists because of the need for predictive techniques for fluid flows, the arrival of the relatively cheap yet powerful desktop workstation and the existence of commercial CFD packages with user-friendly pre and post-processing tools. Hence CFD is today being used for a vast range of industrial, environmental and medical applications.

Although CFD is undoubtedly a powerful tool, it is important to understand that engineering CFD applications are based on a number of simplifying assumptions and approximations. It is not possible to assess the effects of all of these assumptions and approximations by scrutiny alone, since the flow equations are highly non-linear and small effects can have large consequences, and vice-versa. Hence validation against measured data remains an important aspect of CFD applications. In addition, the possible need for sensitivity studies of key input parameters or CFD sub-models requires careful consideration. Furthermore, the use of a CFD package still requires considerable user expertise, physical insight and experience if meaningful results are to be generated.

Overall, CFD is an attractive tool for assessing and mitigating the hazard posed by the build-up of flammable clouds in GT enclosures. In outline, a model of the geometry of the contents of an enclosure must first be created. CAD data may be available for this purpose. A mesh of grid cells is then created in the fluid space. Some details, such as small bore pipe-work, may be too small to represent explicitly by the CFD grid. Their effect on the flow must therefore be approximated. Suitable physical models for phenomena such as turbulence, buoyancy, and heat transfer, are then selected. Boundary conditions, at ventilation inlets/outlets, and walls, are also applied. Potential sources of gas leaks are identified and introduced into the model. Numerical solution schemes are selected and the equations solved iteratively until global conservation of quantities such as mass and energy, are adequately resolved. The resulting three-dimensional predictions of the flow and concentration field can then be analysed, for example to determine the volume of a flammable cloud or assess the impact of alternative ventilation strategies.

3 AIMS, BENEFITS AND LIMITATIONS OF A CFD APPROACH

HSE's Guidance note PM84[3] - Control of safety risks at gas turbines used for power generation (2003), describes how dilution ventilation is the preferred basis of safety against explosion hazards in GT enclosures. The ventilation arrangements should be designed such that there are no stagnant or poorly-ventilated spaces, particularly in the vicinity of potential sources of leaks; and that any leak small enough to go undetected by the gas detection system is effectively mixed with air and the resulting mixture transported out of the enclosure without being allowed to build-up. The minimisation of recirculation and re-entrainment are key aspects of effective dilution ventilation.

Gas turbines within spacious halls are unlikely to present an explosion hazard, since foreseeable flammable mixtures are not sufficiently enclosed. In turbine halls the use of dilution ventilation is less applicable and the focus shifts towards gas detection as the basis of safety. However the ventilation of such large halls should still be designed, and checked, to ensure that large accumulations of flammable mixture would not arise from foreseeable leaks, and that such leaks can be detected. CFD has been found to be of value for such applications [4].

In most cases the effectiveness of dilution ventilation in controlling gas leak hazards is best predicted by CFD modelling. CFD also permits a quantitative assessment of ventilation effectiveness against a criterion. This criterion is based on the principle of limiting any foreseeable accumulation of flammable mixture, so that its ignition would not present a hazard to the strength of the enclosure or people. The current criterion[3] states that the size of the flammable cloud - as defined by the iso-surface at 50% of the Lower Explosive Limit (LEL), should be no larger than 0.1% of the net enclosure volume. This criterion has been developed to permit a common basis for assessment of ventilation effectiveness. It has been shown to be both conservative[5] and attainable.

This criterion is presently under review as a result of a substantial Joint Industry Project. However it is very likely that any revised criterion would follow along similar lines. Certainly the present best practice guidelines on CFD will be equally applicable to both the present and any proposed revised criterion.

NOTE: A revised criterion was published following the Joint Industry Research Project.
Full details are available in HSL report CM/04/09.

In summary then, the prime aim of a CFD approach is to ensure and demonstrate the effectiveness of dilution ventilation by assessment against a quantitative criterion.

There are many benefits of a CFD approach. Clearly it provides a means to both design and demonstrate effective dilution ventilation; it provides a means of quantifying gas leak hazards against the HSE criterion; it provides a cost-effective means to optimise ventilation systems - as a remedial measure if necessary, or even before the plant is built; it allows detection strategies to be tested and optimised. These benefits make CFD an attractive approach compared to other approaches based on either simple models or on in-situ measurements alone.

In addition, the CFD model can be used and extended to optimise plant efficiency[6]. Thus if the turbine casing is also modelled, then the interaction between ventilation and casing temperatures can be studied - to ensure that blade tip clearance is controlled. Furthermore, the thermal loads on the supporting structure can be evaluated and the insulation requirements on enclosure walls determined.

However it should be remembered that a CFD model is nevertheless an approximation to reality: There is always uncertainty associated with use of the technique. This arises from simplifications required in representing the wide range of geometric scales of objects in the enclosure, numerical errors - essentially due to discretisation schemes and grid resolution, the applicability of physical sub-models - in particular the turbulence model, and uncertainties in prescribed boundary conditions. However, in principle, much of this uncertainty can be overcome through sensitivity analysis and validation, addressed in Section 10 below.

4 OVERALL APPROACH

An outline is given here of a suitable overall approach for the application of CFD to GT enclosures. Other approaches could also be taken. However, the intention is not to review all such possible approaches. Rather it is to provide a framework to guide CFD modelling; outlining the key steps which should lead to a soundly-based, fit for purpose, engineering analysis. More detail on specific issues is given in subsequent sections.

1. Initially the flow domain must be prescribed. This can, in general, be limited to the boundaries of the enclosure. However there may be benefit in extending the domain to include a section of the outlet duct(s), to demonstrate that gas is well-mixed across the duct at detector locations, so that the detector does not 'miss' a region of high gas concentration. In practice in most cases any stratification in gas concentration is likely to break down rapidly in an outlet duct - due to the relatively high ventilation rates commonly seen in enclosures and what should be the relatively low gas concentrations at that point. In these circumstances it should simply be sufficient to site a detector at a distance of about 10 duct diameters from the entrance to ensure well-mixed conditions, and there will be no need to extend the computational domain into the outlet duct. However, it is just possible that more stable stratification could occur in the duct, for example if a gas leak is relatively close to an enclosure outlet. In that case this possibility can be investigated by extending the flow domain into the outlet duct.

2. An important next stage in a CFD approach is the selection of those objects to be explicitly resolved by the CFD grid and those to be ignored, as well as identifying those smaller objects whose effects on the flow must be taken into account - but for which it is not currently practical to resolve by the grid. These smaller objects will then require representing by modelling at a sub-grid level; typically by a porous media sub-model. Engineering judgement, backed up by the knowledge which comes from experience of modelling this class of flows - and which in particular has been gained through modelling which has been validated against measurements, is vital in making these decisions.

It is difficult, and not even necessarily helpful, to be overly prescriptive in recommending which objects should be resolved by the CFD grid. Clearly the gas turbine must be represented, as should combustion units - since they will be a source of heat which should be accounted for in the model. In addition the turbine supporting structure and any turbine exhaust gas ducting should be represented, as they will present a substantial obstruction to the flow. It may well also be practical to explicitly resolve the largest diameter pipe-work and any larger objects that have a significant effect on the ventilation flow. However, this depends to some extent on the relative size of pipe diameter to enclosure dimensions and the likely effect of the object on the jet development and/or ventilation flow. More detailed explanation and guidelines are given in Section 5.

Of far lesser importance are simplifications which will inevitably need to be made in the shape of complex objects which are resolved by the grid.

3. The number and distribution of grid cells throughout the flow domain also needs careful consideration. It is again unhelpful to be prescriptive as to the number of grid cells to be employed, since a simulation with a large number of poorly-distributed and high aspect ratio cells could well be less sound than one with far fewer cells overall, but whose distribution more carefully reflects the key flow features. Some more detailed guidelines are given in Section 5.

4. The number, and location, of ventilation inlets and outlets should be correctly represented in the model. Flow rates, directions and incoming flow temperature should be based on measurements, or if this is not practicable, the design specification for the ventilation system until such time that measurements can be taken. Note that the flow field through the inlets and outlets is often not uniform.

5. In many cases natural convection - from the hot turbine casing, can be the dominant mechanism driving air movement in the enclosure(6). Realistic modelling of the thermal boundary conditions is thus important. However this does not necessarily mean that a radiation model is required: If the surface heat fluxes or temperatures can be specified - based for example on in-situ measurements, then there will be no need for a radiation model - unless the detail of heat transfer from and within, say, the turbine casing is required. More details are given in Section 6 and 7.

6. Where possible the first aim once a CFD model is constructed should be to provide some validation of the model by ensuring that it predicts broadly representative ventilation flows under normal operating conditions, by comparison to in-situ measurements. Ideally this should be carried out under hot conditions, although this will not always be possible.

7. Once confidence has been gained in the model, the simulated ventilation flow under normal operating conditions should be analysed to identify any obvious deficiencies in the flow distribution. In particular to detect the presence of stagnant regions or flow recirculation - either of which could lead to gas build-up and may need to be remedied. To help in this part of the analysis it can be useful to calculate a local 'age of air' or 'air change rate'.

8. The resulting flowfield under normal operating conditions can then be used to guide the choice of potential gas leaks to be modelled. The aim here should be to demonstrate that the ventilation is effective for credible worst case conditions for gas build-up. Since it is not possible, a priori, to know which combination of factors will lead to the largest flammable cloud, a small number of alternative leak locations and orientations should be simulated. Typical numbers of leaks (combination of location and orientation) to be simulated would be between a minimum of two (for a very simple enclosure with minimal gas supply pipe-work and fittings) to six (typically three locations and two orientations). These leak scenarios should be investigated in turn to avoid interactions, rather than all modelled within a single simulation.

The leak location should be from a credible source, e.g. a flange, valve casing, or other fitting in the gas supply system. The leak orientation should be such as to seek out areas in which gas build-up is most likely, taking into account the effect of impingement on pipes and surfaces. The 'worst case' leak locations and orientations can be obtained from a qualitative assessment of the flow patterns under normal operating conditions. However it may also prove possible to use a quantitative screening method.

The leak rate should be the largest leak which would just pass undetected. This can be calculated as that gas release rate which, when fully mixed in the ventilating air passing through the enclosure, just causes an alarm for a detector located in the ventilation outlet(7). Larger leaks than this should be readily detected and appropriate action can be taken. Smaller leaks could pass undetected, but present a lesser hazard.

Current guidance, PM84(3), proposes that this leak rate should be modelled at alarm conditions. However there is a move towards use of the turbine trip detection setting(8) - which obviously implies the modelling of larger leak rates. This is, in any case, the more conservative approach.

Incorporation of detector error and drift may also be built into the analysis by simulation of additional leak rates.

9. The way in which the gas leak should be introduced into the CFD model is covered in detail in Section 7.3. A number of approaches are possible and generally a pseudo-source approach will be required, in which correlations or a simple jet model are used to provide a larger source – preferably resolved by the grid, a small distance downstream from the leak location. Use of a point source methodology, in which sub-grid scale sources of mass, momentum, energy and possibly turbulence are introduced as sub-grid sources in a single cell, may also be used. However this latter approach is, in general, less reliable than use of a grid-resolved pseudo-source.

10. More detail on specific aspects of the geometrical representation, physical and numerical sub-models, and boundary conditions, are given in Sections 5 to 8.

11. Consideration should be given to the need to demonstrate the effectiveness of ventilation at cold start-up, as well as during normal operating conditions. Thus at turbine start-up, thermally-induced flows which are present during normal operation may be absent and the flow patterns in the enclosure may be very different. The likelihood of gas leaks may also rise at start-up, for example following maintenance operations. However the likelihood of ignition in the event of a leak would be reduced, due to the absence of hot surfaces.

If the flow patterns in the enclosure are very different in cold and hot conditions then it is recommended that gas leak simulations should be carried out in both cases. Alternatively, the need for a CFD-based demonstration of ventilation effectiveness at cold start-up should be advised by a risk assessment.

12. Steady-state simulations will be an adequate basis for demonstration of ventilation effectiveness. However if the turbine is sited in a large hall - with a consequent shift in focus towards demonstration of effectiveness of the gas detection system, then transient simulations are advised. These will allow time to detection to be determined.

13. The resulting CFD simulations can be post-processed to calculate a cloud size to compare to the HSE criterion. The method used to post-process the gas cloud volume can affect the result. Therefore, an appropriate and valid methodology should be used or, at least, one that is conservative.

14. For enclosures with multiple outlets, and dependent on the design of the ventilation and gas detection system as flow exits the enclosure, it is important to investigate whether there are significant non-uniformities in gas concentration present between each outlet

15. There may be a need for sensitivity tests to address areas of uncertainty in the modelling. In particular the sensitivity of the flammable cloud volume to the mesh resolution should be addressed. This can, for example, be achieved by local grid refinement, see Section 10.

16. Gas turbines sited within a large hall represent a special case. The flow in such a hall is potentially influenced by external weather conditions. In principle these could be taken into account by a coupled CFD simulation of the internal and external flows. However, in practice, this is not likely to be practicable. If the internal flow is influenced by weather conditions, then any measurements used for validation of the CFD model of flow inside a turbine hall should ideally be carried out under still atmospheric conditions.

The flow in a turbine hall is more likely to be dominated by natural convection than that in an acoustic enclosure. This places greater emphasis on the need for a correct representation of thermal boundary conditions. As a consequence there is also likely to be an increased need for CFD analysis under cold start-up, as well as normal operating conditions.

To ensure adequate grid resolution, the overall number of grid cells may also need to be significantly higher than needed for a gas turbine sited in an acoustic enclosure. The need for local grid refinement - in the vicinity of the leak, is also likely to be higher.

As mentioned above, transient CFD analysis is also recommended - to allow time to detection to be determined, and detection strategies optimised.

5 GEOMETRY AND GRID

5.1 GEOMETRICAL RESOLUTION

One of the most important issues to address for modelling high pressure gas releases in GT enclosures is the choice of which objects to resolve by the mesh, which to represent using a porosity approach and which to ignore. Clearly large objects within the enclosure will have a significant effect on the ventilation as well as the flow field and subsequent dispersion of a high pressure gas release. All sizes of objects will also have an effect on heat transfer and turbulence generation within the enclosure.

The choice of which objects to resolve by the mesh should be made by an experienced CFD user taking into consideration possible leak locations and the effects of obstacles on ventilation. A rough rule of thumb is that pipework and objects that have a characteristic length scale greater than $1/20^{th}$ of the cube root of the enclosure volume should always be resolved by the grid. A typical characteristic length scale would be a pipe diameter. Objects whose diameter is $1/100^{th}$ of the cube root of the enclosure volume are about the current size limit of obstacles which can be resolved by the grid in practical simulations. These smaller objects may only need to be resolved if they are likely to be impinged on by the gas jet. As an example, for a 1000 m^3 enclosure, objects of the order of 500 mm should always be resolved by the mesh and objects of the order of 100 mm may be resolved by the mesh, depending on their location and likely effect on the ventilation. Objects that are not resolved by the mesh should be modelled using a porosity type approach if they are likely to have a significant effect on the ventilation flow or the propagation of the gas jet. The level of congestion, in addition to the obstacle size, also needs to be taken into consideration, since a larger number of small pipes may have more effect than a small number of large pipes.

If an object is expected to lie within the path of a gas jet then it becomes more important that the object is explicitly resolved by the mesh. Objects that occupy a significant fraction of the jet's cross-sectional area should be resolved by the grid. As a rough rule of thumb if the object is less than 10% of the jet diameter at that distance from the source then there is no need to resolve the object by the mesh(9). But if the jet interacts with an obstacle which is more than 33% of the jet diameter at that point then it should be resolved. The jet diameter is estimated here by calculating the radius at which the (volume) concentration falls to 10% of the centreline value. A similar type of analysis should be carried out for objects lying in the path of an air inlet stream.

5.2 COMPUTATIONAL GRID

The computational grid must be constructed so that it adequately resolves the gas leaks and their dispersion. General guidance on computational grids can be found in the ERCOFTAC CFD Best Practice Guidelines(1). In addition to adequately resolving the geometry of the objects to be modelled, the grid must be sufficiently fine at the source location and in the region where the jet is expected to be. This ensures that high gradients of the flow variables are sufficiently resolved. Unstructured and hybrid meshes are currently popular as they allow local refinement of the mesh in these areas.

For large turbine enclosures and turbine halls more compromises will need to be made with the grid resolution. In these cases the grid distribution will need to be defined carefully so that the gas release is sufficiently well resolved. In general large meshes will be required. The grid resolution at the source location will depend on the method used to represent the gas leak, see Section 7.3 below.

Below a certain size it is not presently practicable to resolve pipe-work, and other obstructions, by the CFD grid. In this case a decision must be taken as to whether to model these obstructions using a sub-grid approach, e.g. as porous media, or whether to simply omit them altogether. If the obstacles are unlikely to present a significant blockage to the flow and are outside of the area in which the gas may build-up, then there is probably little to be gained by applying a porous media model. Indeed recent research work[9] suggests that even where a gas leak interacts with an array of pipe-work, then adopting porous media modelling may lead to little improvement in model realism. However, consideration should also be given to the heat transfer from pipe-work that has not been explicitly represented by the CFD mesh as this can have a significant effect on the overall heat balance and air movement within the enclosure. Again, a sub-grid approach can be adopted to model these effects.

The overall number of computational cells used in CFD simulations of GT enclosures continues to rise. A minimum of ¼ million cells would be expected to be used in a modern computation and grids using ½ to 3 million cells are fairly typical. Clearly larger meshes will be required for larger enclosures to obtain the same resolution. However, it is also important to ensure that an appropriate distribution of cells is used. The ‘quality’ of the mesh can also have a significant effect on the accuracy of the resulting solution. This means that the computational cells should not be overly skewed or, for a structured mesh, have excessively large aspect ratios etc.. More details on mesh quality can be found in the ERCOFTAC Best Practice Guidelines[1].

Hardware and software developments in the future will lead to the ability to use much larger computational meshes. Further use of techniques such as adaptive mesh refinement would also be expected to be used.

6 PHYSICAL SUB-MODELS

6.1 TURBULENCE

The flows in a GT enclosure are invariably turbulent. The Navier-Stokes equations, which govern the fluid flow, cannot be solved directly (i.e. using Direct Numerical Simulation (DNS)), for flows of industrial interest. This is due to the fact that all relevant length and time scales need to be resolved, leading to intractable, long calculations. It is therefore necessary to assume that the flow varies around a mean value. Averaging the Navier-Stokes equations, via Reynolds averaging, produces a set of equations describing this averaged flow. A degree of freedom is lost in the averaging process, leading to fewer equations than there are unknowns – the so-called closure problem. The closure problem is overcome by using a turbulence model.

A number of turbulence models of varying degree of complexity are available. Zero-equation models, such as the mixing length model and one-equation models, i.e. the Baldwin-Lomax model, are not suitable for flows in GT enclosures. The k-ε model is recommended as a minimum standard for modelling flows in GT enclosures and more advanced turbulence models can be used if they are known to be appropriate; more details are given below.

The industry standard turbulence model is the k-ε model, a two-equation model, which involves solving a transport equation for turbulent kinetic energy (k) and a transport equation for the dissipation rate of the turbulent kinetic energy (ε). A large number of variants of the standard k-ε model exist, e.g. the low Reynolds number Launder-Sharma(10). It is by far the most commonly used turbulence model for the types of flows considered here. The model assumes that the turbulence is isotropic, which is not true for impinging flows, flows with curvature or swirl, etc. A disadvantage of the model is that it does not reliably predict the correct heat transfer to walls, although this is in part also due to inadequate wall heat transfer boundary conditions.

Wilcox(11) proposed a k-ω model, which offers a better representation of the flow near a wall. The variable ω is the turbulence frequency, which is defined as $\omega = k/\varepsilon$. However, the far-field boundary condition on ω tends to infinity, which is unphysical and causes numerical problems with the flow solver. Menter(12) proposed a model called the Shear Stress Transport (SST) model which is in effect a blend of the k-ω model in the near wall region and k-ε model in the bulk flow/far-field. A blending function is used to ensure a smooth transition between the two regions. The definition of turbulent eddy viscosity is also modified, accounting for transport of turbulent stresses. Compared to the k-ε model the SST model yields better heat transfer predictions and improved predictions of flows with adverse pressure gradients, flow separation and reattachment.

Second moment closure models, also known as Reynolds stress transport models, offer much more realistic representation of the flow physics. However, the second moment closure model introduces another five transport equations, which increases both the information required for the boundary conditions and the computational overhead. Grid resolution and quality are also major issues for Reynolds stress models – simpler turbulence models would appear to be more “forgiving” to meshes with skewed cells, whereas a Reynolds stress model may lead to diverged solutions. Simulations using a Reynolds stress model are frequently numerically unstable, which precludes convergence. Reynolds stress models are therefore rarely used for GT ventilation flows. Modelling of scalar transport has not been subject to the same level of research as the Reynolds stresses. It is often assumed that the scalar transport is analogous to that of the stresses, although this is strictly not the case.

A further, more advanced alternative known as Large Eddy Simulation (LES) is beginning to be applied to ventilation flows, LES models require sufficiently fine grid resolution to resolve the important flow structures. Many of the LES calculations published in the literature have been carried out on meshes that are too coarse for the results to be useful. The treatment of boundary conditions, particularly walls, are a weakness of the LES methodology at present and this issue has not been fully resolved. It is also necessary to ensure that the initial flow field is well-chosen. LES calculations are inherently transient; ten eddy turn-over times is an absolute minimum duration to build up reliable flow statistics - there is a tendency to run simulations for too short a time. LES is not, at present, a viable tool for calculations of flows in GT enclosures.

Despite their limitations the two equation approaches, k-ε in particular but also possibly SST are the current 'standard' for this application.

A value of 0.7 is recommended for the Turbulent Schmidt number in the scalar transport equation for the gas concentration. This recommendation is based on experimental measurements[13] and a comparison between CFD predictions and experiment[9].

6.2 COMPRESSIBILITY

For high pressure gas leaks in enclosures the high Mach number region is confined to a relatively small region in the immediate vicinity of the source. Therefore, the flow is often assumed to be incompressible throughout the enclosure. Strictly this assumption is only valid where the Mach number is everywhere less than 0.3 and this will only be the case where the gas leak has been modelled as subsonic. In general it is recommended that compressible flow calculations be carried out and most modern commercial CFD codes can model the flow as such without any loss of efficiency. Furthermore a compressible flow calculation may be required by the specific CFD code if buoyancy and heat transfer are to be included.

6.3 BUOYANCY

The effects of buoyancy should always be incorporated in a CFD model for GT enclosures, since thermally-induced natural convection flows can be significant. Whilst the main fuel - natural gas, is inherently buoyant, a high pressure release will typically induce rapid mixing such that the resulting gas cloud may be at relatively low concentration. In these circumstances the gas cloud could then be more affected by the background ventilation - including any thermally-induced and thus buoyant flows, or flows induced by the release momentum.

The difference in flow behaviour between a calculation where buoyancy is ignored in the mean momentum equations and where buoyancy is taken into account can be significant[14]. It is also important to take into account the effects of buoyancy in the turbulence model; the standard k-ε model does not do this. Modifications to the k-ε model have been proposed and tested[15,16] which involve an additional source term in the turbulent kinetic energy and energy dissipation equations. An additional constant, C_3, is also introduced. Other buoyancy modified k-ε turbulence models also exist and may be equally suitable

Reynolds stress transport models can represent buoyancy effects in a more realistic fashion than k-ε models. However, these models still require a modelled energy dissipation equation which will still need to include the same buoyancy source term as for the k-ε model.

6.4 HEAT TRANSFER

It is important that an overall heat balance for the turbine-enclosure system is satisfied to ensure that natural convection, which often dominates the flow field, is correctly modelled[6].

Ideally in-situ temperature measurements should be obtained to give an indication of the likely temperatures in the enclosure during normal operation. These measurements can be used in setting up an overall heat balance for the enclosure, see below. In-situ measurement techniques are described in detail in a Best Practice Guidance on in-situ measurements[(17)].

It is possible to prescribe wall temperatures, obtained from in-situ measurements. The term wall here implies either an external wall, the casing of the gas turbine or any other equipment in the acoustic enclosure. However, problems of satisfying overall heat balance might arise with this approach, since it depends on the adequacy of heat transfer models for the near wall flow. It also requires fine grid resolution in the near-wall region to ensure that these wall layer models are used within their bounds of applicability and the heat flow into the enclosure is correct. The required grid resolution may be such that it is not feasible to carry out CFD calculations in a real scale enclosure. A better alternative would be to apply an overall heat flux that would yield good overall heat balance, but may yield incorrect wall temperatures.

Rough hand calculations are also advised, based on a calculation of a Rayleigh number[(6)], to indicate the extent to which the flow is dominated by natural convection, and thus the attention that may or may not need to be placed on thermal effects. Standard wall heat transfer functions are usually based on forced convection and are therefore not applicable to flows that are dominated by natural or mixed convection. This is often the case in large enclosures where the heat transfer is considerably lower than in the forced convection case. It is advisable to modify the wall heat transfer functions to take into account natural convection in these regions.

The use of a radiation model should be considered if predictive information is required for local surface temperatures. It may also be desirable to carry out coupled heat transfer calculations through the turbine casing for performance purposes. Ordinarily, however, it is not necessary to use a radiation model.

6.5 PHYSICAL PROPERTIES

The composition of natural gas varies from source to source, and will also vary over time – Table 1 shows a typical gas composition for a North Sea field, while Table 2 shows the physical properties of methane.

Table 1 Typical composition of North Sea natural gas[(18)]

Component	***Chemical Formula***	***Mole fraction***	***Mass fraction***
Methane	CH_4	82.0	65.6
Ethane	C_2H_6	9.4	14.1
Propane	C_3H_8	4.7	10.3
Butane	C_4H_{10}	1.6	4.6
Pentane+	C_5H_{12}+	0.7	2.5
Carbon Dioxide	CO_2	0.7	1.5
Hydrogen Sulphide	H_2S	0.0	0.0
Nitrogen	N_2	0.9	1.3

Table 2 Physical properties of methane at 0 °C and 1 bar[19]

Physical property	***Symbol***	***Value***	***Unit***
Molecular weight	Mw	16.043	kg $kmol^{-1}$
Density	ρ	0.71	kg m^{-3}
Kinematic viscosity	ν	$1.44 \cdot 10^{-5}$	$m^2 s^{-1}$
Dynamic viscosity	μ	$1.02 \cdot 10^{-5}$	N s m^{-2}
Specific heat capacity (constant Pressure)	C_p	2.18	kJ $kg^{-1} K^{-1}$
Specific heat capacity (constant Volume)	C_v	1.66	kJ $kg^{-1} K^{-1}$
Ratio of specific heats (C_p / C_v)	γ	1.31	–
Thermal conductivity	k	$2.5 \cdot 10^{-2}$	W $m^{-1} K^{-1}$

If the gas consists to a large extent of methane then it is acceptable to assume that the gas mixture is made up of methane alone. However, if there is a significant amount of heavier hydrocarbons, C2's and beyond, or other, possibly inert, components, it may be necessary to treat the gas as a mixture with its associated properties. The LEL for a gas mixture can be calculated from

,

where n is the number of species in the gas mixture, x_i is the mole or volume fraction, and $x_{LEL,i}$ is the LEL of species "i", respectively. The CFD predictions of gas cloud volume are sensitive to the value used for the LEL and so it is important that the value is calculated as accurately as possible, see Ivings et al[8] for more details on choice of LEL.

6.6 POROSITY

Gas turbine enclosures typically contain large amounts of pipe-work and other obstructions. It is not practical to represent all of these objects explicitly by the computational mesh. Therefore, practical approaches are required to model the effects of these objects using a sub-grid scale approach or porosity model.

In GT enclosures these congested regions will be, from a modelling point of view, of relatively high porosity. That is, the congested volumes will be mainly free-space. In such cases an appropriate method for accounting for the congested region within the CFD model is to introduce source terms into the momentum equations describing the resistance to flow in this region. These source terms will actually be momentum sinks. It is also possible to derive source terms for the turbulence equations describing the generation of turbulence in this region but this is less important and subject to greater uncertainty. Finally, consideration should also be given to the possible heat rejection through the porous region.

There are a number of ways of deriving the momentum sources. For example the differing approaches described by Ivings *et al.*[9] and Gilham *et al.*[6] derive the momentum source terms in terms of a pressure drop and the drag on the fluid respectively. In either case the source terms depend on the local flow velocity. It is important to note that this flow velocity, which the CFD model is computing, is the superficial velocity which is the velocity based on the volumetric flow rate through the total area. The interstitial velocity is the true (higher) velocity that exists between the obstructions.

If the momentum source term is derived in terms of a pressure drop, then a pressure loss coefficient is required. This coefficient can be calculated from a number of standard correlations either for packed beds[20] or tube bundles[21]. For more complex obstacles and / or to provide a sounder basis for the porosity model, separate CFD calculations can be carried out. These calculations involve simulating the flow past the obstacles to determine the pressure drop across them and hence a value for the pressure loss coefficient. Ivings et al.[9] provides further technical detail.

6.7 TIME-DEPENDENCY

It is generally sufficient to carry out steady-state calculations to assess gas cloud sizes.

Transient or time-dependent calculations can be used to calculate time to detection and optimise detection strategies and are a particularly useful strategy for large enclosures / turbine halls. Transient calculations could also show how the gas cloud size varies with time, especially how the ventilation flow dilutes the released gas after the leak has been detected and the gas supply to the gas turbine has been shut down. The need for any of these additional calculations should be determined by risk assessment.

7 BOUNDARY CONDITIONS

7.1 VENTILATION INLETS AND OUTLETS

The number and location of ventilation inlets and outlets should be correctly represented, as should the flow rates and direction. Where practicable, in-situ measurements should be used to determine the flow rates, inlet temperatures and also any non-uniformities in the flow through the inlets.

The ventilation inlets and outlets will usually be modelled by specifying a flow rate either into or out of the enclosure using an inlet or outlet boundary condition respectively. A pressure boundary condition will then be applied at the other boundary. This approach can therefore take into account the effect of leaks on the ventilation flow.

Care should be taken with setting up the ventilation boundary conditions if the enclosure is ‘leaky’. A leak test should be carried out on the enclosure on commissioning. This may be combined with the "door fan test" associated with the commissioning of CO_2 fire suppression systems.

7.2 WALLS

When setting wall boundary conditions the effects on both momentum and temperature should be taken into consideration. A wall function approach is most practical. Key issues include the mesh resolution next to the wall and the selection of appropriate wall functions dependent on the turbulence model used. Surface roughness and heat transfer also need to be considered, including the possibility of radiative heat transfer.

The permissible y^+ value (the wall-normal distance, normalized by the shear stress, of the first node from the wall) for the standard k-ε model is dependent on the type of wall function used. The equilibrium wall function puts a lower and an upper limit on the acceptable y^+ value. The range is implementation specific, but is likely to be in the range 20 to 200 – the user manual for the code being used should be consulted for appropriate values. The y^+ values should therefore be checked to be in this range – at least for key regions within the flow, i.e. as affecting the gas cloud build-up. The equilibrium wall function is not valid in the viscous sub-layer and it is not advisable to place the first node too close to the wall. Special care is also needed when carrying out a mesh resolution analysis to ensure that the y^+ value is in the acceptable range.

A type of wall function that is not sensitive to the location of the first node is now available. These so-called scalable wall functions can be used with fine meshes and hence low values for y^+. The SST model offers better representation of rough and smooth wall flows, flow separation and reattachment. Calculations of wall-bounded flows with the SST model are in better agreement with experiments than those with the standard k-ε model, especially with respect to heat transfer to the wall. The y^+ limitation when using the SST model, however, is code specific.

If a low-Reynolds number k-ε model, e.g. Launder-Sharma[10], is employed it is necessary to resolve the boundary layer in the near-wall region. This means that the y^+ value, should be of the order 1, and certainly no greater than 4, see Casey and Wintergerste[1]. This approach is therefore not generally practical for routine use due to the large mesh that is required.

Wall surface roughness can play an important role in the fluid flow and the heat transfer. It is difficult to quantify how much influence surface roughness will have, as it is very problem specific, suffice it to say that it would be advisable to consider taking surface roughness into account.

7.3 GAS LEAK

In practice it is not currently feasible to resolve the leak directly at its source in the context of flow in a far larger enclosure. This is partly due to its small size, but also due to the complex under-expanded shock structure which will be present immediately downstream from leaks at typical gas system operating pressures. Hence a pseudo-source approach will typically be required. In this approach, instead of the modelling the actual leak source, the leak is modelled from a point or plane downstream of the leak position. This pseudo source is defined such that the flow behaviour further downstream closely resembles that resulting from the actual leak source.

This pseudo-source will be modelled using one of two means. Either the leak (i.e. pseudo source) is resolved explicitly by the CFD grid, or, the effects of the leak are introduced as sub-grid scale sources of mass, momentum, energy, and turbulence. In either case, the jet can be modelled from the either the ‘sonic point’ or some point further downstream where the flow is subsonic. If the jet is modelled from a subsonic plane then an empirical correlation is required to define the flow parameters for the jet at that point. To model the jet from the sonic point some simple assumptions can be made that allow the jet to be represented by a sonic jet at atmospheric pressure with the same mass flow rate as the original high pressure jet(22).

Recent research(9) has compared a number of the above approaches and has shown that a resolved sonic approach appears to give the best results. Details of gas leak source modelling can be found in Ivings *et al.*(9).

For a resolved pseudo-source, the inlet boundary should be resolved by at least 10 cell faces and probably a lot more if the jet is modelled as subsonic rather than sonic. For a point source the cell size should be approximately the same as the jet width. In either case a fine mesh will be required along some initial length of the jet where high flow-variable gradients exist.

The above is valid for leaks from round holes. Leaks from flanges and slots with a large aspect ratio behave differently. However, there is little research in this area to indicate the best approach for modelling such leaks. The most common approach is to approximate these leaks by a round hole with the same area.

8 NUMERICS

8.1 DISCRETISATION

The discretisation scheme used to model the convection terms in the Navier-Stokes equations plays an important role in determining the accuracy of the overall numerical solution. The discretisation error is equal to the difference between the scheme and the exact solution represented as a Taylor series expansion. For a first order differencing scheme the error is dominated by the quadratic term in the expansion and this is known as numerical diffusion. These errors lead to overly diffuse solutions and their use should therefore be avoided.

In all but a few cases first order schemes will lead to less accurate solutions than higher order discretisation schemes. It is therefore recommended that higher order discretisation schemes are used to solve all the transport equations in a CFD simulation. One of the disadvantages of using higher order discretisation schemes is that it will lead to oscillations in the flow properties near to steep gradients. Therefore more sophisticated discretisation methods, such as total variation diminishing (TVD) schemes, are required to ensure that the solution remains bounded and oscillation free. Most general purpose CFD packages will incorporate such a scheme.

8.2 CONVERGENCE

The iterative procedure used in CFD simulations to obtain a solution requires a measure to determine when a satisfactory solution has been reached. This is known as a convergence criterion. Convergence is generally determined by monitoring the residuals for each equation solved. Different codes use different definitions for the residuals and so it is not instructive to give a definition of convergence here in terms of the residuals. However, as the gas concentration of interest is approximately 2 orders of magnitude smaller than the value at the jet source, it is worth paying particular attention to the convergence of the gas concentration conservation equation.

In addition to monitoring the residuals to determine convergence, the global balances of conserved quantities (e.g. mass, momentum, energy) should also be checked.

Monitor points can also be usefully used to see whether flow variables are still changing as the solution progresses. However, the monitor point location needs to be chosen carefully to ensure that it provides useful information. A further useful guide for monitoring convergence is to record the gas cloud volume at each iteration.

9 USER

CFD is a knowledge-based activity; the user therefore plays a key role in most CFD analysis. This certainly holds true for the present application. Thus the adequacy of a CFD analysis of flow and gas dispersion in a GT enclosure will, in large part, depend on the expertise and competency of the user.

So although these guidelines outline the key modelling issues which need to be addressed, they do not seek to teach an inexperienced user how to undertake CFD. CFD analyses of high pressure gas releases in GT enclosures must be carried out by suitably qualified CFD experts, even when following these guidelines.

In summary, the skills which a CFD user needs for this application area are: an in-depth understanding of fluid flow phenomena encountered in GT enclosures; knowledge of the capabilities and limitations of physical and numerical CFD sub-models relevant to the simulation of flow in GT enclosures; expertise in the application of CFD software. Ideally, more general experience in the simulation of internal ventilation flows and gas dispersion in enclosed spaces should have been obtained before CFD is applied to the simulation of ventilation and gas leak hazards in GT enclosures.

10 VALIDATION AND SENSITIVITY ANALYSES

The CFD model should be demonstrated as being representative of actual conditions by comparison of simulated velocity and temperature fields with in-situ measurements. This is an important step in carrying out a CFD analysis and therefore should always be done.

Ideally validation of the CFD model should be carried out under hot *and* cold conditions. However, in practice it is not always possible to make in-situ measurements under hot conditions. The validation study should ensure that the CFD model is able to correctly predict the general background ventilation flow within the enclosure. This means that the main flow paths through the enclosure and areas of recirculation should be correctly identified. If in-situ velocity measurements cannot be made under hot conditions, then the 'cold' velocity measurements should be used in conjunction with temperature measurements made within the hot enclosure for model validation.

In addition to validation of the CFD simulations of the enclosure ventilation, consideration should also be given to the validation of the individual sub-models that have been used. This particularly applies where a departure has been made from sub-models that have been recommended in this guide or new or less well known sub-models have been used. In these cases reference should be made to validation work. For example, the capabilities of the k-ε turbulence model are well known for modelling round jets and therefore specific validation of this model is not required. However, if a new approach is being used for modelling the jet source then validation of the approach is required.

An additional approach for checking the CFD solution is by carrying out sensitivity analyses for areas of significant modelling uncertainty. This type of analysis will demonstrate the effect of uncertainty in the assumptions that have been made in creating the CFD model on the results of simulations. In practice only a small number of such sensitivity analyses can be carried out. These may include sensitivity studies on the mesh resolution, boundary conditions and modelling assumptions made in setting up the porosity model.

11 DOCUMENTATION

Below is a list of information that should be included when reporting the results of CFD simulations of high pressure gas leaks in GT enclosures. This information will be required by the regulator when trying to assess the adequacy of the analysis. Note the similarity of the structure of the list compared to the checklist in Section 12.

Data and records to be kept following a CFD study should be decided in consultation with in-house QA procedures.

The following items should be documented:

- Geometry and grid:
  - List of objects, including sizes, that have been resolved by the computational mesh
  - List of objects, including sizes, that have been represented using a sub-grid approach
  - Number of computational cells (control volumes) used in each simulation
  - Dimensions of enclosure and net enclosure volume
- Gas Leak:
  - Gas leak rate (including gas detector settings and volumetric flow through enclosure)
  - Method used to model leak including assumptions made
  - Justification of choice of leak positions and orientations
  - Method use to calculate gas cloud volumes
- Physical sub models:
  - Time dependency of solution, i.e. steady-state or transient
  - Turbulence model
  - Compressibility assumptions made
  - Buoyancy model
  - Heat transfer model
  - Physical properties of the released gas; including value for LEL
  - Porosity model used; description of how the pressure loss coefficients were calculated
- Boundary conditions:
  - What boundary conditions have been used
  - Flow properties at each boundary condition
  - Heat transfer or temperature boundary conditions
  - Uniformity of gas concentration at gas detector site or outlet boundary
- Numerics:
  - Convection discretisation scheme
  - Description of convergence criteria and extent to which they have been met
- Results:
  - Description of background ventilation flow
  - Validation of CFD model
  - Volumes of gas clouds

12 CHECKLIST

The checklist below summarises the key points for consideration when undertaking a CFD analysis in this area of application. The list has been divided into topics and is therefore not a step-by-step guide for carrying out the CFD analysis.

CFD User	
	Has the CFD user the necessary expertise to undertake this work?
Geometry and grid	
	Has a structured or unstructured gridding approach to be used?
	Has consideration been given to where the leak positions are in creating the mesh?
	Which objects are to be resolved by the computational mesh, taking into account possible jet impingement?
	Which objects are to be represented using a sub-grid approach?
	Where are the inlet and outlet boundary conditions specified; where the duct meets the enclosure or further down the duct?
	Does the mesh have sufficient resolution to adequately resolve the main geometrical features of the enclosure and capture the background ventilation flow?
	Does the mesh have sufficient resolution to resolve the jet and gas cloud build-up?
	Has a good ‘quality’ mesh been generated?
Gas Leak	
	The leak rate should be the largest leak that would just pass undetected.
	Has a small number of leak positions and orientations been chosen representing credible worst case scenarios? These should be based on an analysis of the CFD model of the background ventilation flow identifying possible stagnant or recirculating regions.
	Has an appropriate methodology been used for modelling the source of the gas leak?
	Has the overall jet structure been correctly modelled in the CFD simulation, e.g. by comparison against an empirical model?
	Has a gas leak been modelled under cold conditions, representing a leak during cold start-up?
Physical sub-models	
	Is the simulation steady-state or time-dependent? For large enclosures / turbine halls a time dependent simulation may be more appropriate.
	Which turbulence model has been used? Have appropriate model constants been used?
	Has the flow been modelled as compressible? The flow can be modelled as incompressible if the Mach number is everywhere less than 0.3.
	Have the effects of buoyancy been included in the momentum equations? Have buoyancy effects been included in the turbulence model?
	How has heat transfer been accounted for? Has consideration been given to whether radiative heat transfer is important?
	What are the physical properties of the released gas; is an appropriate value of LEL being use? For methane assume that LEL = 4.4% v/v.
	What porosity modelled has been used? Have the (pressure loss) parameters been calculated using appropriate correlations?

Boundary conditions	
	Have the inlet and outlet boundary conditions been set up with reference to in-situ measurements?
	Have any non-uniformities in the inlet flow been represented in the CFD model?
	Has wall heat transfer been modelled? Is the overall heat balance correct?
	Have the results of the CFD simulation been analysed to check the uniformity of the gas concentration where the gas detectors are sited?
	Is an appropriate value of y^+ obtained at the wall boundaries?
Numerical model	
	Has a bounded higher order discretisation scheme been used for all the transport equations?
	Has the solution converged sufficiently and has the global imbalance for conserved quantities reached the specified criteria?
Validation	
	Has the model of the background ventilation flow been validated against in-situ measurements? Ideally this should be carried out under hot conditions.
Post-processing	
	Has the gas cloud volume been calculated using a reliable and/or conservative approach?

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