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GUIDANCE FOR NSD ON THE ASSESSMENT OF CFD SIMULATIONS IN SAFETY CASES

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SUMMARY

This report provides guidance for NSD inspectors to aid in the assessment of Computational Fluid Dynamics (CFD) simulations in safety cases.

It assumes familiarity with fluid flow processes, but not CFD.

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1. INTRODUCTION

Computational Fluid Dynamics (CFD) is a powerful, rapidly evolving, simulation tool used for the prediction and analysis of fluid flows. The reliance which can be placed on results of CFD simulations depends on a number of issues, such as the modelling of physical processes, numerical sub-models employed, user expertise, etc. Satisfactory assessment of CFD simulations in safety cases requires that these issues are addressed.

The main objective of this report is therefore to provide guidance to assessors of safety cases on the main issues which should be covered in CFD submissions, and their significance.

2. OVERVIEW OF CFD MODELLING

2.1 Background

CFD is the use of computer-based simulation to obtain an approximate solution to the equations which govern fluid motion for particular applications. 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. The solution consists of values of flow parameters of interest, such as velocity or temperature, calculated at each of the grid cells.

The technique originated in the aerospace sciences field in the 1960’s with the arrival of the digital computer. Development and application in the next decade tended to be confined principally to academia and the aerospace industry, but with the nuclear industry also taking an interest. During this time the use of CFD methods was restricted to those with access to the most powerful computers.

During the 1980’s, CFD began to be used by a wider range of industries and applied to an increasingly diverse range of problems. This was a direct result of increased accessibility to more affordable computers coupled to a growing appreciation of the commercial benefits of computer modelling. Thus by the end of the decade CFD was being used to compute, for example, flow around automobiles (Shaw 1988) and inside internal combustion engines (Le Coz, 1990), natural ventilation inside open atrium office buildings (Alamdari et al, 1991), the performance of gas-fired furnaces (Bai et al, 1992), fires (Fennell, 1988) and explosions (Bakke and Storvik, 1988).

More recently there has been very rapid growth in the uptake of CFD modelling, such that even small to medium enterprises can 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.

CFD is presently used for a vast range of industrial and environmental applications: It plays a major role in the aerospace, power generation and automobile industry; it is used for short and long range weather forecasting - including the simulation of global warming; to compute dispersion of pollutants in rivers, the atmosphere and ocean; in biomedical engineering for arterial and venous flows; in sports science; building ventilation; in the chemical process industry; as well as hazard analysis across a range of industry sectors - including the nuclear industry.

CFD has thus become a useful tool for use alongside more traditional techniques for investigation of fluid flows, such as experimental or analytical methods. It 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 - such as required by the aerospace industry. 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 less cost than experiment.

The difficulty in undertaking experimental work in the field of nuclear engineering means that CFD is an obvious tool. Areas of application for CFD are thus diverse and include simulation of reactor thermal hydraulics under normal operating conditions (Burns et al, 1989; Collins and Henry, 1990) and fault conditions such as loss of cooling (Markatos et al, 1983); prediction of thermal hydraulics of steam generators (Singhal et al, 1980); natural convection around rod bundles (Robinson and Lonsdale, 1989; Splawski, 1990), fires (Cox, 1983; Kadoya et al, 1994); flows in fuel storage ponds (Lea and Kelsey, 1997), amongst others.

The widespread availability of powerful workstations, efficient solution methods and sophisticated graphical pre- and post-processors which are now packaged with commercial CFD software, has led to a rapidly growing user base for CFD simulation and analysis. Although these codes offer impressive features and the capability to model flows in and around highly complex geometry, the physical and numerical sub-models embodied or applied by the user, are, in many cases, often little removed from the relatively crude techniques developed in the early 1970's(Leschziner, 1989). In addition, the codes still require considerable user expertise, physical insight and experience if meaningful results are to be generated.

2.2 CFD Methodology

The governing equations of fluid flow cannot be solved analytically except in special, highly simplified cases. It is the task of CFD to generate approximate solutions to these equations by numerical means.

Firstly a mathematical model is constructed. The exact fluid flow equations, known as the Navier Stokes equations (Panton, 1984), are used as the starting point. These describe the conservation of mass, momentum and energy. For engineering flows of practical interest it is not possible to solve these exact equations directly, so simplified forms are employed, outlined in Section 3.3. It is important to note, therefore, that in engineering CFD simulations the exact flow equations are not solved. Submissions should therefore address the consequences of these simplifying assumptions on the end results.

Boundary conditions are needed for the specific application. These can be of several types, outlined in Section 3.4. In some instances the boundary conditions will not be well-defined or may even be unknown. It should therefore be expected that a submission will state all boundary conditions and include an assessment of the effects of any uncertainties.

To obtain a solution to the simplified flow equations, a discretisation method is used. This is a means of approximating the differential flow equations by a system of algebraic equations which can be solved on a computer. The approximations are applied to small domains in space; the grid or mesh cells referred to earlier. A solution algorithm is used to solve the system of algebraic equations, giving results at discrete locations in space, i.e. at each grid cell, and in time.

The accuracy of the overall numerical solution method depends on a number of factors; the sub-division of the region of interest into grid cells; the accuracy of the discretisation method; the effectiveness of the solution algorithm in solving the algebraic equations. Safety case submissions which include CFD modelling should therefore include an assessment of each of these factors. These topics are covered in more detail in Section 3.5.

Engineering CFD applications thus incorporate 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. It can therefore be expected that submissions should be supported by validation studies, which can be applications of the CFD code to well-documented flow situations which include elements of the main geometrical and physical flow features seen in the case of interest. In addition, sensitivity analyses can be employed, whereby the effects of uncertainties in, for example, boundary conditions, are studied by carrying out further simulations which investigate the consequences of realistic perturbations to values of key controlling parameters.

2.3 Resource requirements

CFD software is available from a variety of sources. The main software packages likely to be encountered by NSD inspectors are general-purpose codes developed and available from commercial vendors or those developed and used in-house by the industry.

In the former category are the four main commercial CFD codes:

FLUENT: Marketed and developed by FLUENT Europe.

PHOENICS: Marketed and developed by CHAM - Concentration Heat And Momentum.

CFX (Formerly FLOW3D): Marketed by AEA Technology.

STAR-CD: Marketed by Computational Dynamics.

In the latter category is the Nuclear Electric code ’FEAT’.

The cost of a perpetual commercial CFD code licence spans a wide range, but may typically be £40K for software which has include all available options and advanced pre- and post-processing tools. Source code is usually only available at substantial extra cost.

The pre-processing tool usually consists of an interactive graphical front-end to generate the mesh of grid cells. Post-processing tools are used to display results in a variety of graphical formats. Since CFD simulations generate an enormous quantity of data, typically values of seven or more flow variables at each grid cell - which may total several hundred thousand (Lea & Kelsey, 1997) , at several moments in time, the necessity for graphical representation becomes clear. In the near-future, virtual reality may be employed as a means of displaying and interpreting data.

CFD software is highly complex, typically in excess of 100,000 lines of code for commercial products. The user usually provides a problem description complete with boundary conditions and solution control parameters by means of a high-level command language. In some circumstances more complex problems may require the user to write source code subroutines which are ' patched-in' to the main code. The high-level command language contains many hundreds of alternative options which can be selected by the user or are set as defaults by the code. To generate meaningful results the user must be aware of the consequences of selecting various options or accepting code default values. This demands that users are highly trained, experienced and have physical insight into the flow being modelled. These requirements are outlined in more detail in Section 3.7.

CFD simulations are computer-intensive, with large memory requirements and the need for rapid floating-point calculation speed. CFD hardware today usually consists of powerful UNIX workstations or servers, for use by single or multiple users. The minimum cost of suitable hardware is realistically about ~£15K for a single workstation. Run-times are commonly such that overnight computations, or longer, will be needed for a single simulation.

Some code vendors, such as CHAM, market PC versions of their software. The memory and processing speed requirements of practical CFD problems means that the results of PC-based simulations should be treated with additional caution.

3. ASSESSMENT OF CFD SUBMISSIONS

3.1 Overview

It should be highlighted that the primary function of this report is to provide assessors with an outline of the main issues which should be addressed in a CFD submission, and the reasons why these issues are significant. In many cases there could be a need to seek additional expert advice or further information, for instance on the applicability of a particular physical model or its known limitations. Section 4 suggests sources of additional information.

CFD results are usually presented in graphical form out of necessity. It should be stressed that graphical data alone is insufficient to allow assessment of CFD submissions. Documentation which describes the model basis and its application is required. Reference to the topic headings in Sections 3.2 to 3.8 should be sufficient to identify whether the requisite supporting documentation needed to allow an assessment of CFD simulations has been supplied by the licensee.

Assessment of CFD simulations cannot be carried out in isolation. A knowledge of the use to which results will be put is also needed to judge the level of predictive performance required, i.e. whether qualitatively correct results would be adequate to provide just an overall indication of flow behaviour, or whether quantitatively-accurate values are required.

It should be noted that it is difficult to put error bands on CFD-computed quantities. This is partly because the governing equations exhibit highly non-linear behaviour such that small errors in some aspects of the physical or numerical sub-models or boundary conditions can either be amplified or attenuated in ways which are not readily predicted, and partly because of the strong influence which the user's modelling decisions exert on the end result. Sensitivity analysis and validation exercises, Section 3.6 and 3.8 respectively, provide a means to quantify errors and reduce uncertainty. However, the assessor should be satisfied that all the most significant sensitivities have been investigated, that validation cases are relevant, that the specific application has been conducted as rigorously as validation studies, and, most importantly, that the work has been undertaken by a competent user - Section 3.7.

The issues which can be expected to be addressed in CFD submissions are outlined below.

3.2 Problem definition

To enable a CFD problem to be set-up and solved, certain parameters must be defined. Usually these parameters will need to be set by the user in the high-level command language which is used by the code to set internal switches for various simplifying assumptions to the governing equations. Appropriate problem definition is thus crucial if meaningful results are to be obtained. For this reason, submissions should include a comprehensive problem definition. In essence this covers all the modelling choices which have to be taken by a user. It is, however, convenient to address issues relating to physical and numerical sub-models, plus boundary conditions, separately in Sections 3.3 to 3.5.

Problem definition should cover specification of the following, which is by no means an exhaustive list:

Compressible Vs. Incompressible flow: If the Mach number is expected to be below ~0.3 at all points in the region to be simulated then the flow can be assumed to be incompressible. If the flow is sonic or supersonic in some regions - perhaps as a consequence of a high pressure gas release, then special solution algorithms will probably be needed to obtain a solution, or alternatively, further simplifying assumptions in treatment of this type of source may have been necessary.

Steady Vs. Transient flow: A decision must be taken before simulations proceed as to whether the flow is likely to be steady or transient. Specification of steady conditions for an inherently unsteady flow may result in the generation of a spurious steady-state solution or may result in failure to obtain a well-converged solution (See Section 3.5.4).

Laminar Vs. Turbulent flow: This is most important. The user has to decide a-priori whether the flow is likely to be either fully turbulent or laminar. If the wrong selection is made, for instance that the flow is specified as being turbulent when in fact it is more closely akin to laminar, then the CFD code will force the computed solution to exhibit the properties of turbulent flow, with the result that rates of mixing and diffusion will be grossly over-predicted. There is great difficulty in problem definition and thus generation of meaningful results if the flow does not clearly fall into one regime or the other.

Single Vs. Multi-phase flow: The user must decide whether the flow is single or multi-phase. If the flow is indeed multi-phase then numerous modelling difficulties arise. This may lead to the assumption that the flow can be represented as single-phase. If this step is made, then care must be taken in ensuring that inter-phase heat, mass and momentum transport effects have been adequately incorporated in the model.

Isothermal Vs. Non-Isothermal: Selection of isothermal flow means that the energy equation does not have to be solved, which reduces computational effort. However, this may be unrealistic, even if temperature differences are small, since buoyancy effects may then become influential.

Buoyant Vs. Non-buoyant: See above. If the flow is buoyant then a decision will have been taken as to whether density differences are sufficiently small that the Boussinesq approximation is valid (Ferziger and Peric, 1996). Cross-checks on final results should ideally be made to ensure that this remains a valid assumption.

Reacting Vs. Non-reacting flow: Chemical reaction, perhaps as a result of combustion, can only be simulated by making many simplifying assumptions. It may be that if the net result is the generation of heat, as in a fire, that the user overcomes the need to compute reacting flow, by specifying both the amount and <u>distribution</u> of the heat load in the computational domain. Since the latter may not be known a priori, the resulting uncertainty in the specification of the heat source will lead to errors in the subsequent flow behaviour, only quantifiable by sensitivity analysis, validation or inclusion of chemical reaction.

Two-dimensional Vs. Three-dimensional flow: Real flows are three-dimensional and must usually be modelled as such. In certain cases an assumption of two-dimensionality may be applicable. However, the validity of this assumption must be carefully scrutinised: If a flow which in reality exhibits significant three-dimensionality is specified to be two-dimensional then the code will force it to be two-dimensional. This may mask important features.

The assessor should be aware that computational run-times are vastly reduced with two-dimensional simulations, essentially because compute time depends strongly on the overall number of grid cells (See Section 3.5.2). This acts as a strong incentive for three-dimensional problems to be reduced to two-dimensions, but to possible detriment of predictive realism.

Extent of the computational domain: The user must fix the region of space in which flow is to be computed - the computational domain. Often the selection of domain boundaries is straightforward, especially for internal flows. However, in some circumstances, external and buoyant flows in particular, or when the two-dimensional approximation is employed, the position of the domain boundaries may be found to influence or even dominate the entire flow solution (Lea, 1996). It should be demonstrated that the domain boundaries have been sensibly chosen. Uncertainty can be investigated via sensitivity analysis.

3.3 Physical sub-models

3.3.1 Background

The fluid flow equations solved in industrial CFD codes are not the exact governing equations. This is because the exact equations either cannot be solved for practical flows of interest, as is the case with turbulent flow - addressed in more detail below, or, because the exact governing equations are not completely known, as is the case with combustion of complex fuels or phase interactions in multi-phase flow.

Simplified physical sub-models are thus employed, in-part derived from the exact governing equations, in-part derived from empiricism and physical reasoning. Since these sub-models form the physical basis for the CFD model as a whole, it is essential that they are critically-scrutinised in CFD submissions.

The main physical sub-model which will be encountered in almost all CFD simulations is that which represents the effects of turbulence. Turbulent mixing is the key process responsible for transport of heat, mass and momentum in the vast majority of fluid flows. For this reason, a very brief outline of the necessity for, basis and limits of applicability of turbulence models is given below.

3.3.2 Turbulence modelling

Solution of the exact equations for turbulent flow, in an approach known as Direct Numerical Simulation - DNS (Ferziger and Peric, 1996), requires all of the length and time-scales of the turbulent motion to be captured by the simulation. Because the ratio of the largest to smallest scales of turbulent motion in practical flows may easily be as large as typically four or even five orders of magnitude, this requires spatial resolution at 10^{-5} or 10^{-6} of the size of the computational domain in each co-ordinate direction. This implies solution on a mesh comprising 10^{15} to 10^{18} grid cells for perhaps 1 million+ time-steps. It is beyond the capacity of present or foreseeable computers to carry out the resulting calculation. DNS is thus currently reserved for research studies of very simple flows at low turbulent Reynolds number, even then it still demands use of the most powerful computers on the planet.

The engineering approach to CFD flow simulation overcomes the above difficulty by time-averaging the exact equations, with the result that the influence of turbulent velocity fluctuations are 'averaged-out' and expressed as new unknown terms in the averaged equations (Versteeg & Malalesekera, 1995). These terms are referred to as the 'Reynolds stresses'. Physically they represent the effects of turbulent mixing on the transport of heat, mass and momentum . Empirically-based turbulence models are then used to close the Reynolds-averaged equation set, either through simple algebraic expressions for Reynolds stresses or by the solution of additional transport equations. There is no universal turbulence model: they all have particular limitations.

The most commonly-encountered turbulence model is referred to as the k-ε model (Jones and Launder, 1972). k is turbulent kinetic energy, ε is the rate of dissipation of k. The model is based on the premise that the Reynolds stresses are linearly related to rates of mean strain by means of a 'turbulent viscosity', which acts in an analogous manner to the physical viscosity of the fluid but depends on local flow conditions. k and ε are used to construct turbulent length and velocity scales which are in turn used to provide local values for the turbulent viscosity. The values of k and ε are found by solving simplified model versions of their exact transport equations. These transport equations and the expression for turbulent viscosity include several unknown 'constants', whose values are tuned to ensure that the model produces reasonable agreement with experimental data for simple flows. Detailed descriptions of the model can be found in Rodi (1993), Wilcox (1993) or Versteeg & Malalasekera (1995).

The k-ε model is thus based on a number of assumptions and approximations, including a degree of empiricism. It is however in widespread use. It exhibits known failings for the following classes of flows: Recirculating flows; Swirling and rotating flows about an axis of radial symmetry; Impinging flows; Flows with streamline curvature; Secondary flows; Buoyant flows.

Since, in many cases, these are the very flows of interest, it is important that validation is supplied which provides an indication of the model's performance for the same class of flow as that presented in a submission, see Section 3.8. Although the k-ε model does have failings, these are mostly well-known and documented (Rodi, 1993; Wilcox, 1993; Versteeg & Malalasekera, 1996; or Launder, 1991). Hence it may also be possible to speculate on the likely consequences of using this physical model for simulation of certain classes of flows.

Many other simpler and more advanced turbulence models exist. In each case, evidence should be provided of the applicability of the turbulence model to the class of flow under consideration, including relevant validation and an assessment of the effects of model limitations.

3.3.3 Other physical sub-models

Other physical models are also likely to be encountered in CFD submissions. For example sub-models known as 'wall functions', are used in the near-wall region to avoid the necessity of resolving the wall-affected flow in detail. These sub-models are based on relationships describing the behaviour of flat-plate boundary layers in equilibrium (Launder and Spalding, 1974) and strictly speaking do not apply in the case of separated flow, or flows subjected to pressure gradients, etc. They are in widespread use however and in many cases give reasonable predictive behaviour, with the notable exception of heat transfer, when they can lead to large errors in computed heat transfer rates (Chieng and Launder, 1980; Yap, 1987). If wall heat transfer is an important process then the near-wall sub-model should receive special attention in a submission. It is possible that more advanced low-Reynolds number models (Launder, 1991), specifically devised to capture wall flows, should be employed.

It is not practical to outline all of the physical sub-models which can be employed in CFD simulations, since these are numerous and cover fields as diverse as combustion, two-phase flows, chemical reaction, thermal radiation, free-surface flows, etc.

The assessor of a CFD submission needs to be aware that physical sub-models will undoubtedly have been used to mimic certain aspects of the flow physics. It can therefore be expected that the sub-models employed should be referenced or described, together with a justification of their applicability - including specific limitations, plus supporting validation.

3.3.4 Physical properties

Physical properties must be specified to undertake a CFD simulation. These can have fixed values, or, be variable and dependent on other flow variables, such as temperature. It is not always the case that properties are well-defined. If there is uncertainty in values of physical properties then it can be expected that a submission will include an assessment of the extent to which the results may be affected. Sensitivity analysis is useful in this respect, Section 3.6.

3.4 Boundary conditions

Boundary conditions must be specified and applied by the user to ensure that the problem to be simulated is physically realistic and well-posed. In a time-dependent simulation these include the initial conditions.

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

Boundary conditions can be of several different types: Prescribed variable values, known as Dirichlet boundary conditions and 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 example, to set a plane of symmetry in the domain by specifying that gradients of all flow variables normal to the plane are zero; Volumetric sources or sinks of heat, mass and momentum, perhaps used to introduce a contaminant stream into a flow or a source of internal heat.

To allow a full assessment of CFD simulations to be undertaken, the specified boundary conditions should be stated in a submission and their basis given.

It is important to note that 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 be encompassed.

Where assumptions are made, these should be stated, together with an assessment of their consequences, including consideration given to the need for sensitivity analysis.

3.5 Numerical modelling

3.5.1 Numerical methods

There are several different numerical methods used to solve the modelled fluid flow equations. The main approach likely to be encountered in application of commercial codes is the finite volume method. Nuclear Electric’s code; FEAT, is based on the finite element method. Descriptions of these methods can be found in the texts by Shaw (1995), Versteeg & Malalesekera (1995), and Ferziger & Peric (1996). There is no need to go into detail here, since, in principle, both of these methods represent well-founded, valid methods. Instead attention is focused on the following three aspects of numerical modelling which are common to all approaches.

3.5.2 Computational Grid

The computational mesh of grid cells has to represent the geometry in the region of interest and be constructed to allow adequate resolution of the key flow features.

Several approaches could be encountered: Stepwise approximation using regular grids - in which curved boundaries are represented by staircase-like steps in the mesh; Body-fitted grids - in which the grid lines follow the computational domain boundary; Structured grids - in which grid lines are continuous across the domain and grid cells are usually hexahedral, or, unstructured grids - in which meshes may be constructed from tetrahedral or more complex-shaped cells and there is no clearly defined grid-line direction; Local grid-refinement may be used in a structured approach -.giving grid lines which are discontinuous across the domain.

The spacing between grid lines can be the same - giving a uniform grid, or varying - giving a non-uniform grid. Grid line intersections may have to be at 90^o - orthogonal, or can be non-orthogonal. Co-ordinate systems can be Cartesian, or follow the local grid line direction.

Clearly many variations are possible.

From the point of view of assessment, the main point to be highlighted is that the simulation results always depend on the number and disposition of grid cells. Generally-speaking, the greater the number of grid cells, the closer the results will be to the exact solution of the modelled equations.

Usually, as more and more grid cells are used in a simulation, the results tend to converge towards a unique solution. In theory, it is possible to carry out simulations on several different meshes with successive grid refinement and find, or extrapolate, to the grid-independent solution. Practically this is rarely, if ever, possible, especially for three-dimensional computations. This is because the compute time depends strongly on the number of grid cells: Typically, compute time varies as the squared to cubed power of total grid cell number, although there is the promise that new versions of commercial codes will exhibit a more linear-like dependency. Grid refinement therefore rapidly leads to unrealistically large compute times, as well as requiring increasing amounts of computer memory. A compromise is usually struck between adequate grid cell resolution and compute time.

Because of its importance, grid dependency should nevertheless be addressed in a submission. This could be achieved by reference to validation exercises and past experience, presentation of results from limited grid sensitivity studies, or, an assessment of the likely consequences of grid refinement on the flow solution.

There are other issues which should be addressed in a submission besides overall number of grid cells. Thus the solution also depends on the 'quality' of the mesh. This is an ill-defined term which covers the need to ensure that grid cell spacing does not increase over-rapidly from one cell to the next; that, if possible, grid lines should be orthogonal for hexahedral meshes and follow the streamline direction; that grid cells are clustered in regions where gradients of flow variables are largest. Access to independent expert advice may be required here.

In addition, it may not be possible to resolve all of the geometrical features, especially if these are of small scale in a large domain (Lea and Kelsey, 1997). In this case, the effects of the unresolved geometry may, for example, be represented by local sources and sinks of turbulence and momentum respectively, with a correction to account for the volume fraction of a grid cell which is occupied by a solid obstruction. This approach is often referred to as porosity-based. If employed, a submission should address the effects of limitations and uncertainties in this approach, possibly by use of sensitivity analysis.

3.5.3 Numerical discretisation

The discretisation methods used to translate the mathematical model into computer code include approximations which result in numerical errors. The significance of these errors depends on the type of discretisation employed.

The most frequently encountered error 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. 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'. Unfortunately, these will usually be set as the code defaults. All of the codes likely to be encountered include 'higher-order accurate' schemes which can be selected by the user, 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 Details can be found in Patankar (1980) and Hirsch (1990).

Because numerical errors arising from discretisation schemes can be of such importance, they can be expected to be addressed in a CFD submission, possibly by statements regarding order of accuracy of the schemes employed, or sensitivity analysis.

3.5.4 Solution control and convergence

The algebraic equations which result from the above discretisation are usually solved via iterative solution algorithms (Patankar, 1980; Hirsch, 1990; Ferziger and Peric, 1996). These start from an initial 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.

These iterative solution algorithms are 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 thus has to specify convergence criteria, which, when met, stop the solution algorithm.

Information should thus be provided in a CFD submission of the criteria by which convergence has been judged. This could include measures of the imbalance in mass, momentum and energy compared to sensible reference values. The change in variable values from one iteration to the next could also be used, with sufficiently small change being used to demonstrate convergence. Note that this latter method is not sufficient if used alone, since this difference may be small when the error in mass, momentum and energy is still significant.

3.6 Role of sensitivity analysis

The role of sensitivity analysis is to vary a model parameter through its range of uncertainty to establish the variation in the model output. It is a useful technique, especially if there is reasonable evidence to suggest that computed flow quantities of concern may be sensitive to parameters which are ill-defined. In such circumstances it can be expected that submissions will include a sensitivity analysis.

Parameters to be included in a sensitivity study could comprise; ill-defined boundary conditions -such as wall heat transfer coefficients or turbulence parameters as flow enters the domain; source terms - such as fire heat output or volumetric heat load and distribution; physical properties; physical sub-model parameters or empirical constants - for example in wall-layer sub-models where surface roughness is uncertain; discretisation methods; even entire physical sub-models.

Sensitivity analysis has several shortcomings: It is time-consuming and so in the case of complex CFD simulations it is likely that any sensitivity analysis will consequently be limited in scope. In addition, uncertainties in the performance of the underlying physical and numerical sub-models can be much larger than those arising from, for instance, uncertainty in boundary conditions. It is usually much easier to carry out sensitivity analysis for the latter, than the former.

3.7 User expertise

CFD-generated results rely strongly on the competence and expertise of the user. It is generally accepted within the CFD community that the user is one of the prime causes of uncertainty in results of CFD simulations (I Mech E, 1994). Versteeg and Malalesekera (1995) explain:

"In solving fluid flow problems we need to be aware that the underlying physics is complex and the results generated by a CFD code are at best as good as the physics (and chemistry) embedded in it and at worst as good as its operator."

To begin to construct a CFD model of a particular flow the user must have a good appreciation of the physical phenomena which are significant. The reason is that at the outset the user must specify, for instance, whether the flow is laminar or turbulent, steady or unsteady, whether the Boussinesq approximation for buoyancy effects is applicable or not, what are appropriate and sufficient boundary conditions, etc. Training in fluid mechanics is thus essential.

CFD codes typically have many diverse options to be set or considered by the user when specifying a problem for solution. These all influence the end result to a greater or lesser degree. The user has to be aware of the consequences of selecting these various options or accepting code default values, including limits of applicability. This demands expertise in not just fluid mechanics, but also the numerical solution of fluid flow equations and the idiosyncrasies of various solution algorithms.

Commercial vendors are making CFD codes more accessible to non-expert users, through interactive graphical pre- and post-processors, the use of automatic grid generation techniques, plus automation of the problem specification by supply of as many default values for physical and numerical sub-models, solution control parameters, etc., as possible. However, at present, these advances are largely made from the commercial perspective of increased sales through increased accessibility, rather than a push towards reduced uncertainty in results as a consequence of in-built intelligence.

User competence is thus a major issue in CFD. Leschziner (1993) concludes that;

"CFD involves a wide range of strongly interacting physical processes and numerical issues, some of which are as influential on predictive accuracy as they are ill-understood. It is for this reason that a high level of training, expertise and insight are essential in order to properly exploit the potential of CFD and, equally importantly appreciate its limitations."

It is must therefore be recommended that submissions which include the results of CFD simulations should include information which demonstrates that the analysis has been carried out by trained, competent users.

3.8 Validation requirements

Definitions (I Mech E, 1994):

Verification is defined as the process of ensuring that the equations in the mathematical model are coded and solved correctly. It gives little or no information on the appropriateness or accuracy of the CFD model to represent particular real world flows.

Validation is defined as the process of demonstrating that the combination of mathematical model, numerical solution method, boundary conditions, etc., provide a sufficiently accurate representation of the real world flows, i.e. that the model is valid.

Verification should be undertaken by the code developer as part of the internal quality assurance procedure. This may be referred to in a submission.

The need for validation is clear from the preceding discussion: CFD models include simplifying assumptions and a range of approximations which mean that there is no guarantee that their results are adequate representations of reality. Supporting evidence of relevant code validation studies should therefore be found in a CFD submission.

Validation is usually undertaken by comparison of CFD results to reliable and appropriate experimental data - often referred to as ’benchmarks’. This data commonly consists of simplified test cases which nevertheless encompass the key physical processes and/or geometrical complexity seen in the problem of interest. Typically more than one validation test case may be required to demonstrate that the CFD model is capable of adequately representing the differing elements found in a real application. For instance, one case may seek to demonstrate that the key physical phenomenon can be modelled acceptably, further cases may be needed to provide surety that other important physical phenomena and complex geometry can be handled.

In some instances it may be appropriate that validation is predictive, with only sufficient data made available from a test case to allow a CFD model to be set-up and run, with the full results withheld from the modellers. A ’blind’ prediction of this type mimics to some extent the way in which a CFD code is used in practice. Exercises of this nature are usually organised by regulators, industry forums or academics. A submission may make reference to a past blind prediction exercise in which the code and user participated. If the test case was simulated by several different code suppliers, or even code users, the exercise can give important insights into both the accuracy and range of results obtainable.

Difficulty arises if there is justified uncertainty in the experimental test case data or if the data is limited or not available. This, unfortunately, may often be the case. In these circumstances, great caution and engineering judgement needs to be exercised when assessing CFD results. It may even be necessary for experiments to be commissioned specifically to provide data for code validation.

Inter-code comparison exercises can be helpful in circumstances in which experimental data is lacking, to assess whether a code is consistent with other predictive CFD models. One important benefit is to help quantify the spread of results which can be obtained. Often inter-code comparisons take place in the context of blind prediction exercises.

It is not uncommon to find that CFD models have been tuned or calibrated by reference to validation data. If this is the case, evidence of applicability of the model to the particular case of interest should then be sought.

It is not always necessary that the code in question be validated directly: If the main requirement of a validation exercise is, for example, that a particular physical sub-model performs adequately, then assuming that the model has been coded correctly - which is the purpose of verification, then it should be acceptable to point to reference works in the literature for evidence of physical or numerical sub-model validation. However, validation of a sub-model for a particular flow may not imply that the results of a simulation can be relied upon if numerical, and other sources, of error have not also been addressed.

Statements such as ’the model has been validated’ are misleading, since in theory only lack of validation can be demonstrated - in much the same way as physical ’laws’ are repeatedly tested for differing situations. In practice most validation studies are limited in scope to certain classes of flow and geometrical complexity.

In a wider context, there are national and European validation initiative’s underway whose aim is to generate datasets of benchmark experiments and CFD results, leading to guidelines for best CFD practice. These are led by NAFEMS in the UK and ERCOFTAC (European Research Community On Flow Turbulence And Combustion). HSL is involved in both of these activities. These initiative’s are at a very early stage and, if successful, will take some years to bear fruit.

It is important to remember that code validation is a necessary but not sufficient condition for ensuring that CFD model results lie within acceptable bounds. The code user must also be ’validated’, as outlined in Section 3.7.

4. SOURCES OF FURTHER INFORMATION

This report provides an overview of issues to be addressed by CFD submissions and of which inspectors should be aware when assessing safety cases which include CFD simulations. In a short report such as this, it is not possible to give a detailed exposition of all the CFD modelling issues which may arise: In many instances access to additional information and advice will be required. This can best be provided by independent CFD experts, or published works.

Until very recently there were almost no introductory texts to CFD modelling. Most either assumed a certain level of knowledge or were aimed at CFD code developers. Introductory-level CFD texts do now exist.

CFD reference books which may be found helpful include;

Introductory

"Using Computational Fluid Dynamics", Shaw, 1995

"Computational Fluid Dynamics: The Basics with Applications", Anderson et al, 1995*

*Primarily aerospace-related

Advanced-level
In some instances these assume little prior knowledge of CFD, but all demand a good understanding of fluid flows and in most cases rapidly become more detailed. In approximate ascending order of complexity are;

"An Introduction to Computational Fluid Dynamics", Versteeg & Malalasekera, 1995

"Numerical Heat Transfer and Fluid Flow", Patankar, 1980

"Computational Methods for Fluid Dynamics", Ferziger & Peric, 1996

"Computational Fluid Mechanics and Heat Transfer", Anderson et al, 1984*

"Numerical Computation of Internal and External Flows", Hirsch, 1990*

Specialist texts concentrating on particular aspects of CFD modelling include;

"Turbulence Models and their Applications in Hydraulics", Rodi, 1993

"Turbulence Modelling for CFD", Wilcox, 1993*

"Turbulent Reacting Flows", Libby & Williams, 1994

"Combustion fundamentals of fires", Cox, 1995

There is a huge body of published literature on CFD, most of which is highly specialised. Review articles do exist, but these tend to concentrate on specific aspects of CFD modelling. Those which are concerned with industrial flows include the reviews by Leschziner (1989, 1993), Launder (1991) and Hanjalic (1994). Many others exist, some of which may be more relevant to nuclear engineering.

In addition, introductory short courses in CFD are held by UMIST and Imperial College.

5. CONCLUSIONS

CFD is a powerful tool for the analysis of fluid flows. It is in widespread use in many varied and diverse fields. It is likely to be employed more frequently as computing costs decrease and commercial CFD codes become more accessible.

However, for meaningful results to be obtained the codes still require considerable user expertise, physical insight and experience.

To allow assessment of CFD simulations, certain issues should thus be addressed in submissions. These include; problem definition; physical and numerical sub-models employed; boundary conditions; computational grid; sensitivity studies; supporting validation; user competence.

This report therefore provides guidance to assessors on the main issues which should be addressed in CFD submissions and their significance.

However, the highly specialised nature of CFD modelling and its continuing development means that it is likely that access to independent expert advice will also be needed. The report includes a list of recommended reference texts.

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