COMPUTATIONAL FLUID DYNAMICS GUIDELINES FOR BEST WORKING PRACTICE

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1 INTRODUCTION

The purpose of computing is insight not numbers - [1]

To be able to use Computational Fluid Dynamics (CFD) with confidence for internal flow analyses within the Rolls-Royce Fluid Systems Group it is necessary to ensure that all analyses are carried out to a high level of quality. The state of development of CFD as a discipline is such that no procedure exists which can guarantee a correct numerical solution to any given fluid problem. However it is possible to lay down guidelines which will reduce the danger of the analyst falling into some of the more obvious pitfalls. It should be understood that the material presented relates to applications specific to work carried out using the FLUENT CFD code within the Rolls-Royce Fluid Systems Group, such as air flow though constrictions and cavities with rotating boundaries. The advice offered has been found to be useful within this context for relatively inexperienced CFD analysts. The author makes no great claim as to the originality of the ideas presented, but notes that there are few documents in the literature that attempt to bring together many of the ideas circulating as to what constitutes best practice in CFD analyses. It is hoped that the current work will prove useful to CFD practitioners recent to the field, and may help stimulate discussion as to what constitutes a generally acceptable methodology for CFD analyses. The experience used in the current work has been gained exclusively using the FLUENT/UNS [2] CFD code, although it is hoped that it may be of benefit for users of other CFD codes.

To assist an analyst in carrying out CFD work this paper includes:

1. Guidelines to ensure best working practice in CFD analyses.
2. A list of some of the main difficulties facing an analyst, and tools to address particular problems.
3. A checklist to help ensure best practice appears in section 5.

1.1 Notation

C_P	Specific heat capacity at constant pressure for air = 1006.43 J.kg^{-1}.K^{-1} at 288.16K.
C_μ	Constant used in definition of turbulent effective viscosity, =0.09.
d	Inlet diameter, m.
g	Acceleration due to gravity, 9.81m.s^{-2}.
k	Turbulent kinetic energy, m^2.s^{-2}.
k_P	Turbulent kinetic energy at point P, m^2.s^{-2}.
L	Typical system length scale, m.
P	Total pressure, Pa.
p	Static pressure, Pa.
q	Non-dimensional dynamic pressure.
R	Gas constant for air = 287.012 J.kg^{-1}.K^{-1}.
T	Fluid temperature, K.
U	Typical fluid velocity, m.s^{-1}.
$\overline{U}$	Mean inlet velocity, m.s^{-1}.
u	Local fluid velocity, m.s^{-1}.
u_τ	$=(\tau_W/\rho)^{1/2}$, the friction velocity, m.s^{-1}.
y_P	Distance from wall to point P, m.
α	Turbulence intensity, dimensionless.
β	Thermal expansion coefficient, K^{-1}.
γ	Ratio of specific heats for air $= \left(1 - R/C_P\right)^{-1} \approx 1.4$.
δ_{Ek}	Ekman boundary layer thickness, m.
ΔT	Surface to fluid temperature difference, K.

ε	Turbulent dissipation rate, $m^2.s^{-3}$.
κ	Fluid thermometric conductivity, $m^2.s^{-1}$.
μ	Fluid dynamic viscosity, $kg.m^{-1}.s^{-1}$.
ν	Fluid kinematic viscosity, μ/ρ, $m^2.s^{-1}$.
ρ	Fluid density, $kg.m^{-3}$.
τ_W	Wall shear stress, Pa.
Ω	Boundary rotation rate, $rad.s^{-1}$.

Gr	Grashof number, $g\beta\Delta TL^3/\nu^2$, dimensionless.
M	Mach number, dimensionless.
Nu	Nusselt number, dimensionless.
Pr	Prandtl number, ν/κ, dimensionless.
Ra	Rayleigh number, Gr.Pr, dimensionless.
Re	Reynolds number, $\rho UL/\mu$, dimensionless.
y^*	$\equiv\rho C_\mu^{1/4}k_P^{1/2}y_P.\mu^{-1}$, dimensionless.
y^+	$\equiv\rho u_\tau y_P.\mu^{-1}$, dimensionless.

1.2 Purpose

The state of development of CFD as a discipline is such that no procedure exists which can guarantee a correct numerical solution to any given fluid problem. However it is possible to lay down guidelines which will reduce the danger of the analyst falling into some of the more obvious pitfalls. This latter objective is the aim of the present paper. The earlier sections discuss some of the issues likely to effect the quality of a CFD solution. At the end guidelines are presented in the form of a checklist for a given analysis. For further reading the author recommends [3].

Philosophy

In principle it is very difficult to know whether a computational fluid dynamics simulation has produced a physically acceptable answer to the required accuracy, thus a CFD solution must be treated with caution until it has been proved reliable. In principle unless validation is carried out over the whole domain this can never be the case, but in practice various tests will reduce the probability that a meaningless or unphysical solution has been found. Such tests can also give an indication of the accuracy of the solution obtained, and demonstrate whether it is likely to prove fit for the purpose for which it is required. For these reasons, inexperienced CFD analysts should work under the guidance of experienced staff.

Consideration must also be given to the purpose for which the work is being carried out, and if need be must conform to any working practices that relate to the nature of that work.

2 THE NATURE OF CFD SOLUTIONS

CFD consists of using a *model* (simplified set of equations) to find a *solution* consistent with a set of *idealised boundary conditions* over a *discretised* domain (the grid) to represent a real continuous fluid system, for which there is, in general, *no uniqueness theorem* (multiple alternative mathematically correct solutions are permitted).

The italicised words indicate the key areas of difficulty for the achievement of successful CFD solutions.

2.1 Overview of Difficulties with CFD Solutions

2.1.1 Model

The model used by the simulation may not be an appropriate representation of the physical system and consequently the solution found may not be a solution to the physical system. A major area of difficulty here is that of turbulence modelling, where there is no guarantee that the model used to simulate the system is correct or appropriate.

2.1.2 Convergence to a Solution

A CFD code uses an iterative procedure to seek a numerical solution to the problem that is consistent with the models and boundary conditions over the chosen grid, i.e. convergence is achieved. This often requires suitable initial guesses otherwise the code may be unable to find a converged solution.

Historically, the choice of iteration scheme influenced the feasibility of achieving convergence. Problems can be expressed in terms of their governing equations as hyperbolic, parabolic or elliptic. Hyperbolic or parabolic problems are such that events at some arbitrary point in the flow may only influence points down-stream (in terms either of flow direction or of time), these were solved by time-marching iteration procedures. In elliptic (steady-state) problems the influence of events at an arbitrary point are also felt upstream from it, and were solved by pressure-correction algorithms (although steady-state subsonic flows could be treated as quasi-unsteady and solved using a time-marching procedure, with the steady-state approached as time$\rightarrow\infty$). An example is pressure-waves in air, which travel at the speed of sound. Providing the flow is steady and subsonic, information about obstacles to the flow will propagate upstream through the pressure-field at the speed of sound, causing the flow to adjust to anticipate the obstacles, although they are down-stream from the current position. In supersonic flow, fluid particles do not know about obstacles until they (more-or-less literally) hit them, thus supersonic flow problems will be hyperbolic in nature and subsonic problems elliptic. More information on elliptic, parabolic and hyperbolic problems is given in [3]. With modern solution algorithms it is generally the case that most types of problems can now be solved using either time-marching or pressure-correction procedures. However, in general terms pressure correction algorithms will be better for solving low Mach number flows and time-marching algorithms for high Mach number and transonic flows.

Thus it is important to be aware of whether the problem under consideration is hyperbolic, parabolic or elliptic, in order to determine whether a particular iteration procedure will be required to achieve a converged solution.

2.1.3 Boundary Conditions

When modelling a physical system, boundary conditions tend to be of a simplified form; walls might be assumed to be perfectly smooth and perfectly insulating, inlet velocity profiles are uniform or have a smooth, prescribed profile, pressures also are uniform, turbulence intensities have specific values, gradients in particular quantities are zero and so forth. In real systems boundary conditions will not usually be as uniform, or regular as in a model, in some cases these differences could alter the form of the resulting flow.

2.1.4 Grid

In order to solve the chosen physical equations, they are solved at a series of discrete points, approximating the spatial domain. Two types of error can occur.

- Representing a continuum by a series of discrete points (discretisation error).
- Calculation of derivatives to a certain accuracy (truncation error).

2.1.5 Uniqueness of Solutions

In general, because the Navier-Stokes equations are non-linear, there is no uniqueness theorem that applies to fluid flow problems. This means that there can be two or more solutions to the set of equations and boundary conditions being considered. There is thus no guarantee that even a "perfect" simulation will give the solution found in nature. In practice, small variations in boundary conditions, which occur in nature, might predetermine the system to one solution or another. One example of this is in hysteresis effects, where the solution obtained will depend on the direction from which the solution is approached. Another way of looking at it is to appreciate that for many fluid systems, if they were to be significantly perturbed from their current state, there is no guarantee that the resulting flow, after it had settled down again, would be the same as the one started with. The best one can do is to check that the broad form of the solution is independent of perturbations to the flow. For some kinds of flow a number of studies scanning through a range of values for the boundary conditions should help to build confidence that a consistent set of solutions have been found. Another approach is to simulate not only the flow, but also the manner in which the flow approached its current conditions.

2.1.6 Summary

In summary there are five major areas for concern:

1. The models used must be appropriate for the problem under consideration.
2. Representation of boundary conditions.
3. Convergence must be achieved.
4. The effect of the grid on the solution.
5. The solution must be the one chosen in nature.

2.2 Guiding Principle

One way of dealing with all of the above areas of concern is to compare the CFD solution with physical data from the system in question. If good agreement is found for a number of parameters over a suitable range of positions and conditions, this makes it extremely likely that all of the above concerns have been adequately addressed in the modelling. However, generally sources of physical data are limited and a different approach is required.

Without a detailed comparison with data from the physical system under consideration, there is no way of being strictly certain that the CFD solution obtained is a good approximation to the correct one. Hence the best approach is to treat the CFD solution with caution and to try to find meaningful tests to determine whether the solution is valid or at least fit for purpose. If the CFD practitioner fails to find fault with the solution, gradually it acquires a degree of respect and a provisional acceptance on the basis that no fault has yet been found with it.

This is a very strict interpretation of the situation, in practice things are probably not quite so bad. However an isolated CFD solution must be assumed unreliable until certain basic tests have been carried out on it. These tests will usually require other CFD runs to be executed, often as a range of sensitivity studies about the initial solution. *As a result a collection of mutually self-supporting CFD solutions are obtained which allow the initial question posed by the CFD practitioner to be answered with a degree of confidence.*

This final point cannot be over-emphasised, the purpose of any CFD study is to answer some technical question posed by the analyst, it is not to produce any single numerical solution to a given model, no matter how perfectly converged.

3 FACTORS TO CONSIDER IN ANY CFD ANALYSIS

The concerns listed in section 2.1 cover the computational modelling side of a CFD analysis, however when dealing with any extended set of data, one must also consider the accuracy of the data (source data for setting conditions, the accuracy required from the analysis and the solution accuracy achieved). In addition it is also sensible to decide the objectives for any analysis before-hand, this helps ensure that these are properly borne in mind when decisions are made regarding the analysis.

These points, together with suitable approaches for addressing them are the subject of the following sections.

3.1 Purpose of the Analysis

The objectives and timescale of any analysis should be agreed in advance (bearing in mind the limits of CFD), and included in any report of the work. It is also valuable to question whether a CFD analysis is really required, or whether there is an alternative route for calculating the required data. This ensures that the user has a clear idea of what they are hoping to achieve as the analysis is carried out. A danger with a CFD solution is that it will present numbers to a great number of decimal places (often interpreted as high accuracy) regardless of the quality of information put into it, or required from it. This can give rise to the temptation to apply the results of one analysis to another circumstance. The most obvious abuse is that the results of a qualitative or comparative study might be used for quantitative purposes. While this may not in itself lead to erroneous conclusions, it is poor practice as it increases the risk.

A way of reducing the danger of mis-use of results is for the analyst to only put data in any written report that is of a form that they would be happy to see used. Thus reports on qualitative studies could contain graphs and pictorial output, but no tables of numbers, so no specific numerical values are available to be taken out of context. The analyst must also be careful to state the limitations of their results and any indication of the accuracy that they are able to provide.

There is no problem in deciding that a particular analysis is 'an initial study, just to get an idea of what the flow might look like', providing that the results are clearly indicated as such. Further studies can then be carried out to examine aspects of the results in more detail. The danger is always that results will be taken out of context and treated as if they had been derived for the quantitative analysis of some obscure sub-feature of the flow.

Another benefit of determining the purpose of the analysis is to consider what new physical insights one hopes to gain. In the case of validation this is a question of 'is the new tool up to the job?'. For other investigations this helps to prevent work being carried out as 'CFD for CFD's sake'. After all, there is no business case for doing CFD just because it can be done.

3.2 Accuracy Required

It is important that the application the results are going to be used for is considered. This in turn determines the accuracy that will be required from the solution. Careful consideration of the accuracy required should reduce the danger of the analyst simulating the problem on a too coarse, too fine or otherwise inappropriate grid, or unnecessarily using a complex turbulence model, saving time and resource. Any report should give an indication of the accuracy of the results, how that accuracy was determined and how the results may be used.

Typical task requirements for accuracy might range from:

- Qualitative data such as flow visualisations for positioning instrumentation, or deciding the areas of interest for more detailed studies. In qualitative studies it is extremely important to consider regions of flow separation and re-attachment relative to geometric features, as these could significantly alter flow patterns. In this respect qualitative studies may prove almost as difficult to execute as full quantitative analyses. (See e.g. [4, 5]).
- Use of relative values for comparative analysis to decide the relative merits of a number of configurations.
- Determination of absolute quantitative values.

Given the large overhead of any CFD analysis it is important to solve the problem at the appropriate level of accuracy adequate for the requirements.

3.3 Values, Measurements and Uncertainties

Strictly, any measured or computed data value (or collection of values, such as a streamline or flow pattern) is of no merit unless there is some indication of the accuracy attached to it. With no associated uncertainty or standard error a person seeking to use that data cannot tell whether their data (or requirements) are in accord with the solution or not.

It is desirable to have an estimate of the probable accuracy of a CFD simulation. This might be obtained by comparison with known test cases (validation case studies), or by translating input uncertainties (uncertainties associated with measured data used for boundary conditions or fluid properties for example) into a spread in CFD solution parameters by use of sensitivity studies (see section 3.5). Usual experimental practice presents uncertainties as ±1 standard deviation (the ~66% confidence limit), unless otherwise stated. This means that one data point in three is expected to be more than one standard deviation from the central value. Uncertainties derived in other manners should have their method of derivation clearly reported.

Validation of a CFD model against experimental data should normally be carried out to the ±2 standard deviation limit (95% confidence limit) of the experimental measurements, so that only 1 point in 20 would be expected to be more than one uncertainty band from the central value.

3.4 Conditions for Convergence

The residual history (a global measure of the local error in the discretised equations plotted against iteration number) gives a convenient indication of the numerical convergence of the model. A necessary (but not sufficient) condition of convergence is that the residuals should remain constant from iteration to iteration, i.e. the residuals should no longer be decreasing (or increasing!).

Further checks on convergence include checking that inlet and exit total mass flows agree to a satisfactory accuracy, that there is heat balance, and that the value of a flow parameter at a given monitor point does not change from iteration to iteration.

The danger in relying on the gradient of the residual history alone as an indicator of convergence is that a solution may 'stall'. This refers to the situation where the residuals do not change from iteration to iteration, but a converged solution with much smaller residual values can be found. Under these circumstances the residuals often oscillate rapidly between two values as the iterations proceed, as if the code is unable to decide which of two possible solutions to head towards. This generally implies that there is some problem with the iteration procedure or model, and can often be resolved by changes to model (perhaps meshing or boundary conditions).

A further possibility is that a series of iterations may produce sudden sharp spikes in the residual plot. This can often indicate that an insufficiently fine or inappropriate grid has been used. As some kind of solution (perhaps not fully converged) can be helpful in determining where problems lie within a model, simulations with stalled or spiky residual histories can often be dealt with by one of two methods.

1. Some codes will allow the user to plot contours of residuals for flow parameters for the whole flow domain. Various approaches can then be used to improve the mesh around locations where the parameter with the highest global residual has its peak local residual value, including local mesh refinement. If iterations are producing a spiky residual history and they can be halted at the top of a spike, this can be a very effective way of preventing the spikes' re-occurrence.
2. An alternative approach is to make the solution scheme more stable by reducing the under-relaxation coefficients. This will usually result in an immediate drop in residual, followed by gradual convergence. However it can slow down the overall process of convergence. In the case of residuals that cycle between high and low values, it can reduce either the cycle frequency (not very useful), or else damp the cycle amplitude.

To deal with stalled solutions a suggested additional requirement for accepting a converged solution is that the residuals should have decreased by a minimum of six orders of magnitude from their initial values. Further advice on achieving convergence can be found in an article by the NAFEMS CFD Working Group [6].

3.5 Sensitivity Studies

In numerical work uncertainties in input boundary conditions (values and types) can be translated into uncertainties in the solution by sensitivity studies. This applies equally to uncertainties attached to types of model used and exploring the effects of the mesh on the solution. Grid refinement is only a form of sensitivity study. In fact, any aspect of a simulation that is open to doubt should ideally have its effect on the solution assessed by a sensitivity study.

Sensitivity studies represent the most useful approach for dealing with questions such as:

- Is the correct type of model being used? Possibilities include 2d vs. 3d, steady flow vs. time-dependent, viscid vs. inviscid flow and 1st order vs. 2nd order discretisation schemes. It should be noted that a 2nd order discretisation scheme should always be used to calculate the final solution. If in doubt the analyst should consult an expert.
- How do the details of boundary conditions and their type effect the solution? (Vary boundary conditions, change velocity profile shapes, change pressure boundary conditions to velocity boundary conditions, vary the inlet turbulence conditions.) Also fluid property values may only be known to an accuracy of a few percent.
- How does the choice of grid effect the solution? (Dealt with in more detail below.)
- Would Nature have chosen the solution found by the analysis? (Vary boundary conditions in a systematic fashion and see if the solution retains the same general form, or vary geometry in a systematic manner and see if the solution changes in the way you would expect.)

Given the comments in section 2, one must expect any high-quality CFD analysis to be accompanied by a number of sensitivity studies addressing various aspects of the simulation and flow.

3.6 The Physics of the Flow

A good understanding of the physics of the flow is one of the few ways of protecting the analyst from presenting solutions that are obviously incorrect. Before commencing a CFD analysis the user should attempt at least a qualitative understanding of the expected solution. After code execution at the most basic level the CFD code user can check basic physical quantities (in the steady-state, does the mass flow rate into the system equal the mass flow rate out of it?). In the other extreme the expert analyst may know perfectly well what the answer should look like, but would just like to firm up on a few numbers.

A list of simple physical checks that can be carried out during or at the end of a run to give a basic level of confidence in the developing or final solution is given below.

- Is the flow entering at inlets and leaving at outlets?
- Are the mass flows as expected / is mass conserved?
- Are the absolute pressures and pressure drops sensible?
- Are the temperatures sensible / is energy conserved?
- Are the density and viscosity values sensible?
- Is the flow doing what is expected for incompressible / compressible flow?
- Does the grid need revising to improve y^+ values? (See section 3.7.3.)

A clear physical understanding also amounts to knowing the solution that nature would select and so reduces the risk of obtaining unphysical results.

In many cases the advice above may be simply expressed as 'if you do not understand a flow - ask an expert about it'. In any case the analyst should not rely on the CFD code to provide a substitute for their understanding of the flow.

3.7 Choice of Models

CFD codes offer a variety of models to simulate different types of flows. Often these take the form of switches, which effectively define which terms in the governing equations will be used. Typical choices and considerations are given below.

3.7.1 Number of Dimensions

It is often possible to construct two-dimensional models of a particular system. If this is possible it is extremely desirable because two-dimensional models can be solved much more rapidly than three-dimensional models. However careful consideration must be given to whether the physics of the problem can be adequately represented in two-dimensions. It is important to appreciate that just because the geometry of the system can be represented in two-dimensions, or has a certain axis of symmetry, does not necessarily imply that the flow solution must also be two-dimensional. Further comments about the geometry and the number of dimensions that should be used are given in section 3.9.

3.7.2 Heat Transfer

Fluid temperature gradients can give rise to buoyancy forces. From a modelling perspective the flow needs to be regarded as one of four types.

1. Isothermal flow. The flow is at uniform temperature so no buoyancy forces can arise. Heat transfer is irrelevant.
2. Forced convection. Heat transfer by fluid advection dominates buoyancy forces. Temperature is effectively a tracer carried by the fluid, buoyancy effects can be neglected. Conduction may be important.
3. Mixed convection. Buoyancy has an effect on fluid motions that is comparable with heat advection. Buoyancy effects will have to be simulated, though they

may only have a minor effect on the flow. Under these conditions it might be worth running a 'pseudo-incompressible' simulation with $\rho=\rho(T)$ only.

4. Natural convection. Buoyancy effects are the only significant cause of heat advection.

Radiative effects may also modify the flow obtained.

To determine whether the flow for a particular configuration is likely to include forced, mixed or natural convection, the dimensionless group $Gr.Re^{-2}$ should be used [7]. For natural (or free) convection $Gr.Re^{-2}>>1$, in which case heat transfer (as denoted by the Nusselt number, Nu) will be governed by $Nu=f(Gr, Pr)$. For forced convection, $Gr.Re^{-2}<<1$, and $Nu=f(Re, Pr)$. Mixed convection will take place when $Gr.Re^{-2}\approx1$, in which case $Nu=f(Re, Gr, Pr)$. As for any particular geometry, the change-over between natural and forced convection is likely to occur at different values of $Gr.Re^{-2}$, the best approach for determining the flow type is to compare the value of $Gr.Re^{-2}$ with the flow for a known solution.

3.7.3 Turbulence Modelling

Steady laminar flow is characterised by streamlines that run in a well ordered manner with adjacent layers of fluid sliding relative to one another, with no motion or change normal to the streamlines. Under certain conditions, such a flow may undergo instabilities and become turbulent. In such instances close examination of the flow will reveal that what appears to be steady motion is actually a time-dependent flow oscillating around an apparently steady mean condition. The point at which the flow changes from laminar to turbulent is characterised by the Reynolds number (Re). Although it is problem dependent, as a rule of thumb, for Re < 2000, the flow can be considered laminar. For pipe flow the transition to turbulence takes place between Re=2000 and 10^5 (Tritton 1988). For natural convection in a vertical slot, the transition from laminar natural convection to turbulent convection takes place for Rayleigh numbers above around 10^6.

It is currently not practical to solve the full Navier-Stokes equations for turbulent flow, hence a time-averaged form of the equations are solved, known as the Reynolds Averaged Navier-Stokes equations. These describe the time-averaged turbulent flow, introducing the Reynolds stresses as new flow parameters. The central requirement of turbulence modelling is then to define and model the Reynolds stresses in terms of other time-averaged flow parameters.

The accuracy to which these Reynolds Stresses are solved to is dependent on the turbulence model chosen. Versteeg and Malalasekera [3] list the five commonly available turbulence models as:

1. Two equation k-ε model which comprises transport equations for the turbulent kinetic energy, k, and its dissipation rate, ε.
2. Zero equation mixing length model, which calculates the turbulent viscosity without employing any transport equations.
3. One equation model, which consists of a transport equation for k and an algebraic expression for the turbulence dissipation rate, ε.
4. Reynolds Stress Model (RSM), which models the transport of turbulent shear stresses (Reynolds Stresses) in each direction, as opposed to treating turbulence as isotropic.
5. Large Eddy Simulation, uses a spatial filtering to remove the small scale fluctuations in turbulence, but captures the larger scale fluctuations, thereby more accurately representing the true flow condition. This however requires a very fine grid to enable these fluctuations to be captured.

Although not strictly a turbulence model, Direct Numerical Simulation (DNS), is being developed as a means of solving the full time dependent Navier-Stokes equations. This technique cannot currently go above Re = 3000 due to limitations in computer power.

All existing turbulence models are inexact representations of the physical phenomena involved, and it is the simplification of the turbulence in these models which limits the accuracy to which CFD can reproduce flows seen in nature. However, it is known that the degree of inexactness of a given model depends on the type of flow it is applied to.

For further details see the chapter on turbulence models in Versteeg and Malalasekera [3].

Turbulence Intensities

The most commonly used model is the two equation k-ε model. In this model a turbulence intensity, α can be used to define inlet boundary condition parameters, (following [3]) the turbulent kinetic energy,

$$k = \frac{3}{2}\alpha^2\overline{U}^2 \text{ (m}^2\text{.sec}^{-2}\text{)}$$

where $\overline{U}$ is the mean inlet velocity, and the turbulent dissipation rate is given by

$$\varepsilon = \frac{C_\mu^{3/4} k^{3/2}}{0.07d} \text{ (m}^2\text{.sec}^{-3}\text{)}.$$

Here d is the inlet hydraulic diameter. It is recommended that turbulence boundary conditions should be specified in terms of the turbulence intensity, α and hydraulic diameter, d. A good general turbulence intensity value might be 5-10%, i.e. α=0.05-0.1. However sensitivity studies over a range of inlet boundary condition α values should be considered. In general terms the k-ε turbulence model has produced adequate results for many applications, however for some specific cases other turbulence models may be required, such as the Reynolds Stress Model (RSM) for orifice flows where the thickness-to-diameter aspect ratio is in the region of 0.5 [4, 5]. In this particular case inappropriate choice of turbulence model lead to a discrepancy with measurement of around 12% in orifice discharge coefficient despite having a mesh independent solution. Use of the RSM instead reduced the discrepancy to around 3%.

One important factor is that on a suitable grid the turbulent profile should not develop significantly along some inlet region. Such development would suggest that inappropriate initial turbulence boundary conditions had been chosen. As a consequence, an alternative approach to deal with k-ε turbulence modelling is to ensure that the velocity profile has the appropriate form as it reaches the regions of interest. This could be done (in a short inlet duct region) by using an inlet boundary condition with a (fixed) velocity α-profile for fully developed flow. Alternatively the flow could be given a long inlet region (up to 40 pipe diameters) so that the velocity profile and turbulence intensity α can develop to their correct values.

In the case of fully developed flow, the desired situation is that when approaching the regions of interest, the k and ε of the flow, being at its fully developed value, should be constant. This can be checked by plotting k and ε along some appropriate axis central to the flow.

y^+ Values

When using a turbulence model, the near wall region of the boundary layers can be simulated using wall functions. The wall functions are correlations which are valid for the range $30 \leq y^+ \leq 300$ (in the absence of pressure gradients), where y^+ is a Reynolds number with a length-scale based on the dimensions of the cell next to the wall (Figure 3.1). However if the pertinent parameters for the solution are demonstrated to be insensitive to the range of y^+ obtained this is also acceptable, as it demonstrates that boundary layers are being adequately simulated for the problem in hand (assuming that other modelling issues have been satisfactorily addressed).

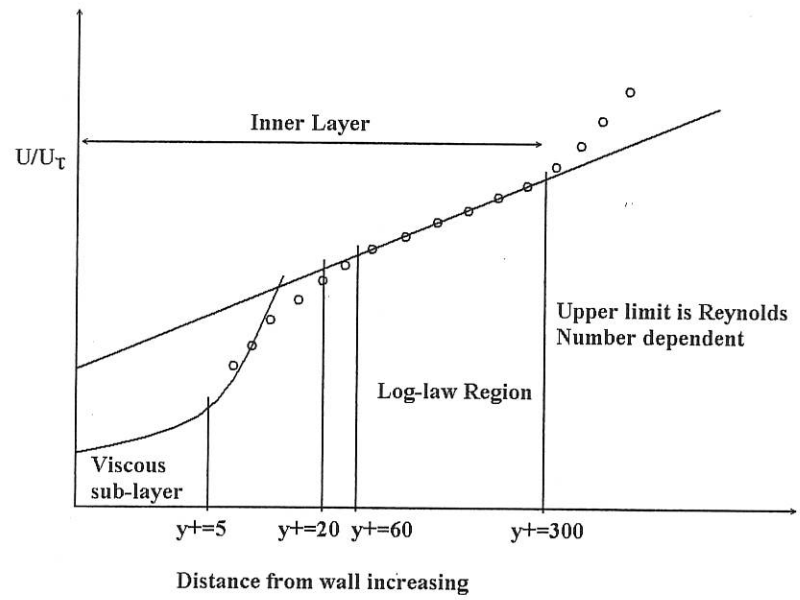

Figure 3.1: Velocity Distribution in turbulent pipe flow. Data points are indicative only.

An alternative to the wall function approach is to use near wall (so-called low Reynolds number) modelling, where the viscously affected region is resolved right down to the wall, including the laminar viscous sub-layer, one example of this is the two-layer model.

The wall units $y^*\equiv\rho C_\mu^{1/4}k_P^{1/2}y_P.\mu^{-1}$ and $y^+\equiv\rho u_\tau y_P.\mu^{-1}$ are defined following [2]. The wall functions are defined in terms of y^*, however both y^* and y^+ have comparable values when the first cell adjacent to the wall is placed in the wall log-layer. In circumstances where the k-ε two-layer model is selected, wall spacing should be based on y^+ rather than y^*. For further details see [2] and [3].

3.7.4 Compressible or Incompressible Flow Models

Various choices can be made within a CFD code to determine whether flow will be incompressible or compressible. Incompressible flows (density a function of temperature only) will generally reach a converged solution more reliably and quickly than the other options. The compressible flow of air is simulated by using the ideal gas law with a compressible option enabled, to determine the density as a function of pressure and temperature.

For isothermal flows an incompressible solution may often prove a good initial guess for a fully-compressible solution. A compressible analysis is required for flows where the non-dimensional dynamic pressure

$$q \equiv \frac{P-p}{\frac{1}{2}\rho u^2} = \frac{2}{\gamma M^2}\left[\left(1+\frac{\gamma-1}{2}M^2\right)^{\frac{\gamma}{\gamma-1}} - 1\right] \tag{3.1}$$

differs from unity by an amount that would cause the whole solution to be in error by more than the accuracy required for the analysis under consideration. In other words, if the overall analysis requires an accuracy of 5% (say), then one would require that $q < 1.05$ at most. However, as there will be other sources of uncertainty in the analysis, and as several of the sources of error may be cumulative, it would be wise to require an error due to compressibility effects of, say, half of that for the overall analysis, in this case 2.5%, i.e. $q < 1.025$. Thus the Mach number limit will be given by the value of M for q=1.025 in equation (3.1). An approximate solution to (3.1) can be found for

$$M < \sqrt{\frac{2}{\gamma - 1}},$$

(so that if $\gamma = 1.4$, $M < \sqrt{5}$), in which case (3.1) can be expanded using the binomial theorem to give

$$q = 1 + \frac{M^2}{4} + \left(\frac{2-\gamma}{24}\right)M^4 + \frac{(2-\gamma)(3-2\gamma)}{142}M^6 + \ldots$$

If $\gamma = 1.4$, this reduces to

$$q = 1 + \frac{M^2}{4} + \frac{M^4}{40} + \frac{M^6}{1600} + \ldots,$$

giving a limit on the maximum acceptable Mach number of 0.3 for air. Thus a compressible analysis will usually be required for flows with a Mach number of 0.3 or greater.

By way of example, consider the case of the flow of air through a duct with a small circular outlet orifice in the side-wall [8]. With a duct Mach number of 0.25, locally occurring Mach numbers in the side-wall orifice of around 0.8 gave rise to significant discrepancies between incompressible flow simulations and measurements. Under practical conditions, these discrepancies amounted to around 21-22% in pressure-difference ratios and 3-4% in cross-flow discharge coefficients.

In the special case of axisymmetric flows in rotating cavities incompressible analyses can often be used for swirl velocity component Mach numbers greater than 0.3, because the analyst will often not be concerned with azimuthal pressure gradients.

3.7.5 Rotating Boundaries

Flows in cavities with rotating walls require some special considerations. One elementary (but confusing) point that is often omitted is to state whether results are presented in a stationary or rotating frame of reference. Clearly if all the walls of a system are uniformly rotating it makes sense to present the analysis in a frame of reference which rotates with the walls. As such a rotating frame is non-inertial this will cause the appearance of two fictitious forces, the Centrifugal and Coriolis forces.

High rotation can also give rise to different forms of viscous boundary layers, notably thin Ekman boundary layers on surfaces perpendicular to the axis of rotation and thicker Stewartson boundary layers on surfaces parallel to the rotation axis. Flows that are highly influenced by rotation often tend to hug the boundaries of a cavity, rather than crossing the interior. If further information on the effects of rotation on fluid flows is required, see any of a range of textbooks, including for example Batchelor [9] and Tritton [10]. The Ekman boundary layer thickness is given by $\delta_{Ek}=(\nu/\Omega)^{1/2}$ for laminar flows, and $\delta_{Ek}=0.525.r.\mathrm{Re}^{-0.2}$ in turbulent flow.

Additionally rotating systems may often have boundary conditions that are symmetric about the rotation axis. Despite the fact that the geometry can be represented as two-dimensional axisymmetric, the analyst should determine whether the resulting flow field is likely to be axisymmetric or three-dimensional, as it is a feature of rotating flows (particularly buoyant rotating flows) that steady two-dimensional boundary conditions often give rise to unsteady three-dimensional solutions.

3.8 Boundary Conditions

Great care must be exercised over the choice of boundary conditions used as only certain combinations of inlet and outlet boundary conditions will lead to convergence and/or physically acceptable solutions (code manuals should be consulted for details).

Once a legitimate set of boundary conditions has been chosen there still remains the danger of local in-flow at an out-flow (zero gradient) boundary, which is generally unacceptable. This problem may be because a region of recirculation is required close to the out-flow. In this case the problem can often be overcome by a combination of extending the out-flow duct to give space for the recirculation to form inside the simulated domain, and increasing the mesh density in the region of the recirculation, to allow better flow resolution. The first case may move the out-flow away from the recirculation, the second may move the edge of the recirculation away from the out-flow.

Rough surfaces, even when surface deformities do not penetrate the boundary layer, will affect the boundary layer thickness resulting in changes to heat and mass transfer. Often this can be represented by using a wall roughness height and roughness constant (which describes the roughness distribution).

The nature of the boundary conditions is also important when considering whether to construct a model in two or three-dimensions. It must be appreciated that two-dimensional boundary conditions can give rise to three-dimensional flows, and that axially-symmetric boundary conditions can cause non-axially-symmetric flows. In particular this can be a feature of buoyant rotating flows.

Care should be taken in selecting boundary conditions, as it is computationally expensive and time-consuming to execute runs with incorrect boundary conditions. Remember that 'rubbish in = rubbish out'.

3.9 Grid Considerations

Testing for the grid independence of the solution is really just another form of sensitivity study, however it is of such importance that it merits special mention. Many meshing problems can be avoided by careful choice of simulation geometry. In general terms quadrilateral or hexahedral cells are to be preferred over triangular or tetrahedral cells for meshing geometry. Hybrid meshing (mixing quadratic and triangular cells in 2d, or hexahedral or prismatic and tetrahedral cells in 3d) can be considered for more complex geometries.

3.9.1 Definition of Geometry

Three main points, which should be considered when defining the geometry to be meshed, are:

1. Geometric complexity can lead to a distorted mesh. This hampers convergence and undermines the quality of the solution. It may be necessary to simplify the geometry to improve the mesh, or use an alternative meshing strategy.
2. Any geometric simplification runs the risk of altering the flow pattern. If there is any doubt, expert advice should be sought on what simplification would be acceptable. One approach would be to run the case both with and without the simplification, perhaps on representative geometries to assess the effect on the flow.

3. Geometric accuracy enhances the credibility of an analysis, particularly to non-specialists.

Discrete holes in a three-dimensional geometry can only be modelled as a slot in two-dimensions. The size of the slot should match the area of the holes it replaces so that the same mass flow and velocities will be achieved as would have been through the holes. This approach is only acceptable if it can be shown that the real flow is not 3d. A characteristic of 3d flows is that a two-dimensional projection of the flow would cause crossing streaklines.

Other factors that should be borne in mind include:

1. The grid spacing of the mesh needs to be fine enough to resolve the features of the flow. This may involve a second attempt to mesh the problem. In certain cases, the only way of knowing whether one has captured all the flow features may be to increase the grid resolution over the entire mesh. If there is no change to the flow this is a fair indication that all the main features have been simulated (see also 'capturing all the flow features' and 'sensitivity studies'). However it must be appreciated that at times very considerable refinement will be required to capture certain flow features, it is for this reason that validation of any CFD model is extremely important, to allow the analyst to anticipate flow features.
2. The chosen mesh should avoid large variations in grid expansion between adjacent cells, as this will reduce the numerical accuracy of the solution. In the resulting mesh, if one proceeds along an arbitrary chosen direction the number of cells per unit length should only change by a factor of between 0.7 and 1.3 between adjacent cells. This advice raises a concern about automatic adaption capabilities within CFD codes, which often result in grid expansions of 2 between adjacent cells. In this case it is hoped that the benefits of refinement will more than offset the reduction in the numerical accuracy of the solution.
3. Long thin elements should be avoided and an aspect ratio of less than 5:1 is recommended where possible. However, in boundary layers long thin elements are acceptable.

4. Cells with a high degree of skewness (>45°) should be avoided.
5. Care should be taken with the size of elements adjacent to wall because of the likely importance of boundary layers. In the case of turbulent flows the cells should have the correct range of y^+ values if wall functions are being used. For other kinds of boundary layers the user needs to ensure that there are sufficient cells within a boundary layer thickness of the wall for the layer to be adequately represented (see section 3.9.3).
6. If it is not possible to coarsen a mesh beyond its original definition (as the original mesh defines the geometry), initial meshes should be made coarser than required, rather than too fine. Another benefit of this approach is that initial problems with the model set-up can be dealt with on a model that converges relatively quickly, saving computing time.
7. The arrangement of the mesh may influence the flow obtained. An example is where a topologically square mesh is used to simulate a circular pipe. The resulting isobars may incorrectly have a deformed square cross-section, rather than being circular. In other circumstances it is possible that a mesh may channel flow so that it follows the mesh.
8. Sharp edges in geometry can lead to unphysically high heat transfer coefficients. In reality the edges in a physical geometry are unlikely to be as sharp as those represented in a computer-generated geometry. In this case it may be necessary to slightly round edges in the simulated geometry.

3.9.2 Capturing all the Flow Features

Of particular importance is the danger that a given mesh may fail to capture a feature at all. If this is the case then no amount of solution adapted local mesh refinement (i.e. mesh refinement based on the solution already obtained) is likely to be of any benefit, as it will only be by chance that additional elements are placed in regions that allow the resolution of the feature in question.

For this reason global doubling of the entire mesh is to be preferred whenever possible to any form of local adaption based on a previous coarse mesh solution.

There is however an exception to this, namely refining the mesh in a particular region because the analyst knows, from consideration of the physics, or for other reasons, that a flow feature is expected there which has not been resolved.

3.9.3 Minimum Grid Requirements for Turbulence Modelling

For most applications turbulence modelling using wall functions is quite adequate. On occasions when two-layer modelling is required (e.g. low Re flows near the turbulent transition), then turbulence modelling tends to have its own additional meshing requirements. These include the need for wall $y^+ \approx 1$.

For a natural convection boundary layer (as illustrated in Figure 3.2a) the flow will generally go from a low interior velocity to a maximum in the boundary layer before returning to zero at the wall. This will probably require about 10 mesh points (i.e. about five points on each side of the maximum - note that the maximum will be much nearer the wall than the quiescent fluid core). For a flow boundary layer (Figure 3.2b), which goes from a maximum velocity in the fluid interior to zero at the wall, probably only about five points will be required.

In the case of the k-ε turbulence model using wall-functions the problem is dealt with for the flow boundary-layer (Figure 3.2b) by ensuring that the grid results in a suitable range of y^+ values. The natural convection type of boundary layer (Figure 3.2a) will require more careful meshing.

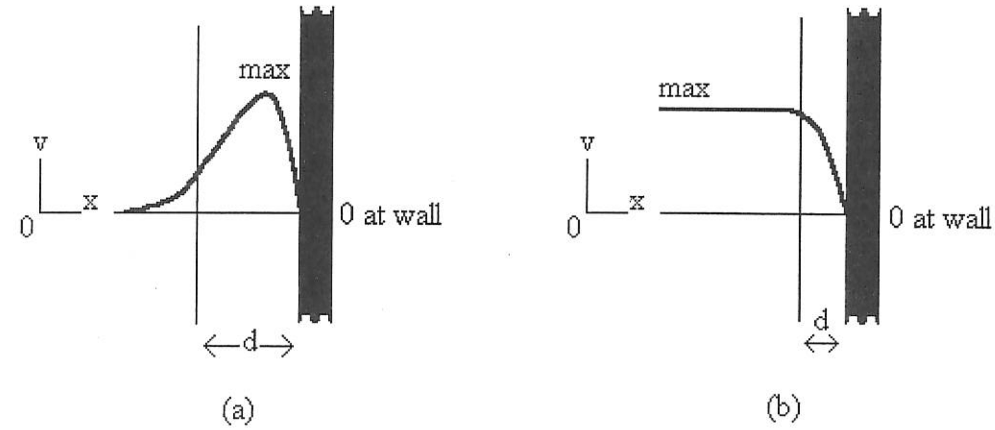

Figure 3.2: Illustration of boundary layers (a) natural convection boundary layers, (b) flow boundary layer.

3.9.4 Grid Sensitivity Studies

The only way that errors caused by the coarseness of a grid can be eliminated is by carrying out a grid sensitivity study. Usually this would be a matter of successive refinements to the grid until the key features of the results do not change. A systematic search for grid-independent results forms an essential part of all high-quality CFD studies [3].

If it is not possible to demonstrate that a given solution is grid independent, it is at least always possible to give an indication of the effect that changes to the grid have on the solution. In other words to see what effect coarsening the grid has on the solution. Thus it is *not acceptable* to argue that grid independence studies were not carried out because resources did not permit the grid refinement. If computational resources do not permit the refinement of a grid, it is always possible to coarsen the mesh. This should at least give an indication of the degree to which the solution is grid dependent.

Thus grid sensitivity studies should be used to show that either (preferably) the solution is grid independent, or (at least) how much the solution changes by if the mesh is refined. This is easy to imagine in the case of mesh doubling, where if you have a base case solution A and then double the mesh and achieve solution B, the results of solution B could be quoted as accurate to the difference between the two solutions. However the concerns about the amount of refinement required to capture flow features mentioned in section 3.9.1 ('other factors', number 1) must also be considered.

If mesh doubling is not possible (perhaps because of machine space limitations) this process becomes conceptually more difficult as local refinement may be the only option. In this case the approach illustrated below may be useful. If, for example, you require a solution accurate to ±5%, you might carry out a series of *local* refinements and find that your new solution differs from the original by 0.5%. In this case you would feel reasonably confident that you probably had a solution that was mesh independent to within the required limits. The key ideas here are:

- The degree of local mesh refinement needs to be enough to stand a reasonable chance of making a difference. Adding only a few cells when doing this test is unlikely to be sufficient.
- Only a small change in the solution is expected, because only a small change was made to the mesh (it was only refined locally). Hence to be acceptable the change in the solution should probably be significantly less than the accuracy required.

If refinement on this basis is required, it should only be carried out under expert supervision.

3.9.5 Problems with Mesh Adaption

Some CFD codes provide a capability to locally refine the mesh based on parameter values obtained by a previous solution, known as mesh adaption. This capability offers the prospect of reducing errors due to inadequate meshing whilst potentially reducing the total number of cells that would be required if refinement was carried out by some other means such as doubling the entire mesh. Local adaption comprises doubling the mesh in the chosen areas, leading to discontinuities in the mesh density. In the case of quadrilateral cells the mesh can only be adapted by leaving 'hanging nodes' (where a new node is created which lies on one of the faces of an already existing cell). Local mesh doubling means that proceeding along some chosen direction the number of cells per unit length increases by a factor of two at the boundary of the chosen area giving a discontinuity in cell density.

For triangular cells 'conformal' adaption is also possible, where new elements have their vertices at previously existing nodes. In this case the meshing density ratio between an unadapted and an adapted region may not be as large as for a quadrilateral mesh as the new elements can be smoothed out into the surrounding mesh.

Good practice suggests that between adjacent cells the mesh density ratio should be kept as small as possible, say to a ratio of about 1.3:1, and certainly less than the 2:1 ratio caused by mesh doubling [11]. Rigid application of this rule would prohibit local adaption using a quadrilateral mesh, however when such an approach is used, it is hoped that successive refinements are such as to render the errors caused insignificant.

Because of these concerns global mesh doubling (or halving) is the preferred route for mesh sensitivity studies, although it is accepted that this may not always be practical. However this route, when possible, may prove more economical of effort than successive local mesh adaptions.

4 MODEL VALIDATION

CFD does not provide a substitute for experimentation, it is a powerful additional tool. To give confidence in any solution validation should be carried out by comparison with experimental data of similar scope. This will allow the level of accuracy available from a given CFD code to be assessed. At a quantitative level this is an important area of CFD research that seems to have been badly neglected in practice.

If the appropriate experimental data is not available then the CFD user will have to rely on

- previous experience,
- comparisons with analytical solutions of similar, but simpler flows, and,
- comparisons with data from related problems reported in the literature.

5 DISCUSSION & CHECKLIST

It is not possible to provide a set of guidelines, which, if followed, will guarantee a perfect CFD analysis every time. The most that can be achieved is that a number of pitfalls may be avoided, and hopefully, by following guidelines better analyses will be carried out than otherwise would have been the case, at a certain minimum level of quality.

The following section gives a checklist, which consists of reminders of the important factors to be considered at each stage. If the reader intends to use the checklist they should then turn back to sections 3 or 4 for more detailed advice. Thus for example the entry 'Code Execution - check physics as solution is developing' is to be taken as a pointer to section 3.6, where a list of suitable checks is given.

5.1 Checklist for CFD Analysis

Inexperienced CFD analysts should work under the guidance of experienced staff. In the following list, section numbers for cross-reference are given in parentheses after the entry.

<u>Defining the problem</u>

- Objectives of the analysis - insight not numbers (3.1)

- Accuracy required (3.2)
- Uncertainties in data (3.3)
- Physics of the flow (3.6)
- Choice of models (2.1.1, 3.7)
- Boundary conditions (2.1.3, 3.8)

Building the mesh

- Definition of geometry (3.9.1)
- Capturing flow features (3.9.2)
- Grid requirements for turbulence modelling (2.1.4, 3.7.3, 3.9, 3.9.3)
- Grid requirements for boundary layers (2.1.4, 3.9)

Code execution

- Attainment of convergence (2.1.2, 3.4)
- How do you know the solution is not stalled? (3.4)
- Check physics as solution is developing (2.1.5, 3.6)

Post-execution analysis

- Sensitivity studies - are additional runs required? (2.1.5, 3.5)
- Grid sensitivity studies (or is the solution mesh independent?) - more additional runs? Resolution of boundary layers? (3.9.4)
- Uncertainty in results (3.5)
- Validation against other data (4)
- Checks against the physics of the flow (3.6)

Reporting of Results

- Purpose of the analysis (3.1)

Remember the objective is to produce a mutually self-supporting set of CFD solutions that give confidence in the overall conclusions reached.

6 CONCLUSIONS

1. Guidelines to ensure best working practice in CFD analyses are given.
2. The main difficulties facing the analyst are reviewed, as well as tools to address particular problems.
3. A checklist is given to help ensure best practice is followed appears in section 5.1.

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