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Computational modelling of complex turbulent flow - expectations, reality and prospects

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Abstract

The paper considers issues pertaining to the capabilities and limitations of computational methods for multidimensional turbulent flows of the type encountered in fluids engineering. It argues that CFD, whilst offering considerable predictive power and potential, is not yet sufficiently well established to be applied routinely to complex 3D flows, unless only a rough qualitative statement is being sought. CFD involves a whole array of ill-defined and ill-understood interacting issues, such turbulence modelling, boundary conditions and the numerical approximation of convection, whose combined influence on predictive realism is never transparent. Illustrative examples are presented to justify the above view. Because of the particular prominence of turbulence modelling as an error source, an indication is provided of current directions in representing turbulence effects by advanced stress/flux closures as a means of improving accuracy. The discussion leads to the conclusion that considerable expertise, physical insight and experience are essential for meaningful solutions to be obtained and for the limitations of computational schemes to be appreciated.

1. CFD - THE CHALLENGE POSED BY PRACTICAL FLOWS

1.1 Substitute for Windtunnels?

Rapid advances in computer technology, mainly over the past ten years, have given strong impetus to the development and validation of 3D CFD algorithms capable of predicting the type of complex flows encountered in real engineering applications. This evolution has given rise to the rather radical view - expressed predominantly among the US aerodynamics fraternity - that the windtunnel is destined to become a "convenient storage cabinet for computer output". A moment's contemplation leads to the conclusion that this view reflects a rather narrow interpretation of CFD, focusing on the particular type of flows most relevant to high-speed external aerodynamics and some turbomachinery applications. Such flows are often characterised by an insignificant level of viscous and turbulent transport, except within thin, attached boundary layers which do not interact significantly with the outer aerodynamic field. In such circumstances, predictive realism is dictated, principally, by the numerical accuracy with which the inviscid processes are represented and by the validity of the boundary conditions imposed. While both these issues are far from trivial, as will be argued later, nearly inviscid flows can be computed with fair to good accuracy by use of high-

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resolution schemes and reasonably dense numerical grids.

The majority of practical flows - and these include virtually all those relevant to wind engineering - are much more challenging than those mentioned above. The critical points of difference are separation and recirculation, both closely associated with the dominance of turbulence processes. Viewed in statistical, time-averaged terms, the position and orientation of separation lines (unless provoked by geometric edges), and the size, shape and structure of recirculation zones, all depend decisively on turbulent mixing. In many circumstances, the detailed flow structure within the recirculation zone is, itself, of primary interest and must, evidently, be resolved accurately. Even if this is not the case, however, the separation and reattachment process must be captured realistically, for the shape of the recirculation zone will profoundly affect the adjacent flow, even if this is nearly inviscid, and hence all global flow characteristics. The main challenge within a statistical framework is then to construct a turbulence model which represents correctly turbulence transport, the anisotropy of normal Reynolds stresses which, in recirculation zones, contribute on a par with shear stresses to momentum transport, and the interaction between fluid viscosity and turbulence, particularly in the semi-viscous near-wall region. As it turns out, this is an exceedingly difficult task, akin to trench warfare. The central problem is a realistic closure of a severely truncated subset of the infinite set of exact time-averaged equations which describe a corresponding hierarchy of turbulence correlations of ever-increasing order. The alternative approach - full or partial simulation of the 'chaotic' turbulent motion in all of its details, is gaining weight, but also involves considerable problems as well as very heavy computing costs. As regards wind-engineering, it is the writer's view that the role of computational methods, whatever approach they adopt to resolving turbulence, will be confined to efforts intended to elucidate the details of processes associated with single or a very restricted set of geometric obstacles and bluff bodies. Hence, windtunnels are here to stay for many years to come and will continue to be the main vehicle for investigating realistic architectural design concepts.

1.2 Turbulence Modelling

Turbulence models of the type required for predicting separated flows have been developed and applied predominantly in the broad area of mechanical, civil and heat-transfer engineering [1-3]. Much experience has been gained, in particular, with a variety of turbulence modelling practices which account for the convective and diffusive transport of turbulence parameters, among them turbulence energy, turbulence vorticity, turbulent viscosity and, indeed, the Reynolds stresses themselves. The large majority of validation studies have been pursued within the two-dimensional framework, however, principally because of the availability of related detailed and accurate experimental data, and the lack of computer resources necessary for numerically accurate three-dimensional computations. Although the latter problem has rapidly diminished over the past few years, applications to massively separated three-dimensional flows are still relatively rare. The problem is not primarily rooted in computational limitations. Fig. 1 shows a facet of a computational study by Lin [4] in which the flow around a group of buildings was investigated with a turbulence-transport model prior to the actual construction of the group in Manchester. Leaving aside, for the moment, the question of large-scale transient features, which have here been subsumed into the statistical framework, one may justifiably query the quantitative accuracy of the calculation. In the absence of experimental data, this question can evidently not be answered. As will be shown later, there is every reason to assume, however, that present modelling capabilities for 3D flows, whilst yielding a broadly valid qualitative view, simply do not suffice for any reliance to be placed on the quantitative statement derived from solutions such as that in Fig. 1. This then leads to the conclusions that CFD for physically complex 3D flows will, at best, supplement wind-tunnel testing for many years to come.

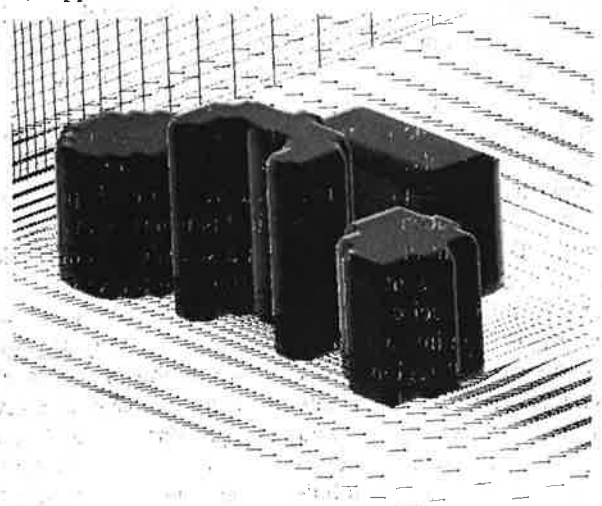
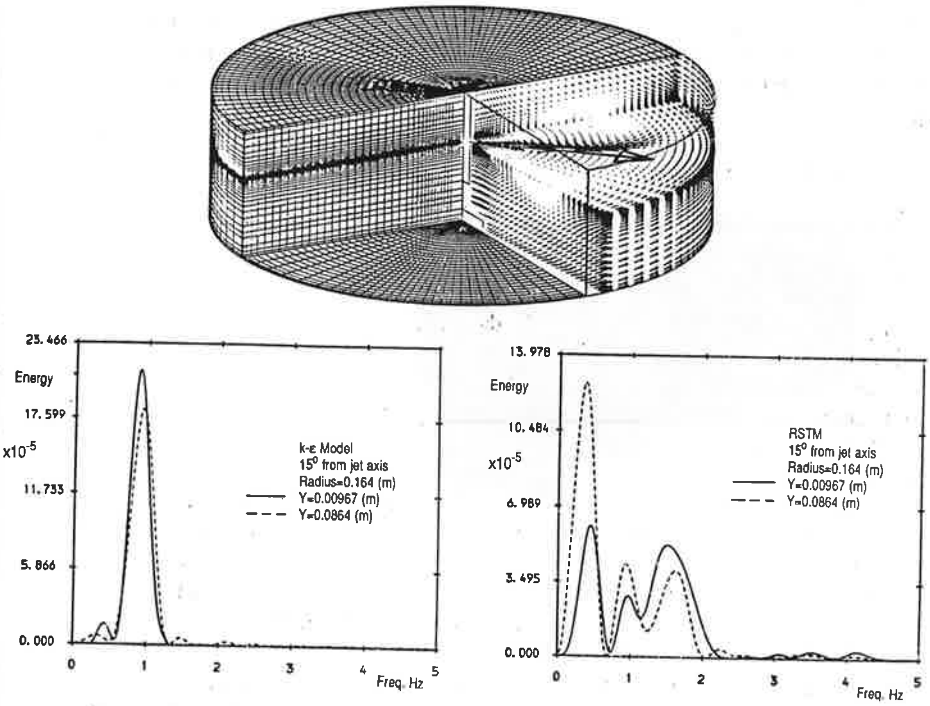


Fig. 1. Predicted flow around building group (Lin [4])

1.3 What about Transients?

A feature which is of particular relevance to wind-engineering is periodic vortex shedding from bluff bodies and associated large-scale structures in wakes. It is generally assumed that the effects of these structures is accounted for within the statistical modelling framework. However, shedding is a period process, rather than turbulence, and there is a range of evidence to suggest that turbulence models yielding steady-state solutions which underestimate the apparent mixing implied by an *a-posteriori* time-averaging of the transient solution derived from a simulation which resolves at least the large-scale structures arising from shedding. An associated problem is that different turbulence models suppress to a variable extent naturally occurring periodicity. Fig. 2 gives an example from mechanical engineering (Lin and Leschziner [5]). Here, a jet is issued from a radial injector into a swirling cross-flow. The interaction between the two flows produces a periodic flapping motion associated with shedding. The flow was computed with two models: an eddy-viscosity variant based on two transport equations, one for turbulence energy and the other for its rate of dissipation, and a Reynolds-stress model consisting of 6 transport equations for all Reynolds stresses. The latter tends to return a lower level of turbulence mixing resulting in a more pronounced flapping mode. This is brought out in Fig. 2 by a comparison of frequency spectra obtained by a Fourier analysis. Evidently, different model variants include different time-scale ranges, suggesting an overlap between turbulence and shedding time scales. In extreme cases (Franke et al [6]), the turbulence model entirely suppresses any transients and returns a steady solution



ig. 2. Jet injected into cross flow and flapping frequency spectra predicted by k-ε eddy-viscosity model and Reynolds-stress transport model (Lin & Leschziner [5])

hich does not conform with the real time-averaged behaviour. It must be said here that the ›ove difficulty is encountered predominantly in unconfined conditions. Confinement and wall ›oximity inhibits periodicity and enhances the validity of the statistical framework.

In the event of peak wind and pressure loading having to be determined, a statistical ›amework is obviously inappropriate, although some very limited information can be derived ›m the predicted (steady) correlations of turbulent fluctuations. In this case, the only ›ernative route is Large Eddy Simulation. This approach, vigorously pursued in Japan and › USA (Tamura et al [7], Murakami et al [8], Reynolds [9]), resolves scales down to the ›e of the (relatively coarse) grid and accounts for smaller scales by way of a sub-grid ›del, the nature of which is similar to conventional statistical models of turbulence. While ›s route avoids the difficulties pointed out earlier, it has its weaknesses: it is especially ›stly, it requires the use of particularly accurate approximation techniques which tend to ›stability in high Reynolds-number flow, it entails the storage of large quantities of data in › form of time series, from which statistical information needs to be extracted by integration ›er time-marching is completed, it requires the prescription of transient boundary conditions ›ich are not available but must be generated numerically, and it involves serious ›certainties relating to semi-viscous near-wall effects and their simulation. This paper is does ›t consider LES further, but confines itself to issues relevant to the computation of flows ›h turbulence models.

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2. CFD - SOME IMPORTANT ISSUES

While CFD offers tremendous potential, the wider exploitation of which is to be encouraged, it is important to recognise that it requires great care, physical insight and continuous validation by reference to experimental data. The large majority of experienced computational fluid dynamicists will bear witness to having experienced frequent, frustrating and perplexing instances of numerical instability, agonizingly slow convergence, insufficient resolution with economically tolerable grid densities, a high level of sensitivity to superficially uninfluential boundary conditions and obvious lack of physical realism in the solutions generated. The writer's favourite example for the fallibility (or, perhaps more charitable, sensitivity) of CFD is the outcome of an computational test exercise organized by the IAHR [10], in which seventeen specialist groups submitted solutions for the relatively simple two-dimensional plenum-chamber flow, sketched in the small inset of Fig. 3, with the same boundary conditions used by all groups. The figure itself conveys an impression of the spread of solutions obtained for turbulence energy (not all have been included) in this relatively simple case and requires no further elaboration. A similar story can be told about a more recent ERCPOFTAC workshop [11], held at Ecole Centrale de Lyon, which focused on impinging jets.

What is it then that makes CFD such a challenge? The essential elements of the answer are shown in Fig. 4 and include, as the most prominent issues, non-linearity, inter-variate coupling, drastic variations in the characteristics of the flow-governing equations within one and the same flow, turbulence, chemical reaction (combustion), and multi-phase interaction.

Putting aside, for (relative) simplicity, density variations, reaction and multi-phase features - each of which is itself a Pandora's box of problems and pitfalls, one may identify the roots of some of the difficulties mentioned above as being the frequent prominence of convection in the balance of processes governing the flow behaviour, the interaction between turbulence - or rather turbulence *model* - and the statistically time- or ensemble averaged strain field, and uncertainties in handling boundary conditions.

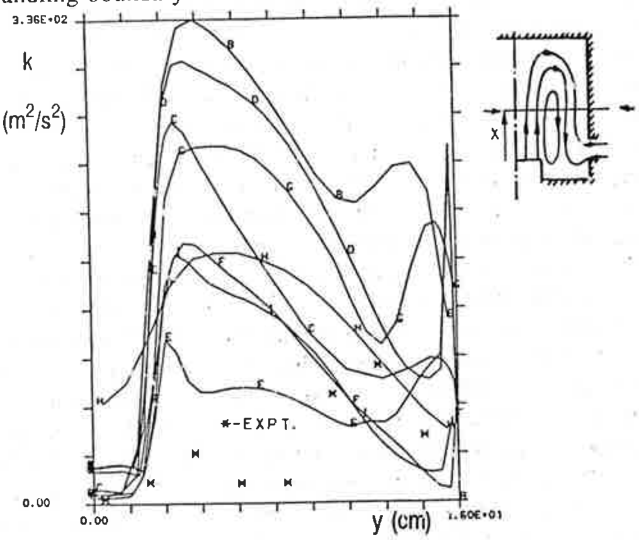

Fig. 3. Computed profiles of turbulence energy in plenum chamber across height 10.5 cm (Grandotto [10])

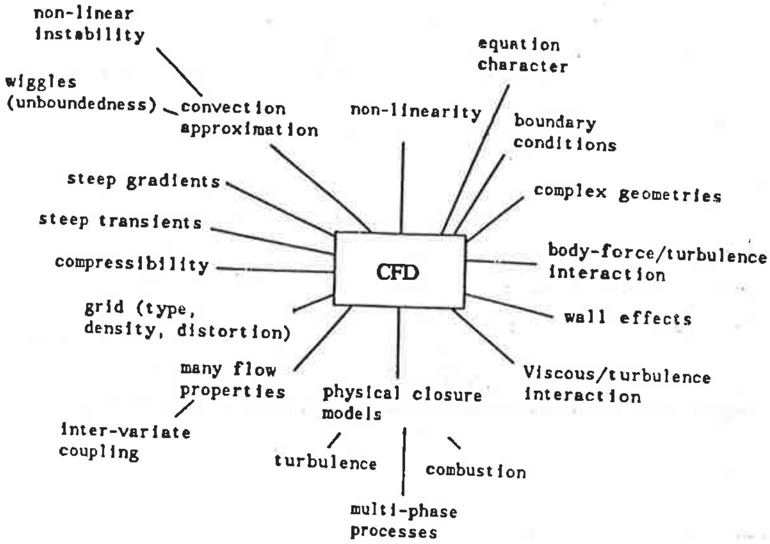

Fig. 4. Major CFD issues

2.1 Fluid Convection

Convection tends to give rise to highly strained (compressed and sheared), often convoluted regions and steep variations in flow properties. In addition, it introduces strong non-linearities into the equations governing the fluid's motion, and is a major source of coupling between the equations - both directly through the appearance of convection-related terms and indirectly through the pressure. If the steep property variations are to be resolved accurately with economically tolerable meshes, convection must be approximated with higher-order numerical schemes, particularly when the steep gradients are significantly skewed relative to the numerical mesh - as is invariably the case in complex flows. The problem here is, however, that such approximations tend to provoke instability and oscillatory solutions - features which must be avoided at all costs in "robust" codes. The frequently adopted alternative is, therefore, to use highly stable low-order schemes, which can introduce unacceptably high levels of numerical error.

Numerical errors are brought out most prominently in time-dependent simulations. As an example, Fig. 5 compares two numerical solutions, arising from two different convection approximations, for the purely convective transport of a Gaussian-shaped conserved scalar by forced vortex (solid-body rotation). Solution 5(a) was obtained with the third-order upsteam-weighted scheme QUICK (Leonard [12]) combined with a second-order ADI time-marching method, while solution 5(b) was generated with a spatially fourth-order spline approximation combined with a time-space characteristics method (Nasser [13]). Although the former scheme is generally assumed to be quite accurate and is widely used, it is evident that it results in serious artificial erosion of the scalar distribution. The latter scheme has been applied to vortex shedding behind a square cylinder and, as seen from Fig. 6, has returned a dependence of Strouhal number on Reynolds number which differs considerably from QUICK-based variations reported by Franke et al [14] and Davis et al [15]. Here again, these differences appear to reflect sensitivity to the convection scheme. In fact, use of a first-order upwind scheme would have led to a total suppression of shedding, resulting in a steady separated wake. The clear implication is then that simulations of turbulence, even if restricted to large-scale features, must adopt highly accurate, numerically non-diffusive schemes.

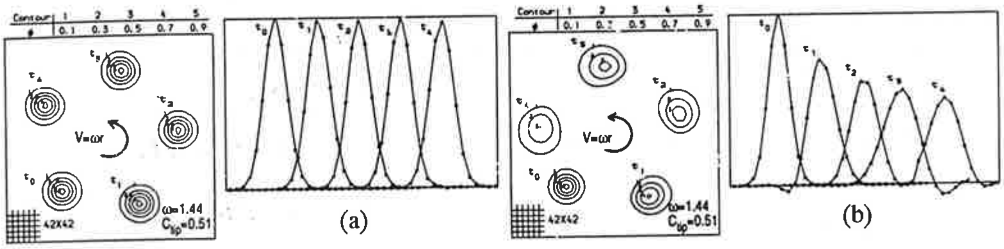

Fig. 5. Convective transport of Gaussian scalar field by a forced vortex; (a) QUICK/ADI scheme, (b) Spline/Characteristics scheme (Nasser [13])

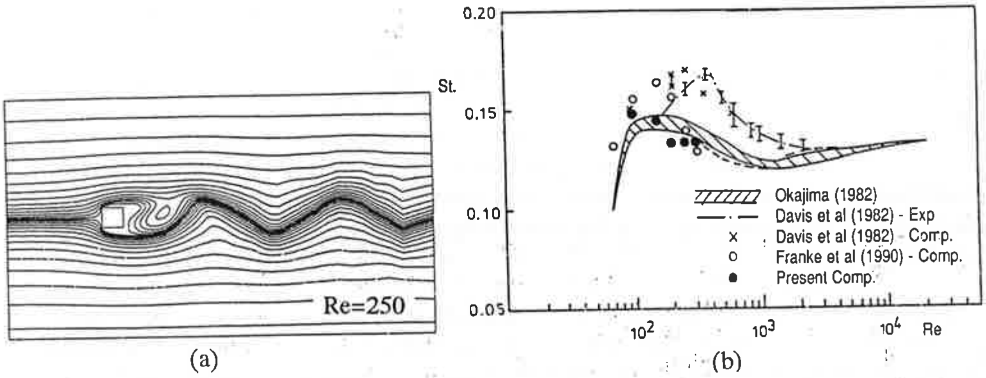

Fig. 6. Laminar vortex shedding behind a square cylinder computed with Spline/Characteristics scheme; (a) flow field, (b) Strouhal number vs. Reynolds number (Nasser [13])

2.2 Turbulence

Turbulence, if tackled by means of a model describing the variation of turbulent stresses and/or related turbulence parameters, leads to a further intensification of non-linearity and coupling - this time via diffusive processes. If turbulence is modelled through transport equations, the computational task is significantly complicated further, for these equations are themselves highly non-linear and coupled among themselves as well as to the mean-flow equations.

Understandably, there is a tendency to keep the turbulence model as simple as possible, if only because its structure can crucially affect the stability, robustness and economy of the computational scheme. However, the simpler a model is, the less realistic it tends to be (unless it is carefully tuned to particular types of flow conditions), and the narrower its width of applicability is. Models which provide the mean-flow equations with an eddy viscosity - the route taken in most industrial applications - tend to display good stability properties, mainly because a property-gradient representation of diffusion allows diffusive transport to be treated numerically in an implicit manner, i.e. coupled to convection, when the related transport equation is discretized and the resulting algebraic set is solved. A serious drawback of such viscosity models is, however, that they are unable to account, in a non-*ad-hoc* manner, for the interaction between turbulence and body forces arising from stream-line curvature in recirculating zones, swirl, rotation and buoyancy. Models which do capture this interaction involve no viscosities and diffusivities, but consist of partial differential transport equations for the turbulent stresses and fluxes themselves. Such models - generally referred to as second-moment closures - offer the prospect of considerably improved generality, but are shunned in the industrial environment, for they provoke substantial numerical problems and significantly increase computational expense. The question of sensitivity to turbulence modelling will be pursued further in Section 4.

2.3 Boundary Conditions

In any continuum problem described by partial differential equations, it is the nature of the boundary and initial conditions which give rise to different solutions to one and the same set of equations governing the behaviour within the solution domain, away from the boundaries. However, in fluid-flow problems, boundary conditions are rarely well defined and, in turbulent flow, *never* complete. This applies to almost all kinds of boundaries, be they walls, fluid outlet ports or an "entrainment" boundary through which fluid flows at a unknown rate which must be determined as part of the solution itself. Taking walls as an example, one is confronted with steep variations in velocity, turbulence-exchange parameters and other flow properties over a semi-viscous near-wall region which is normally too thin to be resolved by the numerical mesh. Yet, this region can exert a crucial influence on the overall solution accuracy, and its representation (by log-law based semi-empirical relations) requires care and insight. At a fluid inlet, the velocity distribution might be available (with luck), but distributions of influential turbulence quantities for which transport equations are solved will most frequently have to be estimated, and this again requires care, skill and a high level of physical insight. Exit conditions can present additional difficulties, if the outlet plane is not placed in a relatively inactive region in which the flow is unidirectional and weakly curved. Special problems arise in simulations which require transient boundary conditions with a spectrum representative of the statistical character of turbulence. This issue may be addressed by periodic conditions, in which the solution effectively generates the boundary conditions, but this is only a tenable approach in particular, geometrically repetitive configurations.

3. CURRENT CAPABILITIES AND LIMITATIONS

The proceedings of CFD conferences frequently feature impressive examples of complicated industrial flow applications involving convoluted geometries, heat and mass transfer and particulate transport, some generated by commercial packages incorporating sophisticated graphics post-processors. Whatever the origin of the 'pretty graphics' might be, the central question the design engineer confronts is how realistic and accurate the predictions are. This question can almost never be answered in complex conditions with any degree of confidence, for lack of experimental data for a configuration which is closely akin to that being considered prevents a proper evaluation of the solution scheme. Validation must thus be carried out by application to the widest-possible range of well-controlled and well-documented laboratory flows. These may be (and usually are) *geometrically simple* but must include those *complex flow features* which are ultimately encountered in the intended industrial applications. It is in the course of validation efforts such as that just considered that current limitations of CFD often come to light most starkly.

The relatively inexperienced CFD user, who might be in the process of applying a code to describe the operation of a complex heat exchanger or the flow around an array of obstacles, may be 'disconcerted' to learn that his code, if incorporating an eddy-viscosity turbulence model, would not be able to return an adequate description of many 'simple' 2D boundary-layer flows in which streamline curvature plays a significant role. Two examples of such flows - one a curved wall-boundary layer and the other a wall jet developing over a logarithmic spiral - are shown in Figures 7 and 8. To achieve a reasonable degree of agreement with the experimental data, a *Reynolds-stress turbulence model* must here be used, which by-passes the eddy-viscosity concept by solving equations for the individual stresses.

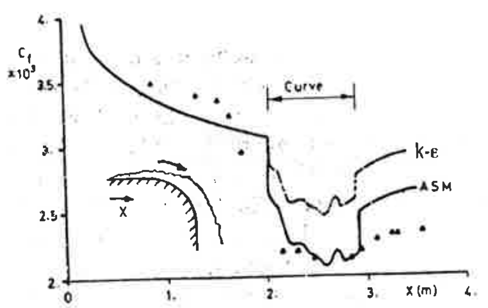

Fig. 7. Friction factor in curved boundary layer (Khezzar [16])

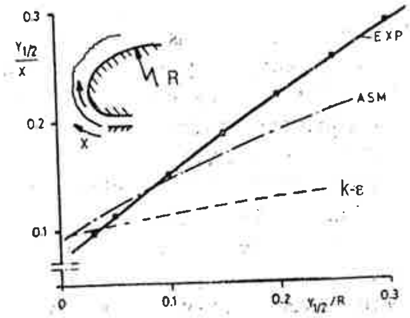

Fig. 8. Spreading rate of self similar wall jet over a logarithmic spiral (Nemouchi [17])

It may be argued that more complex flows, such as those involving recirculating regions, are, essentially, collections of curved shear layers, jets and wakes subjected to pressure gradients. It is not unreasonable to expect, therefore, that the defects observed in simple boundary layers will carry over - indeed, manifest themselves in a more serious form - in complex conditions. There is ample evidence, gathered in many validation studies, to show that this expectation is often met. Indeed, there are instances where even the most advanced turbulence closures fail to yield an acceptable level of agreement with experiment, and just two such examples are shown in Figs. 9 and 10. That defects are not reported in *all* flows is often a consequence of a 'judicious' choice of boundary conditions and the use of *ad-hoc* (or even flow-specific) turbulence-model modifications which are unlikely to perform well beyond a very narrow range of conditions.

What then can be done to improve the degree of confidence in flow predictions in a general sense? The answer is multi-faceted and complex, but three issues may be identified as playing a primary role. The attainment of a high level of numerical accuracy is one crucial requirement, and this can be achieved, in principle, by use of higher-order approximations, coupled with careful grid-independence checks involving tests with several mesh densities. This is undoubtedly an expensive route, but an essential one, particularly if refinements to models of turbulence and other physical processes are under examination. In this context, it is useful to remark that, in general, eddy-viscosity closures tend to over-estimate, often seriously, the level of diffusive transport, which then leads to an excessive erosion of property gradients. This, in turn, 'eases' the task of the numerical mesh of supporting the solution adequately. A corollary of this observation is that more advanced turbulence modelling usually require denser meshes for a given level of numerical accuracy.

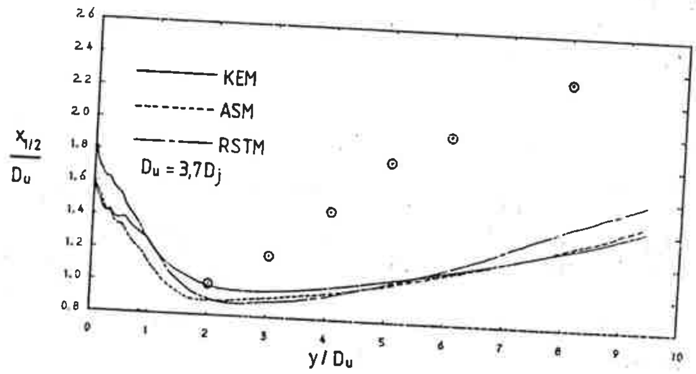

Fig. 9. Spreading rate of fountain produced by collision of two 2D plane jets, computed with eddy-viscosity and Reynolds-stress turbulence models (Huang [18])

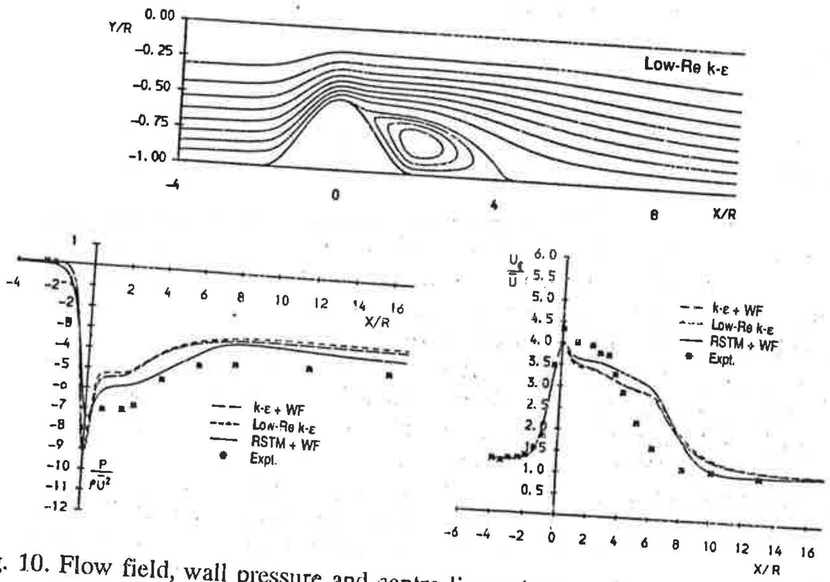

Fig. 10. Flow field, wall pressure and centre-line velocity variations in a sinusoidally constricted tube, computed with high-Re and low-Re eddy-viscosity and Reynolds-stress turbulence models (Lien and Leschziner [19])

Careful attention to boundary conditions is the second major requirement. Because this issue is wholly flow specific and because boundary conditions are virtually never complete, this is an area in which physical insight, a high level of expertise and experience are absolutely essential if the computational simulation is to provide a meaningful statement. The use of more refined turbulence models is the third major issue contributing towards improving the predictive capabilities of CFD procedures. Of the three issues considered here as being of primary importance, turbulence modelling is the one requiring by far the greatest input, not only in terms of fundamental research, but also as regards a stable implementation of alternative models into any existing numerical framework. Much work in this area is in progress, and its detailed review would go well beyond the framework of this paper; instead, a superficial indication of current directions and achievements is provided in the following section and should suffice to justify major conclusions.

4. CURRENT DIRECTIONS IN TURBULENCE MODELLING

As already indicated, eddy-viscosity models are not able to represent the interaction between body forces and turbulence. A highly over-simplified (and partial) explanation of this failure is that the isotropic nature of the eddy viscosity does not permit the strong curvature/buoyancy-induced enhancement of normal-stress anisotropy to be captured. This anisotropy, created by different levels of stress generation and turbulence-energy redistribution among the normal stresses, then feeds into the shear stresses and fluxes through a complex interaction between all the stress, flux and strain components.

The lowest level of turbulence closure which offers a real prospect of accounting for the above interaction is one based on the solution of separate equations for all independent stresses and fluxes [2,3]. Exact forms of such equations can be obtained by lengthy manipulations of the Navier-Stokes, Reynolds and energy equations. Adopting a simple descriptive representation and denoting the stress and flux components by τ_{ij} and ϕ_i (i=1,2,3 for x,y,z directions), one may write the resulting stress or flux equations as follows:

$$\text{Convection}\ (\tau_{ij}\ \text{or}\ \phi_i) = \text{Diffusion}\ (\tau_{ij}\ \text{or}\ \phi_i) + \text{Production}\ (\tau_{ij}\ \text{or}\ \phi_i)$$
$$+\text{Redistribution}\ (\tau_{ij}\ \text{or}\ \phi_i) - \text{Dissipation}\ (\tau_{ij}\ \text{or}\ \phi_i)$$

While diffusion, redistribution and dissipation all require modelling, production does not, for it only involves stresses, fluxes and mean-flow gradients. As the stress and flux levels respond sensitively to the related production levels, it can be concluded tentatively that a model based on the above principles offers a superior range of generality.

Much work has been done, in particular over the past five years, on the development of stress closures and their application to complex flows [3]. At UMIST alone, some twenty recirculating and strongly swirling flows have been examined, some three-dimensional and others involving large density gradients and combustion. Further studies, mainly in three-dimensional and compressible conditions, are in progress.

The gains achieved by switching from an eddy-viscosity to a stress closure are not uniformly high, and Reynolds-stress closure is by no means a panacea. Yet, no case has been encountered which does not benefit from the switch. Swirling flows and those dominated by large recirculating regions seem to derive the greatest benefits. Figs. 11 to 13 serve to illustrate the level of improvement which is often achieved. Fig. 11 shows solutions by Leschziner et al [20] for a separated flow in an expanding annular section following a backward-facing step ("ASM" denotes an algebraic Reynolds-stress model). The close agreement in respect of pressure recovery indicates that the recirculation zone shape is well predicted, not just its length. Figs. 12 and 13 show calculations by Ince and Leschziner [21] and Ince [22], respectively, for two different three-dimensional impinging jets, one with and the other - a twin configuration - without cross-flow ("DSM" denotes a differential Reynolds-stress model). While neither flow is closely allied to building aerodynamics, both contain features which are frequently encountered in the contex of wind engineering. In both applications, Reynolds-stress modelling yields considerable improvements in predictive realism, due to its ability to resolve curvature-turbulence interaction.

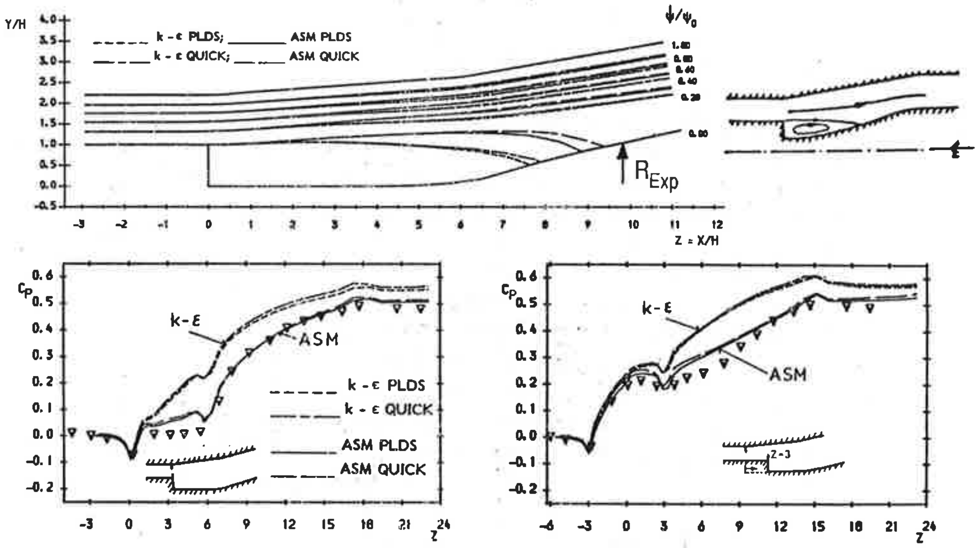

Fig. 11. Streamfunction and pressure recovery in separated flow in expanding annular passage: response to turbulence model and numerical approximation of convection (Leschziner et al [20])

5. CONCLUDING REMARKS

CFD involves a wide range of strongly interactive physical processes and numerical issues, some of which are as influential on predictive accuracy as they are ill-understood. It is for this reason that a high level of training, expertise and insight are essential in order to properly exploit the potential of CFD and, equally importantly, appreciate its limitations. This might be perceived as posing a serious hindrance to a widespread industrial application of CFD. Even if this perception is justified to some extent, the intolerable alternative is, at least in some instances, an uncritical, overly optimistic approach to the subject which, in the long run, will prove to be damaging to its reputation and progress.

It is the writer's view that CFD for general turbulent flow is unlikely ever to evolve to a "computational wind tunnel", and that a good measure of expertise will always be essential if value for money is to be derived from CFD software.

Algorithms incorporating turbulence models, increasingly at second-moment level, will continue to play the main role in industrial applications for some years to come, but there is likely to be a continuous shift of emphasis towards LES, if only because transients arising from periodicity and turbulence are, in some situations, as important as the mean behaviour. Is is unlikely that LES will replace turbulence modelling altogether. The need to arrive at acceptably accurate answers at minimum cost will probably secure at least a spacious niche within CFD for model-based algorithms.

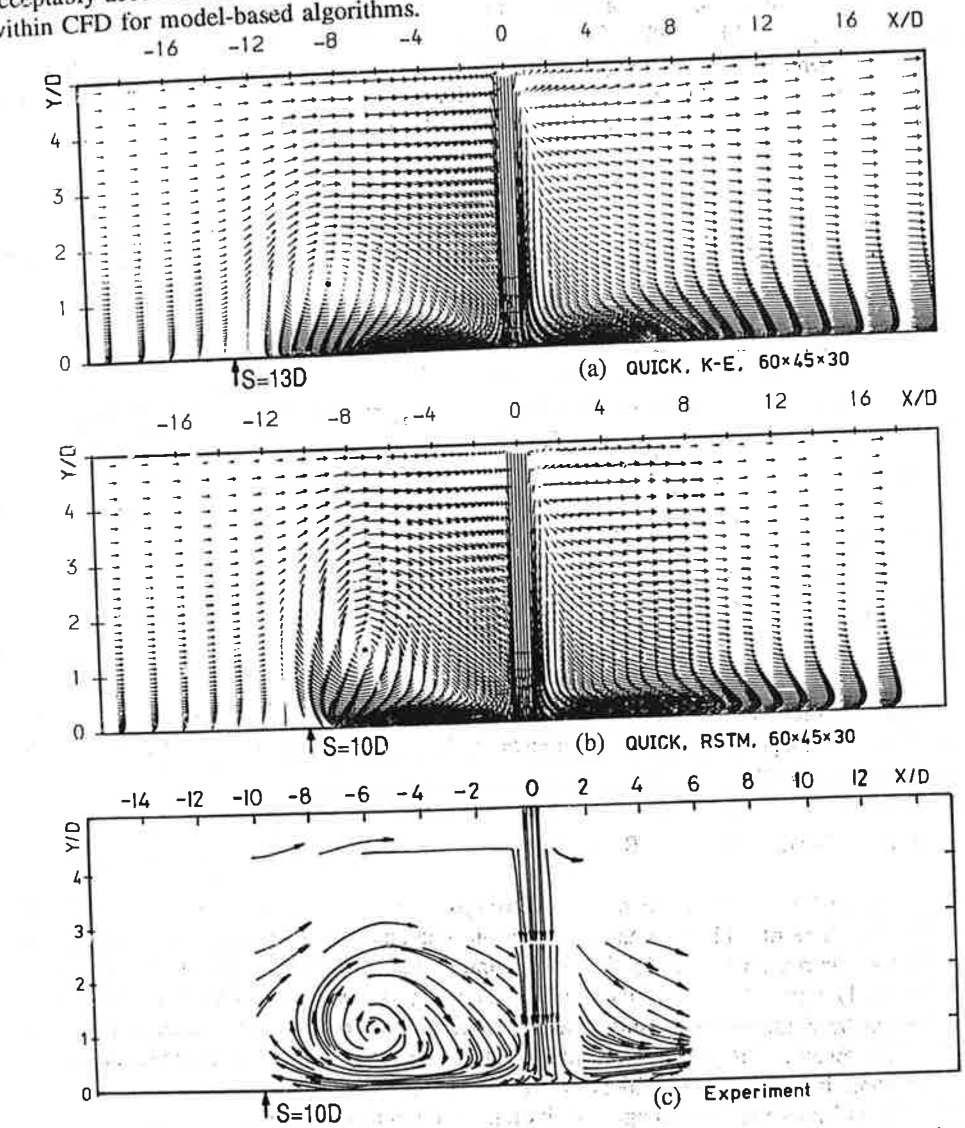

Fig. 12. Flow field in central plane of 3D impinging jet in cross-flow; (a) k-ε eddy-viscosity model, (b) Reynolds-stress-transport model (c) experiment (Ince and Leschziner [21]).

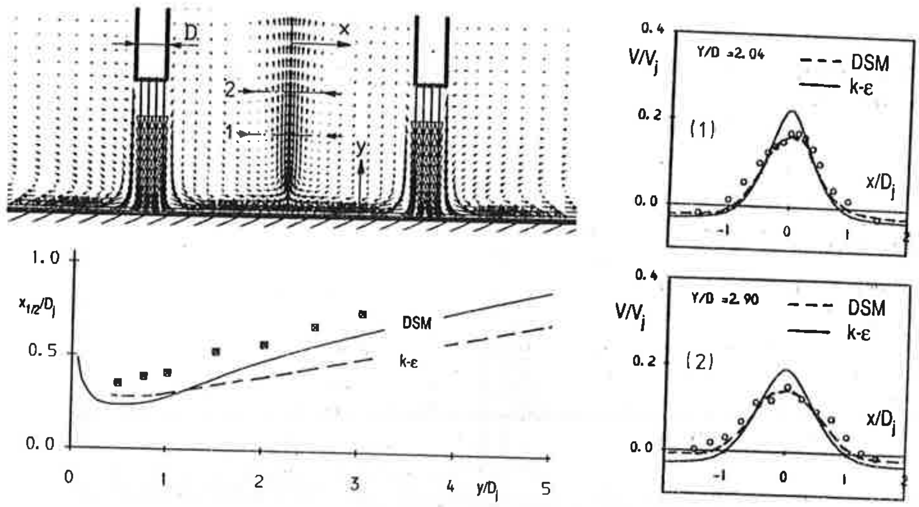

Fig. 13. Flow field, fountain half-width and fountain-velocity profiles in centre plane of twin-impinging jet, computed with k-ε eddy-viscosity model and Reynolds-stress-transport model (Ince [22])

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