Computations of turbulent flows for industrial and environmental applications

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Prof. dr. J.C.R. Hunt, FRS

TU Delft

Faculty of Design, Engineering and Production
Laboratory for Aero- and Hydrodynamics

Delft University of Technology
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Introductie

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Op 3 Mei 2000 door

Prof.dr. J.C.R. Hunt, FRS
Mijnheer de Rector Magnificus,
Leden van het College van Bestuur,
Collegae hoogleraren en docenten,
Andere leden van de universitaire gemeenschap,
Zeer gewaardeerde toehoorders,
Dames en Heren.

"Rector Magnificus, members of the board of governors,
Fellow professors and other members of the university community
Esteemed listeners
Ladies and gentlemen"
1 THE IMPORTANCE OF FLUID FLOWS AND THE GROWTH OF CFD

The main aims of sustainable economic development are to improve living standards, secure people's health and safety and expand people's capabilities and horizons, especially through education, travel and communications. For the development to be sustainable, it is also essential to preserve and enhance the environment. These aims can only be achieved by the widespread and deep application of science and technology and advances in the practice of engineering and medicine, as well as by the more widely recognized practice of economics, management and effective politics. Fluid mechanics, with its adjacent sciences of thermodynamics and chemistry, is a striking example of a field of science and technology that is making valuable contributions to economic and social development and the solution of environmental problems. The theme of this lecture is to show how its contributions are spreading more widely and becoming more valuable and creative by the use of appropriate computational methods.

The main reasons why fluid flows are important in industry, technology and the environment are that:

(a) in the manipulation of materials most processes partly or wholly involve fluids, for example metallurgy, food manufacture, chemicals, etc., and
(b) these activities generally involve the utilization of natural fluids in the atmosphere, ocean, rivers and ground water, for example for transport (ships, aircraft), combustion (which of course relies on air), dispersion of pollutants, wind and wave energy, and for cooling buildings.

An extensive review of the role of industrial and environmental applications of fluid mechanics was written by Hunt (1).

How important is it to apply the latest research to these fluid flow problems? Would standard methods not be sufficient? The answer is that the considerable resources put into research and development studies of fluid motion, together with those in other technologies (notably materials and computers), have been effective in improving products and in helping to create new markets. There have been notable technological breakthroughs:

1. In material processing, new extremely strong composite materials are made as a result of mixing liquid metals or the use of metallic sprays.
2. Engines of ships, planes and vehicles have more than doubled their fuel efficiencies and, in the case of space vehicles, the engines have become significantly more reliable.
3. The fluid dynamic drag of aircraft, trucks and ships have been reduced by factors of three or more by careful design (and new lighter materials).
4. The aerodynamic noise of aircraft and cars has likewise been reduced.
5. Weather forecasts for five days are now practical using the largest computers, running currently at about 10^7 flops.
6. New bioengineering fluid flow devices have been produced for saving, prolonging and enhancing human life.

Even in industries where the design and the technology of fluid flow systems have changed little over the past 10 years there have also been considerable economic and environmental benefits simply from the wider understanding of fluid flow processes, the wider use of computational models and the faster and more reliable design of fluid flow systems; for example, in the design of mechanical pumps, filters (see Fig. 1) and mixers, and in engineering and aeronautical engineering, less time is now spent on experimental testing or wind tunnel tests. Indeed, some commercial aircraft have been designed using only computational methods. In environmental studies calculations can now reliably be made of pollution levels from proposed industrial/urban developments to within a required accuracy. As computers become faster, the computational fluid dynamics (CFD) have arisen from the development of basic understanding and modelling of fluid mechanical phenomena, especially turbulence, two-phase flows (for example gas-liquid mixtures), combustion and chemically reacting flows, and then their simulation in practical computational schemes. The improvements in numerical methods have been a vital part of this progress. The term CFD is used here in a more general and futuristic way, to include all practical computational methods and turbulent flows, which also extend to the large eddies simulation methods codes for turbulence spectra etc.

Since the main practical applications of CFD are in assisting the competitive provision of goods and services, those practising, managing or commissioning CFD need to understand the capabilities and limitations of different methods. They should also know about what progress in practical CFD is expected in the next few years on the basis of current research work.

They should probably ask some of the following questions. What kinds of complex flow involving mixtures of fluids with different compositions will it be possible to simulate, and with what accuracy? Will one single type of code be suitable for all applications? Will improved computational techniques and new techniques
for measuring and contrasting flows lead to quite new technological possibilities? How is Europe addressing this challenge?

This lecture has benefited from reviews by Rodi (2), Ulmert (3) and Holmes et al (4) from practitioners of CFD and the conclusions drawn from recent meetings on turbulence fluid (5), Nieuwoldi (6). There seems to be a good degree of consensus, which I have attempted to reflect in this lecture. I have also aimed to use as little mathematics as possible?

2 MODELLING TURBULENT FLOWS

2.1 Current ideas about turbulence

The first question to ask about a flow is about the fluid or fluids involved, for example whether it simply involves a single liquid or gas, or a mixture, and whether thermodynamic or chemical processes are involved. Assuming there is a single homogeneous fluid moving at speeds much lower than the speed of sound (compressibility and other complex fluids and processes will be touched on later), one should then ask whether the flow is dominated by inertial or by viscous forces, or, in engineering terms, whether it is an aerodynamics flow or more like a lubrication type of flow.

To answer this question we need to know the value of the Reynolds number, Re, in the particular flow in question (Fig. 2a). This dimensionless quantity is defined by the formula

\[ Re = \frac{U L}{\nu} \]

in terms of two quantities of the flow itself, an average velocity U, and an 'average' distance, or length scale, L, over which the velocity changes (for example the width of a jet or a pipe), and in terms of a relevant property of the fluid (which is approximately independent of the flow), namely the kinematic viscosity \( \nu \) (equal to the ratio of the viscosity to the density). The magnitude of Re in engineering flows varies from 10^3 in some lubrication problems, to 10^5 in typical power hydraulics, to 10^6 for air flow round an aircraft or ship (see reference [7]).

However, as the Reynolds number increases, the nature of these flows changes so much that quite different approaches to their computation are necessary. The first most characteristic change is that of the smallest distances over which the velocity changes decrease (because the gradients in velocity increase as the relative effect of viscous stresses decreases), so that more detailed (and therefore more computationally expensive) calculations are necessary for a flow over which temperature at the front of a turbine blade decreases in the order of \( (Re)^{-1/8} \) or typically one-hundredth of the thickness of the blade in operating conditions. The second characteristic change as Re increases is that the flow becomes unstable in the sense that the flow pattern changes and fluctuates. With further increases in Re, these perturbed motions themselves become unstable so that the velocity becomes progressively more chaotic, in the sense that it is unpredictable in both its variation and over time. For high enough, but finite, values of Re, this process is continuously repeating, leading to fully developed turbulence in some part of the flow, for example along an aircraft wing or, possibly, everywhere, as, for example, in a stirred tank.

The flows in which this turbulence occurs are generally shear flows, such as jets, wakes, pipe flows, shearing flows between boundaries, etc., because they persist for long enough for the initial instabilities to build up into turbulence as they travel downstream. The critical Reynolds number Re_c for jet, is quite low in free-shear flows where there is no boundary to suppress the fluctuations (for example Re_c = 10 (to within a factor of three) for jets and wakes), while in flows near rigid boundaries Re_c is much greater (for example Re_c = 100 for boundary layers and pipe/channel flows). When the Reynolds number is increased above its critical value, the nature of the turbulence changes; most notably, in any other kind of motion, the length decreases over which the smallest scale variations occur, which in this case corresponds to the sizes of the smallest eddies.

What is a turbulent flow? It consists of a large set of eddy motions, which are vortices, which are only loosely correlated with each other and which range in size from those comparable to the mean flow itself, for example the width of the jet, to those at the smallest scales (as explained above). This ratio of sizes might be about 10 when \( Re = 10^4 \) (for example in an engineering pipe flow) and rise to 10^5 or 10^6 for jet exhausts or atmospheric flows. Also the larger eddies persist for a substantial time as they are carried along the flow (for example for more than 10 diameters along a pipe), whereas those on the smallest scale are distorted and evolve quite rapidly. Even though there are luminous flows that are not steady and may even have example rising bubbles in oil, turbulence usually poses serious engineering problems, and also creative possibilities, by changing the nature of the flow to one that is unsteady and random on a wide range of scales and frequencies.

Lewis Fry Richardson in 1922 described the essence of the dynamical interaction between these eddies in his famous parody of Swift's rhyme on flow:

Great whirls have little whirls
That feed on their velocity
And little whirls have lesser whirls
And so on to viscosity
(in the molecular sense).

Engineers need to understand the features of turbulent motion and allow for it in their calculations; but only to the extent that it has a significant effect for their particular problem. In some flows, or in particular local regions of a complex flow, the turbulence is merely a small disturbance on the mean motion—a kind of molecular motion, and has little engineering impact. However, this is not generally the case even though turbulent fluctuations (whose r.m.s. value is denoted by \( \alpha \)) are usually small compared to the mean velocity \( \bar{U} \), which is usually defined as the velocity averaged over time in a steady engineering process or over many cycles in an unsteady process such as an engine. In typical engineering flows, the r.m.s. magnitudes of the fluctuations \( \bar{u} \) are about 15 per cent of \( \bar{U} \), although they sometimes rise to about 40 per cent in flows behind buildings, or other bluff obstacles. The reason for weak turbulence having a significant effect is that along the length of the flow or over its duration, just like the much smaller stresses caused by molecular viscosity, the effective Reynolds stresses caused by the fluctuations change the mean flow, and hence determine the critical engineering parameters, such as pressure drop or surface drag. Because the size of turbulent eddies are so much larger, of the order of \( L \), than those of molecular motion (in a gas the mean free path - 1 \( \mu m \)), the turbulence always significantly increases the rate of heat transfer, mixing, etc.

Practical methods of calculating these changes, from Boussinesq (8) onwards, have usually been based on drawing an analogy between the motions of eddies and of molecules in a gas (for example that eddying simply leads to a larger value of viscosity or of thermal diffusivity). From the pioneering atmospheric and laboratory studies of Taylor (9) and Prandtl (10) it was clear that this approach could only be applied to a limited range of flows. Moreover, even in the last twenty-five years that measurements and direct simulations of turbulent flows have been detailed enough to enable students of turbulence to specify these limitations and, where it is relevant, to propose new concepts and better practical models.

The new ideas and the types of models used can best be understood from the answers to the two basic questions:

1. Is turbulence a universal state of nature, with general laws of behaviour or equations of state governing its statistics, similar to those of the behaviour of gas molecules?

2. If not, can turbulent flow be classified into different types or subclasses, for example distinguishing flows (such as flows impinging on an obstacle) or shear flows (in a pipe, jet, etc.)? In that case each flow of a given type should have certain similarities, whether in their statistical descriptions (or equations governing the variations of these statistics) or in the form of the eddy motions.

The answer to the first question might have been qualified 'yes' forty years ago; for example, Landau and Lifshitz (11) stated that turbulent flows tend to some general state in certain ideal conditions. However, current fundamental and applied research in turbulence has shown that in quantitative terms the answer is 'no'; even though all well-developed turbulent flows have certain qualitative statistical and physical properties (5). Notably these are:

(a) three-dimensional random motion on many length scales (for reference future let these three velocity components have root mean square values \( u', v', w' \) and let the specific kinetic energy be \( E = \frac{1}{2} \rho \bar{U}^2 \), such that \( u' = n^{-1} u', v' = n^{-1} v', w' = n^{-1} w' \); (b) the energy spectrum \( E(k) \), of different sizes of eddy \( - k \), has a single maximum, corresponding to the dominant eddy motion with length scale \( L \) (see Fig. 2b); (c) the eddy diffusivity \( D_e \), which defines the diffusion of heat or matter, is finite and of the order of \( \nu L \). The reason why the answer is 'no' is because these statistical properties can differ significantly between flows; notably there are differences in the values of the ratios of different r.m.s. components \( u'/w' \) and in the forms of the spectrum \( E(k) \) (these affect the relationship between the rate of viscous dissipation per unit mass \( \nu \) and \( L \), as defined by the ratio \( \varepsilon = u'^3/L \) and between \( u \), \( L \) and the turbulent diffusivity \( D_e \)).

The reason why these statistical properties and differential equations of turbulence models vary between different types of turbulent flow is essentially because turbulent eddies are large and not like gas molecules; firstly, because of their size, the eddies scales tend to be comparable with those of the mean flow scales \( L \). and, secondly, because they have a significant memory—or correlation time scale \( T \), which is determined by how
long it takes for large eddies of scale $l_x$ and velocity $u$, to interact with each other, it is found experimentally that $T_r \sim L/u$. In unconfined flows such as jets or wakes, $L$ increases and $u$ decreases along the length of the turbulent flow and therefore the memory time $T_r$ increases. In fact, it increases at the same rate as the time $T$ for an eddy to travel along the flow, that is $T_r \sim T$. Therefore, the statistics of the larger energetic turbulent eddies are always partly dependent on how the turbulence is initiated.

On the other hand, if the turbulence is confined, for example in a pipe, the statistics of the flow reach a steady state, so that $L$, and $u$, do not vary along the flow. Then $T_r$ is much less than $T$, and the initial state of the turbulence is forgotten. \( 12 \) However, in this case the same eddies are limited by the size and shape of the pipe and therefore cannot be universal. Thus, other because of its growing memory in unconfined flows or because of its distortion by particular boundaries. The large-scale turbulence cannot have a completely general form. Note that, although the current answer to the first question is no, it does not contradict Kolmogorov's \( 13 \) hypothesis that certain aspects of the small scales of turbulence have a universal structure-a result that is of great practical value for models of chemical mixing and the propagation of waves through turbulence (see the reviews in \( 14,5 \)).

If turbulence does not reach a universal state by internal random motion, why should one expect, even in a particular type of flow, any features in the large scale eddy motions to be the same or to be modelled by similar methods in different flows. As shown in Fig. 3, based on laboratory flow visualization studies and direct numerical simulations, the answer is that characteristic large-scale eddies or coherent structures-often called in a distinct way in different types of flow, such as those affected with mean shear (that is where $\xi(L) \neq 0 \( 15 \)), with curvature in the mean streamlines, with rigid boundaries, or those affected by unstable or unsteady buoyancy forces \( 12 \). In each case it is found that the form of the eddies is broadly the same irrespective of how the turbulence is initiated or how it enters the flow region being considered.

In other words, there is a tendency towards self-organization rather than statistical equilibrium.

In the case of shear flows the eddies are elongated vortices sloping in the direction of the shear, which in curved flows are parallel to the mean motion. It is therefore natural, as well as being theoretically justified \( 10 \), to expect that certain turbulence statistics, or the approximate turbulence model equations used for their derivation, are similar for all flows within each of these types.

### 2.2 Turbulence mechanisms that need to be 'modelled'

Having noted the need to estimate certain basic statistics of turbulence in order to calculate the practically important aspects of engineering flows one should go on to review the parts of the CFD models that provide these statistics. Use is made of the fact that turbulence has particular features in different types of flow to describe the key mechanisms that determine how the turbulence statistics vary in these flows (see Fig. 4).

#### 2.2.1 Production

Where there are variations of the mean large-scale flow (with mean shear/stretch components such as $\partial^2 u$ or $\partial^2 v$, each of the vortices in the eddies are stretched or compressed, leading to an increase in the variance of some velocity components (for example the transverse component $v^2$ in an accelerating flow, where $\partial^2 v$ is negative) and a decrease in others, at a rate proportional to this variance and to the mean strain (for example $-\partial^2 H(u)$). There are obvious analogues to the increase in the energy of elastic solids under strain. In most engineering flows the largest rate of strain is caused by mean shear $\partial^2 u$, where the eddies are stretched and rotated. The net effect is an increase in all the turbulence components, $u^2$, $v^2$, $w^2$.

#### 2.2.2 Dissipation

As turbulent eddies interact they may merge, leading to larger eddies, and hence an increasing 'memory time' $T_r$, but they also tear and distort each other so as to generate a cascade of energy to smaller scales which, as explained already, determines the rate of dissipation by viscous stresses \( 16 \) viscosity. This is why the rate of dissipation $\epsilon$ can be modelled in terms of the large-scale turbulence and of variations in the mean flow that strain it, without needing to model the details of the small scales. However understanding these unsteady motions involving the life cycle of small scale eddies \( 16 \) is necessary to estimate mixing, chemical reactions and two phase flow processes.

The rate of dissipation $\epsilon$ is of the order of the ratio of $u^2$ to the length scale $L$, but the numerical factor varies (typically by a factor of two) between different types of flow. When turbulence is in a state of 'local equilibrium' the rates of production and dissipation are in balance, as occurs in turbulent boundary layers near a rigid surface.

#### 2.2.3 'Diffusion' of turbulence

Intense eddy motion in one region of the flow diffuses outwards into other regions of the flow as a result of the self-induced motions of the vortices and their mutual interactions. This is why the thickness of wakes and jets increases along their axis. At the same time there is a mixing between fluid that is turbulent and the external fluid that may have a different temperature or concentration, which is not turbulent. This takes place at the randomly moving but very thin interface between rotational dissipative motions on one side and irrotational velocity fluctuations on the other. Most mixing occurs where the interface rolls up and engulfs the external flow. The result of these random motions is a net transport of turbulent energy outwards at a mean boundary velocity $U_L$ of the order of $u_*$. This transport phenomenon is modelled as a diffusive process proportional to the mean gradient of $u_*$, except very close to the interface, this is a valid approximation near flow, for example at the outer edge of jets. But also in is not necessarily a good approximation for transport in flows that are far from equilibrium and with rapid variations in length scale, such as near bluff obstacles where there is a strong production of turbulence by straining motion.

#### 2.2.4 Action at a distance

In many practical flows there are adjacent regions where the mean flow and turbulence are quite different, for example when the wake of one row of turbine blades impinges on the boundary layers of a downstream blade or where a sideways jet enters a larger volume (Figs 4 and 1). The vortices, say with length $L$, in the adjacent regions of turbulence can directly induce eddy motions in the other region over a limited distance (of order $L$), i.e. this 'action at a distance' is generally reduced by the shielding action of strong shear. The spreading of these externally induced motions have to be considered carefully to be presented. To model these interactions tends to thicken the layer and change the profile (i) by causing a sharper gradient near the surface so as to increase the skin friction. By contrast external turbulence has little effect on the pressure fluctuations in a wake or below roughness elements \( 17 \). Understanding and modelling these mechanisms is proving to be one of the greatest challenges for CFD \( 22 \).

#### 2.2.5 Rate of change and advection of turbulent energy

When turbulence is not in a state of local equilibrium and the diffusion of turbulence is not balancing the difference between local production and local dissipation, it means that the turbulent energy locally is changing, either with time or spatially, as it is advected into or away from the local region by the mean flow. This occurs in turbulent wakes of obstacles and in most shear flows except very close to boundaries.

#### 2.2.6 The effects of rigid walls and gas-to-liquid surfaces

Since on any rigid surface the velocity is zero relative to the surface, the velocity fluctuations are zero. However, because of the large variations of velocity over small scales (associated with high Reynolds number flow), there are significant velocity fluctuations very close to the surface; indeed, the magnitude of the energy of the parallel component $u^2$ has its maximum value at a distance above a smooth surface of the order of 10$^2$ $L/R_e$ (less than 1 mm for a large gas pipe) where the viscous stresses are still significant. These rapid variations in mean velocity and in the turbulence are associated with similarly rapid variations in the rates of production and dissipation relative to their local maxima. As flow visualization shows, the intensity of these fluctuations is caused by local bursting instabilities of the eddy motion near the wall \( 23 \). When $Re$ is much greater than $10^5$, each eddy interacting with the surface produces its own internal layer in which the lengths of the vortical structures may extend over 10 boundary layer depths.

Despite the rapid variation in the form and scale of turbulent eddy motion in this region, because the local dynamics are dominant, the 'diffusive' effects are relatively less significant. Aspects of these motions have still to be understood, especially, for example, how large eddies do or do not affect, through 'action at a distance' shear shielding the fluctuating contribution to surface shear stress and how surface roughness elements change the turbulence around them. At a gas-liquid surface, the mechanisms are different, there are no rapid variations in the rates of production and dissipation because the mean shear $\partial^2 u$ is small. However, as also occurs near a rigid
surface, the distortion to the turbulence arises from the blocking effect acting on the larger scale motions, especially those normal to the surface.

2.2.7 Adjustment of anisotropy

There are usually significant differences in the strength of the three components of turbulence ($u'$, $v'$, $w'$) and in the length scales in the different directions. These may originate from the initial or upstream state of the turbulence or the anisotropic production in a steaming flow, or the blocking effect of the boundaries. In most flows, notably shear flows, pressure fluctuations tend to transfer energy from the most energetic to the least energetic components. However, because turbulent eddy motion is not like that of gas molecules, this is not a universal tendency, as vortex dynamics readily explains. Second-order models now reflect this non-universality (24).

3 REQUIREMENTS OF CFD CODE

3.1 Output and other types of requirement

Any practical method of calculation should be designed so that its output is compatible with data available and so that the method is appropriate for the user in terms of its operational convenience and availability of necessary resources (see Table 1). It is also necessary to define the flow domain or volume where the calculation is to be performed (see Fig. 2). This decision depends on other factors, such as knowing the flow entering the domain and the computational capacity available.

For many users of CFD codes the output required is information about the broad features of the mean flow pattern and quantitative estimates of the variables, such as mean flow-rate, pressure drop or heat transfer rates. This approach supplements or replaces the more traditional engineering approximate calculations based on non-dimensional coefficients, for drag or heat transfer, or those based on equivalent one-dimensional integral equations which cannot account for variations across the flow. Well-designed and user-friendly CFD codes enable the designer of engineering devices to examine the consequences of various designs on the fluid flow aspects of their performance. Figure 1 shows the results of simplified calculations of flow through a liquid filter with a central bubble plate. Showing how the flow changed as the location of the bubble plate changed led to a decision on the optimum design. Although only a basic level of output may be required (which is denoted as level 1), depending on the type of flow and the accuracy that is required, quite different levels of input data of complexity of the model are necessary (which are discussed below).

At the next level (2) in terms of improved output for practical flow calculations either the mean flow has to be considerably more accurate (for example the drag of a wing calculated to within 1% per cent) or basic statistical features of the turbulence are required (such as the intensity of turbulence and its broad effects on combustion and mixing).

To provide the third level (3) of output, calculations are required for more complex aspects of the turbulence, such as the variation in the spectrum of energy, (E(x)) which is necessary to calculate unsteady loads on structures or the production of noise, or the form of the eddy structures of turbulence (for example because of their influences on bubbles and particles, in two-phase flows (25) and on the efficiency of combustion devices).

3.2 Input

Having decided on the required level of output, the next step in planning the use of CFD is determining whether sufficient input data are available to perform the necessary calculations. Even this is not straightforwardly decided because it depends on the nature of the flow within the flow region to be calculated as it enters. In two common situations, the input is known; the first is where the entering flow is essentially non-turbulent (for example for an aircraft in flight) and the second occurs when the entering turbulence has a well-established form whose details are well known (for example flow from a straight pipe section entering a complex flow region (as in Fig. 1). More often, however, the input flow is only known rather approximately (as in Fig. 5). The practical reasons may be because of the lack of specification of other components in a design or because it may be difficult, or costly, to measure or possibly calculate it, such as the flow within the curved pipes entering an internal combustion engine. In these cases assumptions may have to be made using data for comparable flows.

For most calculations the input data are required at a comparable level of detail and accuracy as the output data. However, there are situations where it may be necessary to have the input data available in greater detail and at a higher level (for example the turbulence length scale) than is required for the output, simply because a higher level model has to be used to ensure the required degree of accuracy in the output (for example in the mean flow quantifications).

How do the practitioners of CFD answer the basic question about the sufficiency of data? It is necessary in principle to know about the sensitivity of (a) the calculation method to type and detail of data input and (b) the given flow. For example, to calculate the mean velocity in the wake downwind of an obstacle (an aerosol or a plate), even to an accuracy of 50 per cent, it is necessary to specify some details of the turbulence in the wake near the obstacle (for example see reference (36)). The simplest level of model cannot make use of this input data and therefore has inherent errors. Recent blind tests of CFD (level 2) codes have shown how for certain flows, especially those near sharp boundaries, the calculations are very sensitive to the specification of the input turbulence (22). A user of this code might then be advised to evaluate the sensitivity of the calculation and consider a range of input data before making any design decisions. However, such precautions tend to be regarded in practice as 'expensive luxuries'. In that case beware of disappointment in the results!

3.3 Turbulence models

It has been seen that, depending on the practical problem to be solved, different levels of output data are required, the form of the input data depends on the output requirements and the turbulence model to be used (see Table 1).

First consider problems with a level 1 output. If the form of the mean velocity profile of a turbulent flow is changing slowly, that is $U(x)$ varies with $x$ (say over 30 boundary layer depths or pipe diameters), so that the forms of the eddy structure do not change significantly, it is quite usual in industrial engineering and environmental work to make basic calculations for the mean profile $U(y)$ and Reynolds stress $\tau$ on Prandtl's mixing length model. This is a simple equation relating $\tau$ to $dU/dy$ and to a length scale (of the order of the correlation length, $L_u$) that has to be assumed at each point (x, y, z) in the flow. The mixing length equation and its variants (for example the Spalding-Almazan model (26) used in aeronomical boundary layers) all involve a mathematical relation between, certain properties of the mean velocity vector U, the position vector x and coefficients that have been derived for particular types of flow, for example shear flows near a wall. These coefficients may have been derived empirically, or by calculation using higher level models or numerical simulation. For modelling the flow very close to the wall, where steepest changes by molecular viscosity are significant, the kinematic viscosity $\nu$ enters the relation.

The mean flow is obtained by solving together the differential equations for the mean momentum (which involve both $\tau$ and $U$) and for continuity (together with that for the passive scalar), etc. The solution requires as input the mean velocity U and the boundary conditions on the walls, say at $y=0$, to be specified. If they are smooth the no-slip boundary condition applies; if they are rough and perhaps mobile (like a water surface) some wall boundary conditions have to be derived empirically to specify the solution, either empirically (eg by specifying a roughness length) or by coupling the fluid flow problem to a model of the physics at the wall.

As with any practical computational model, it tends then to be applied to more complex types of flow; it is generally found that inaccuracies grow the greater the difference in the way that the turbulence is distorted and adjusted compared with the original type of flow. Thus if equations for a flat boundary layer are applied to flows over undulating walls or boundaries, or for gas flows over water waves (a problem for chemical engineers as much as oceanographers), as the undulations steepen the distortion of the flow increases and fluctuates, so that the errors using the mixing length increase. Another case where the mixing length approach cannot be applied is the common engineering problem of turbulent flow in non-circular pipes.

The next level of turbulence model most widely used in practice is similar to the mixing length model in that there is a relationship between the mean shear stress $\tau$ and the local gradients of the mean velocity (that is $dU/dy$ in pipe flow), but the difference is that it explicitly models the dependence on the kinetic energy K and length scale L (in $K^{-1}$) of the turbulence. Thus in a shear flow

$$\tau = -\frac{1}{2} \rho U' \nu \frac{dU}{dy}$$

(1)

where $\nu$ is a coefficient (the other important feature of the model is that it represents the way in which the turbulence usually develops at a different rate to that of changes in the mean velocity as a result of the different nomenclature. The turbulence and those of the mean flow (see Section 2.2). These processes require the introduction of two new partial differential equations for the kinetic energy K and for the dissipation rate $\epsilon$, which together effectively define the length scale of the turbulence, as explained in Section 2.1. The two equations for K and $\epsilon$, first introduced by Kolmogorov (14), were developed for widespread engineering practice in the 1970s by Launder, Spalding, Rodi and their colleagues at Imperial College (see references (27) and (28)). The equations contain terms that model most of the dominant processes. The mathematical forms of the terms and the coefficients involved are based respectively upon physical arguments and comparison with a range of
experiments (particularly shear flows) (see Fig. 6). In principle this method requires details of the turbulence, viz. K and ε, for its data input which are not required for level 1 models. In many cases they are not available, and therefore have to be estimated based upon knowledge of similar entry flows. Since this model is often only required to provide level 1 output, some uncertainty and rough approximations about input data are allowable, given this level of user requirements. Mean flow patterns calculated using this model may well be broadly correct, even where there are isolated boundaries and where there is a number of inflows and outflows into the flow region, such as in an aerodynamic combustor (30). However, calibration of the code with a similar flow is generally desirable. The success (or the use of this model) was the correctness of the flow pattern and path of the flame front that was calculated to simulate the events in Kings Cross underground station during the fatal fire in November 1987 (31).

Recent discussion between industry and the research community (32) has led to conclusions about the limitations on the use of the K-e model in flow regions where the mean velocity gradients are changing in magnitude and directions, such as in three-dimensional shear flow over a curved surface (for example over swept wings) or where there is intense, anisotropic turbulence that significantly affects the mean flow, for example in wake flows or disturbed jets; see Fig. 7), or in flows with strong swirl, even where they impinge at stagnation point, or where the turbulence intensity changes rapidly over distances much less than the scale of the large eddies (as in thermal convection) (35). Then it preferable to use a more complex model involving fewer assumptions, but up to seven new model equations for the separate components of the Reynolds stress, \( u_1 u_2 \), of the turbulence, together with an equation for the dissipation rate for \( \epsilon \). The forms of the equations for models of this type first developed by Launder et al. (36) and by Lumley (37) continue to undergo developments, under the extension to the applicability of the models (for example to flows with higher strain rates, higher anisotropy or wider ranges of Reynolds number) or to improve the accuracy of the model for particular types of flow (for example those with stable density gradients, which have internal wave motion as well as turbulence). These second-order models are less widely used in engineering and environmental flows than the K-e models, because they require more detailed input data or more assumptions and are more sensitive to them. Also they require significantly more computational effort and can be more sensitive to the computational methods used in their solution. Probably the most advent is in their highly reduced and simplified form of algebraic stress models, where the equations give rise to a useful relation between the different stress components (\( u_1, u_2, \ldots \)) and the local mean velocity gradients. This is a marked improvement over the simpler form used in the K-e model. Both types of level 2 model are only appropriate for the types of flow where the scale of the most energetic turbulent eddies are of the same order or smaller than the distance over which the mean velocity is changing (this is satisfied in a shear flow where \( L_e \geq \sqrt{u_1 u_2} L_{1/2} \)). Also it is necessary to neglect the effect of action at a distance of larger eddies, which is particularly important near boundaries or in the presence of large-scale free-stream/turbulence outside a shear layer (see Fig. 8 and reference (40)).

To illustrate how certain features of turbulence structure are common to similar types of flows, consider how the dissipation rate \( \epsilon \) and the relevant integral length scale vary in slowly varying shear flows \( U \) away from and close to boundaries. This example also illustrates the problem in turbulence models of relying on local relationships. In a wide range of shear flows \( U(y) \) (away from boundaries) the dissipation rate is related to the mean velocity gradient by \( \epsilon = \frac{2}{3} \langle u' v' \rangle / L_e \), where \( L_e = - \frac{1}{u'} \frac{d U}{d y} \). Note that the expression \( \epsilon \) denotes an average value, \( \epsilon \), at a distance \( z \) from the boundary, defined as \( \epsilon(z) \) (which is approximately equal to \( L_e \)), is also influenced by the blocking effect. In a wide range of shear flows near boundaries these two effects can be combined in a single formula for \( \epsilon \) (for very high Reynolds number flows, outside the surface viscous layer).

\[ \epsilon_L = \frac{L_e}{L_{1/2}} \approx A_L \epsilon_L + \frac{1}{2} u' \frac{d U}{d y} \]

where \( \epsilon_L \) denotes an average value. This effectively combines Prandtl's concept of a local model for turbulence near a wall and a spatially averaged model for shear layers, wakes, etc. (12, 41). A similar approach to modelling length scales in turbulence models has been introduced by Orszag et al. (42) based on purely statistical physics concepts of turbulence. The eddy structure in turbulence changes when it is driven by thermal convection or in strongly accelerating flows. It produces a different value of the coefficient \( \beta \), and in the latter case very different (al if a distance \( y \) from the surface of the ratio \( u' / v' \) (33)). Differential equation turbulence models can usually account for quite rapid changes in the variation of the different velocity components across different flows; they rely on the diffusion of turbulence to model some mechanisms that may correspond more closely to those caused by 'action at a distance'.

The limitations of the local models mean that a reasonable accuracy of level (2) output cannot be achieved for the same computational effort when used for level (2) models. Turbulent flows round obstacles are a good example (see Fig. 9). This requires a higher level (3) model based on a few, more generally applicable assumptions. For the physical reasons explained in Section 2.1, the only reasonable general assumptions about turbulence are those concerning the smallest scale motions. This is the basis of large eddy simulations (LES) in which finite size motions are directly calculated, while the smallest scales but not approximately treated.

However, if no assumptions are made about the statistics of the resolved or largest scale motions greater than those of the assumed 'sub-grid scale motions', it means that their random space-time variations must be calculated directly and any required statistics must then be derived from the large periods of integration (say 1000 natural periods of the turbulence). These calculations or simulations can be performed at different levels of accuracy depending on the relative size of the sub-grid motion to the resolved motion. However, generally this approach requires large computational resources and/or longer periods to perform the calculation. For moderate Reynolds number pipe flows (it is possible in some cases to pipe flows (it is possible in some cases to compute the flow with complete accuracy (provided the initial conditions are known) without using a sub-grid motion this is a direct numerical simulation (DNS)).

A comparison is shown in Fig. 11 between the numbers of grid points required for computing a significant engineering flow using LES and DNS. It is clear why DNS is not yet a practical option, even using the largest computer systems. Both LES and DNS models can also be used to calculate other statistical information about the eddy structure of the turbulence, for example the extreme values of fluctuations (of great importance in environmental models) or how the velocity is correlated over intervals of time and space, and its spectrum.

Reviewing models at different levels shows how more computation is required as the model level increases or, given the same computer capacity, how only relatively idealized turbulent flows can be computed with a high level of accuracy and detail (see Fig. 45).

3.4 Numerical methods

All the governing partial differential equations (PDES) of CFM (momentum, continuity and turbulence models) assume that the statistical variables (such as moments of velocity, pressure, etc.) are continuous functions of space and time. For all but a few very simple situations, it is necessary to solve these equations approximately by defining the variables, \( \psi(z) \), as a series of values \( \psi(z) \) at a number of discrete volumes (or finite elements). Then (with finite difference methods) the derivatives in the PDES can be approximated as differences between the nodal values at different points (for example \( \partial \psi / \partial z \)). This converts an insoluble calculus problem for defining \( \psi(z) \) into a tractable problem of finding the variables \( \psi(z) \), in a large number of nodes, and their effect on the normal velocity components, and therefore reducing the distances between them (for example \( \psi \), \( \psi \), \( \psi \)). In general brings the solution of the algebraic equations closer to the actual solution of the PDES. Nevertheless, however large the number of points used, may exceed 10\(^6\) in some large aerospace calculations, some errors always exist. Users of CFD need to be aware of them and what needs to be done to minimize them, or at least allow for them, in assessing computational results.

Firstly, even small numerical errors can lead to significant errors in the solution to the flow problem, especially where the flow is affected by regions with sharp changes in the shapes of boundaries (for example rounded blades in a stirred tank reactor) or where the flow region and/or flow time are large enough that errors can build up. The errors are similar to those that are caused by an insufficiency or inaccuracy of input data, whether of the velocity entering the flow region or of the shape of the boundaries. They may even lead to choric and unpredictable solutions (47).

Secondly, different numerical methods (for example the way that derivatives are approximated) have their own particular types of error and also make different computational demands (see Fig. 12). Therefore, in assessing the performance of any CFD code it is essential to know which numerical methods have been applied and also the size and nature of the grid. The latter is becoming increasingly important as new numerical methods are developed for distributing the grid points through the flow region. In some cases quite simple improvements in the grid point distribution in CFD codes have led to significantly greater accuracy for the same number of grid points. Can such improvements be predicted in advance or planned? Fortunately, at this stage, still relatively simple methods may facilitate the prediction of the advance of the benefits of new numerical schemes (an approach practised more strongly in France). However, the usual approach is empirical, especially because the benefits are not generally applicable to all flows and are generally related to the particular model equations. [A notable example at the Meteorological Office was the 50% reduction in the error of the forecast position of tropical cyclones obtained by improving the model and the]
4 DEVELOPMENTS IN CFD

4.1 Operational and resource questions about CFD codes

The wider and deeper application of CFD for practical engineering is following the same path as that of other branches of science and technology. First, quite complex ideas and theories are converted into algorithms and robust computer codes. These need to have been thoroughly tested and quality assured, so that the user can be confident that all the intellectual and practical steps in producing the delivered code (Fig. 13a). In general such codes have to be produced so that they can be used by operators who only have a superficial understanding of all the ingredients and whose main job is to run the model for specific flow problems and then apply the results for particular purposes (see Fig. 13b). The latter step usually has several components: one is an assessment of the accuracy and general reliability of the model output for this particular problem (based on a previous similar calculation and a knowledge of similar flows), and then either an interpretation or communication of the result to those who wish to use the result. For this stage to be effective usually requires the fluid flow expert to have a good understanding of the technology and general requirements of the model user. Discussion with engineering and computer practitioners of CFD show that their assessment, communication, and application of the results is largely based on combining an understanding of the basic scientific principles with a case-by-case knowledge of how any particular CFD scheme works. The interpretation is seldom in practice influenced or helped by detailed knowledge of how the algorithms and code were constructed.

The intuitive insight of CFD users, of fluid flow designers and of those involved in practical environmental fluid flow problems (such as weather forecasters) is rapidly improving with developments in graphical presentation of computer results (49). One possibility now being explored is the use of visual reality so that the user can visualize being in the fluid flow field, hurrying round the vortices or 'passing' in a stagnation region, etc.

The appropriate use of these visualization approaches is only just beginning (58).

While generally well tried and tested, some engineering designs fail to take into all particular types. Therefore the users of CFD need to interpret the results for particular applications, and engineers specializing in a particular technology associated with certain types of flow should ensure that their CFD system has been developed and tested for these types. To become effective designers they need to become familiar with the use of the CFD system as a natural adjunct to their other techniques.

What level of resource, however, should be appropriate for this adjunct to engineering (and environmental) design? For those dealing with the development stage of major design projects a vital consideration is the time to run the calculation so as to maintain a programme of trials, for example, in a grid of 100 x 100 x 100 or 1000 points a mainframe supercomputer is necessary (operating at say, 10^10 flops) to obtain a result within two hours. For other kinds of project where the pressure of time is less, work stations (currently running at about 180 megaflops) are adequate to solve lesser problems in a few hours, or major computations in days.

For many organizations, from the largest to the smallest, the decision on the resources depends just as sensitively on the cost of staff to write the code and maintain it, or to run a commercially available code and use it effectively with reasonable results. In either case the staff level depends on the size of the code that is necessary. If the code has to be written 'in-house', a typical estimate is that one experienced programmer takes about one day to write 25 fully validated bug-free lines of code, so that the key engineering design code is a large aerospace organization, which extends to about 10^5 lines (e.g., aerodynamics, structures, thermodynamics, and electromagnetics), is worth about £10^7 just for the computer time and the resources associated with research and testing. Maintaining and updating such a code requires about one experienced programmer per 20000 or 30000 lines of code. Even smaller consulting organizations have codes with 50000 lines and the manpower resources costs can be calculated on a similar basis. The important point is that serious financial and human resource decisions are most often taken about the level of code that is to be used, in the light of all the requirements.

4.2 Progress in CFD codes for turbulent flows

One objective measure of the progress in CFD of turbulent flows over the past 25 years has been the increase in complexity of the 'frontier' fluid flow problems that have been studied in the comparisons of the codes. These are the problems where most vigorous research and development code is focused at any given time.

At Stanford in 1968, the main emphasis was on calculating turbulent boundary layers on flat plates in pressure gradients, whereas in 1990, at the next international workshop, the emphasis had moved on to more complex shear flows, such as wall jets and corner flows, and to recirculating flows at the expansions of pipes. In the same time the codes had changed. In 1988 these were essentially variants of level 1 codes (with some embryo level 2 codes) and in 1980 the emphasis had changed to level 2 codes.

At the ERCOTAC (European Research Community of Flow Turbulence and Combustion) workshop at Lousanne, 1990 (16), the frontier problems changed again to the important aeronautical engineering problems of accurate calculations of three-dimensional turbulent boundary layer and transition as a result of external turbulence. Rolls-Royce donated data from their test programme for this study.

The first problems were computed most successfully with level 2, 'second-order' equations, because all the separate Reynolds stresses could be calculated. However, the transition problem was most effectively modelled at level 1 by a large eddy simulation code of Voke (50) which does not involve assumptions about the large-scale eddies which change dramatically at transition. However, although statistical level 1 and level 2 models for fully developed turbulence cannot be used for flows in transition between laminar and turbulent flow, it has been found that special adaptations of level 2 (K-e) models, are suitable for engineering problem range of flows a clear demonstration of the benefits of focusing modelling effort rather than attempting to develop all-encompassing models for a wide range of turbulent flows. Level 5 models (especially DNS, but also 'two-point' models such as the exact idealized RDF calculation) have given valuable insight into the limitations in level 1 and level 2 models and have led to improved approximation for particular classes of flow. In other words, a 'cascade' of modelling methods may be the most cost effective strategy. Combinations of these types of modelling are being introduced for certain industrial problems.

4.3 The new 'frontier' problems

The growing use of fluid flow technology and information about environmental flows not only necessitates more accurate predictions of the mean fluid flow than turbulence (v, w, y), but also an understanding of the range of turbulence. The range of applications that require objective methods for defining the eddy structure have been compounded (and found to be less different than was thought at first). Now the basic fluid mechanics and the technology of this aspect of turbulence can progress more systematically (51). Also in specific classes of flow these structures can be modelled for practical purposes at a less complex level than large eddy simulation, for example using discrete vortex models.

The eddy structure is equally important for modelling combustion, particle motion and bubbles in turbulence. Vortices are efficient at concentrating and transporting bubbles, by sucking them in. In some cases solid particles are also trapped, because if they are present when the vortex is formed they tend to diffuse outwards at a slower rate than that of the growth of the vortex. Vortical eddies can also enhance combustion. Ad hoc CFD models for these flows have been developed. There is now a common consensus as to whether LES, although the most general method, is the most practical method for computing flow problems that are sensitive to the eddy structure.

The computer power and expertise required is considerable.

It is certainly true that some complex flows, including two phases, electromagnetic body forces, strong rotation, fluid/fluid/solid interactions, etc., are being successfully modelled at levels (1) and (2). However, industrial engineers (specifically in the oil and ship-building industries) state that for these applications the codes have not yet been significantly well validated to give industry the confidence it is looking for. Even the methods of validation of codes and of their inter-comparison have not yet been generally agreed. Nevertheless, although experienced engineers are using CFD codes for complex problems, in some industries doubts prevail and the use of CFD is vestigial. Overcoming this problem is where the networks of research specialists and interested industries can contribute. This is one of the major roles in Europe of ERCOTAC. [Updating (52) set out in some detail the extensive (level 3) information about the flow. It should also be possible to use CFD more effectively to develop concepts and better fluid flow technology solutions, which may well require more extensive design (integration of fluid flow and other technologies, such as those listed in Section 1.)

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(a) Three-dimensional wakes of a porous disc and solid sphere with the same drag. Note the differences in eddy structure and magnitude of turbulence (8).

(b) Random turbulent signal represented by Fourier wave modes with random amplitudes $a_1, a_2, ...$, and the connection with the energy spectra $E(k)$. The largest scale eddies (specific to these flows) are $k_{max} = 1/L_Y$. The energy containing eddies (with characteristic form) have wave number $k$ or $k$ wave number (with a more general structure) are $a_1$ and $a_4$.

Fig. 2 Typical turbulent flow.

(c) “Small”-scale eddies with their typical form of enstrophy vertices (w) with spiral streamlines stretched by local stretching motions $u_0$, which occur in flows at high Reynolds number. Despite their non-isotropic form (the eddies have approximately isotropic orientation, leading to isotropic second-order statistics).

Fig. 3 Eddy structure of turbulence at different scales and in different flows (12).
Fig. 4 Schematic diagram of the main mechanisms that determine the eddy structure and statistics of turbulence.

Perturbed laminar boundary layers

Fig. 5 Wake turbulence from one set of aerofoils impingings on to another. Note how the turbulence is not fully developed, the different types of turbulence that are present and that transition to turbulence occurs on the blade. B is the boundary of the domain D where the flow calculation might be performed.
Fig. 6 Flow around a two-dimensional car model 

Fig. 7 Flow in plane plenum chamber; solid and dashed lines correspond to different level 1 calculations (32); circles show experiments (25) (taken from reference (24)). ASM = algebraic stress model, RSE = Reynolds stress equation.
Fig. 9 Demonstration of limitation of turbulence models involving local gradients. Graph of dissipation length scale $\ell_\lambda$ at the wall $y=0$ computed by P. Spalart using direct numerical simulation compared with the model equation $\ell_\lambda = \frac{\nu}{u'}$ and $\ell_\lambda = \frac{\nu}{(u'^2/\partial u/\partial y)}$. Note the implementation using the spatial averaging of $u'/\partial u/\partial y$.

Fig. 10 Schematic graph showing the degree of detail of the computation as a function of the complexity of the turbulent flow for different levels of the computational model, from coarse to fine. The graph is divided into levels:

- Level 1: Basic turbulence model (e.g., RANS)
- Level 2: Advanced turbulence model (e.g., LES)
- Level 3: Direct numerical simulation (DNS)

The complexity of the flow increases as we move from Level 1 to Level 3, reflecting the increased detail in the models.

Fig. 11 Number of grid points required for different types of turbulence simulations. The graph shows the number of grid points needed for RANS, LES, and DNS simulations, indicating a significant increase in grid points required for DNS compared to RANS and LES.

Fig. 12 Comparisons between (a) wind tunnel measurements of kinetic energy around a cube in a turbulent flow ($\partial \bar{u} / \partial t$) and two kinds of computation using (b) a level 3 statistical model $k-\varepsilon$ and (c) a level 5 simulation model (large-eddy simulation) (LES). The graph shows the distribution of kinetic energy at different locations around the cube, highlighting the differences between the experimental data and the computational models.
Fig. 12 The importance of numerical methods in CFD