Eighth Australasian Fluid Mechanics Conference, University of Newcastle, N.S.W., 28 November/2 December 1983.

FUNDAMENTAL CONSIDERATIONS IN COMPUTATIONAL FLUID MECHANICS

G.D. TONG

CONSULTING ENGINEER

25 HUNTINGDON DRIVE, GLENALTA, S.A. 5052 AUSTRALIA

SUMMARY This paper addresses two fundamental and related issues in the numerical modelling of high Reynolds number, incompressible flow; the treatment of advective transport and the modelling of turbulence. Both problems are shown to arise from the need to consider numerical solutions to the governing (Navier-Stokes) equations. Discretisation suggests the need to average physics in order to work in terms of economically resolvable lumped or averaged quantities and mean mechanisms (Reynolds decomposition and Boussinesq eddy viscosity concept) while formal identification of discretisation error shows the possibility of spurious numerical mixing. These considerations identify the important area of physics/numerics interaction. Flows containing zones of recirculation are shown to be a stringent testing ground for model development and results of the author's computations are used to illustrate the arguments in the context of environmental hydrodynamics (flow past a barrier) and a wind tunnel simulation (backward facing step).

NOTATION

C_μ optimised constant in the Prandtl-Kolmogorov law
$C_1, C_2, \sigma_k, \sigma_\varepsilon$ optimised constants in the k-ε equations
k turbulence kinetic energy
p pressure
q_{ij} Reynolds stress tensor
t time
u_i vector of time averaged (mean) velocity components
$\hat{u}_i$ vector of instantaneous velocity components
u'_i velocity fluctuation components
x_j Cartesian co-ordinate system (x,y,z)
ε dissipation rate of turbulence kinetic energy
λ penalty parameter
ν kinematic viscosity
ν_t eddy viscosity
ρ density of the fluid
ω_j vorticity

1. INTRODUCTION

Fluid Mechanics has traditionally been a subject rich in classical applied mathematical technique. It is therefore not surprising to find, since the advent of the digital computer, a vast literature on computational techniques in fluid mechanics. The old difficulties, with their unforgiving nature, remain, but the search for solutions proceeds as optimistic workers advance into battle with their established and evolving computational armoury. Progress has been made in achieving numerical solutions to classically intractable equations however it is the purpose of this paper to review two outstanding problem areas and their interaction which currently characterise difficulties in computational fluid mechanics; the representation of the physics of turbulence and the numerical treatment of advective transport.

2. THE ORIGIN OF THE PROBLEM

The starting point is the non-linear terms (2nd term) in the Navier-Stokes equations.

$$\frac{\partial \hat{u}_i}{\partial t} + \hat{u}_j \frac{\partial \hat{u}_i}{\partial x_j} + \frac{1}{\rho}\frac{\partial \hat{p}}{\partial x_i} = \nu \frac{\partial}{\partial x_j}\left(\frac{\partial \hat{u}_i}{\partial x_j}\right) \qquad (1)$$

These represent advective transport and are sometimes referred to as the convective acceleration or inertia terms. Being non-linear these terms, (e.g. $u\frac{\partial u}{\partial x} \equiv \frac{\partial \frac{1}{2}u^2}{\partial x}$), have the ability to transfer energy through the entire range of scales of motion from kilometres to millimetres. The transfer mechanism is best seen from the vorticity equation, easily obtained from the Navier-Stokes equations and containing a vorticity/strain-rate interaction term (3rd term) as a direct consequence of the non-linear terms in the Navier-Stokes equations.

$$\frac{\partial \hat{\omega}_i}{\partial t} + \hat{u}_j \frac{\partial \hat{\omega}_i}{\partial x_j} - \hat{\omega}_j \frac{\partial \hat{u}_i}{\partial x_j} = \nu \frac{\partial^2 \hat{\omega}_i}{\partial x_j^2} \qquad (2)$$

With reference to the conceptual vortex line model, (Bradshaw, 1976), the term represents energy transfer by the stretching and re-orientating of a vortex filament. Indeed, in three-dimensional motion, energy cascades to smaller and smaller scales of motion until it is finally dissipated away to heat energy against molecular viscous action.

If it were possible to obtain a general closed-form solution to the Navier-Stokes equations, in principle, there would be no further problem. This, unfortunately is not the case and recourse must be made to some averaged or mean description of the physics resolvable on a discretised domain.

3. ON AVERAGING EQUATIONS

3.1 Statistical Averaging

The traditional approach to averaging the physics is the so-called "statistical" approach (Reynolds, 1895) comprising the decomposition of each instantaneous dependent variable into a mean and a fluctuating component, e.g. $\hat{u} = u + u'$, and time or ensemble averaging each term of each equation. Essentially the averaging process filters the explicit behaviour of certain scales from the motion resulting in a mean flow field perturbed by additional fluctuating component terms. For an averaging time which is long, compared to the time scale of the largest eddies, a mean flow field is obtained which is completely devoid of any eddy structure (Rubesin, 1975).

Now in terms of the Navier-Stokes equations it is the non-linearity of the advective terms which produce correlations of the component velocity fluctuations that are not zero after application of the averaging rules (Hinze, 1959). These terms are identified as effective stresses (Reynolds stresses) and appear in the averaged Navier-Stokes equations, the Reynolds equations, with the role of influencing the mean motion in a manner consistent with the particular decomposition and averaging.

Following through this line of derivation one obtains the Reynolds equations as:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} - \frac{1}{\rho}\frac{\partial q_{ij}}{\partial x_j} + \frac{1}{\rho}\frac{\partial p}{\partial x_i} = \nu \frac{\partial}{\partial x_j}\left(\frac{\partial u_i}{\partial x_j}\right) \qquad (3)$$

where $q_{ij} = -\rho\, \overline{u_i' u_j'}$ is the Reynolds stress tensor.

The final step to the usual working equations is to introduce the Boussinesq eddy viscosity assumption which links turbulence (Reynolds) stresses and mean strain-rate in a manner analogous to a viscous fluid in laminar motion,

$$-\rho\, \overline{u_i' u_j'} = \rho \nu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \qquad (4)$$

where ν_t is the flow dependent eddy viscosity which becomes the coefficient for the whole process of instantaneous turbulence energy or momentum transfer now represented as a diffusion mechanism.

On neglecting viscous stresses, $\nu << \nu_t$,

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} + \frac{1}{\rho}\frac{p}{\partial x_i} = \frac{\partial}{\partial x_j}\left(\nu_t \frac{\partial u_i}{\partial x_j}\right) \qquad (5)$$

The point to appreciate here is the huge departure from the physics of energy transfer between different scales of motion (the energy cascade) as represented by non-linear advection in the Navier-Stokes equations and the mean flow behaviour with only facility for diffusion of momentum as represented by the Reynolds equations and Boussinesq eddy viscosity concept.

3.2 Large Eddy Simulation

It is to be noted in passing that considerable advances have been made over the traditional approach outlined above in the form of direct simulation of the large eddy structure, see for example Leonard (1974) or Ferziger (1977). This approach is based on the sound idea of controlled filtering of the basic equations such as to sub-grid model only the small eddy structure up to a predetermined level leaving the large scales for explicit determination from an unaveraged description. The method shows enormous potential but, predictably, computing demands are heavy and the method is yet to be established as a practical engineering tool for the computation of turbulent flows. For the remainder of this discussion attention will be confined to the statistical approach.

4. NUMERICAL MIXING

Attention has so far been directed to the representation of physical processes in a computational model of turbulent flow. Having gone through some severe simplifying stages, equation (5) evolved as representing both mean flow advection and non-linear diffusion of momentum.

It is appropriate now to focus on the numerical discretisation of such an equation. Here again it is the advective (hyperbolic) part of the equation that is the most troublesome. It is not so much the non-linearity of the advection term which is the problem (regardless of the discretisation method some enforced linearisation is required), but rather the discrete representation of first derivatives.

To illustrate the problem a first-order discrete approximation to the one-dimensioned, linearised, equation representing pure advection is analysed.

$$\frac{\partial u}{\partial t} + \bar{u}\frac{\partial u}{\partial x} = 0 \qquad (\bar{u} > 0) \qquad (6)$$

Taking simple first order differences in space and time yields the discrete equation:

$$u_j^{n+1} = (1 - C_r)\, u_j^n + C_r . u_{j-1}^n \qquad (7)$$

where $C_r = \bar{u}\frac{\Delta t}{\Delta x}$, the Courant number.

Expanding in Taylor Series about the central discrete point (j,n) returns the differential equation:

$$\frac{\partial u}{\partial t} + \bar{u}\frac{\partial u}{\partial x} = \nu_N \frac{\partial^2 u}{\partial x^2} + D_N \frac{\partial^3 u}{\partial x^3} + \text{higher order terms} \qquad (8)$$

Comparison with (6) shows how such a first order difference scheme introduces two additional error type terms which add spurious physics; numerical diffusion (second derivative) and numerical dispersion (third derivative) with their grid dependent coefficients ν_N and D_N respectively.

It is precisely these discretisation error terms which lead to unsatisfactory numerical results. Diffusion generally results in an over-damped solution field whereas dispersion manifests itself in the form of phase error. Thinking of a solution field in terms of component modes, dispersion is the spatial spreading of modes, one with another, due to errors in wave propagation speeds, and underlies the often encountered oscillatory behaviour of numerical solutions. Of course the effects are most severe where gradients in the solution field are steep, i.e. grid resolution least, however the two effects should be considered together while recognising them as separate distinct mechanisms. For a more complete discussion of this see Tong (1980).

The discussions so far have elucidated the problem areas stated in the introductory remarks. It is apparent that in the computation of turbulent flow one must be looking for a turbulence closure to set mean flow dependent eddy viscosity (representing turbulence momentum transfer) throughout a flow field and to be using computational methods relatively free of numerical mixing.

5. A COMPUTATIONAL PROCEDURE

One computational procedure developed by the author on the basis of the forgoing requirements is the use of the two-equation k-ε turbulence model developed at Imperial College, London and the finite element method applied to both the mean flow (Reynolds) equations and the two further field equations, one for k the turbulence kinetic energy and the other for ε, its dissipation rate.

The k-ε model was chosen because it is derived directly from the Navier-Stokes equations with only three main assumptions further to the Reynolds decomposition. They being:

(i) isotropy,
(ii) the Boussinesq assumption (introduced earlier),
(iii) the Prandtl-Kolmogorov relationship,

$$\nu_t = C\mu \frac{k^2}{\varepsilon} .$$

Derived on this basis, the k-ε model is then the simplest turbulence model not requiring an imposed length scale (or equivalent) input and thereby it attains a unique position within the hierarchy of turbulence models. Details of the model can be found in the primary reference, Launder and Spalding (1974) and a full self-contained derivation is given in Tong (1982)[1].

The finite element method was chosen primarily on its facility for ease of grid refinement in regions of steep gradients and its ability to handle irregular geometries. The nature of the finite element as an integral formulation and hence the so-called natural boundary condition, (arising from a Greens Theorem reduction of second derivatives), later became an important link in the solution algorithm between the mean flow model and the turbulence model. Details of the special boundary module developed to handle flow along a solid boundary can be found in Tong (1982)[2].

It is sufficient here to give the broad outline of the algorithm in terms of the two-dimensional mean flow equations (penalty function formulation) and the k and ε equations. The mean flow model feeds a velocity and strain rate field to the turbulence model and in turn receives an update on the eddy viscosity field.

Mean Flow Model

$$u\frac{\partial u}{\partial x} + w\frac{\partial u}{\partial z} - \frac{\lambda}{\rho}\frac{\partial}{\partial z}\left(\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z}\right) = 2\frac{\partial}{\partial x}\left(\nu_t\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial z}\left(\nu_t\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)\right)$$

$$u\frac{\partial w}{\partial x} + w\frac{\partial w}{\partial z} - \frac{\lambda}{\rho}\frac{\partial}{\partial z}\left(\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z}\right) = \frac{\partial}{\partial x}\left(\nu_t\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)\right) + 2\frac{\partial}{\partial z}\left(\nu_t\frac{\partial w}{\partial z}\right)$$

Newton-Raphson non-linear iteration

Turbulence Model

$$u\frac{\partial k}{\partial x} + v\frac{\partial k}{\partial y} = \frac{\partial}{\partial x}\left(\frac{\nu_t}{\sigma_k}\frac{\partial k}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{\nu_t}{\sigma_k}\frac{\partial k}{\partial y}\right) + P_h - \varepsilon$$

$$u\frac{\partial \varepsilon}{\partial x} + v\frac{\partial \varepsilon}{\partial y} = \frac{\partial}{\partial x}\left(\frac{\nu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{\nu_t}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial}\right) + C_1\frac{\varepsilon}{k}P_h - C_2\frac{\varepsilon^2}{k}$$

$$\text{where } P_h = \nu_t\left\{\left(\frac{\partial u}{\partial x}\right)^2 + 2\left(\frac{\partial w}{\partial z}\right)^2 + \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)^2\right\}$$

Picard Substitution non-linear iteration

Figure 1 Series Solution Algorithm

6. EXAMPLE COMPUTATIONS FOR RECIRCULATING FLOWS

Finally some results of example calculations are given. Flows containing zones of recirculation are chosen for the reasons that they are a class of flow which exercises to good effect the ideas presented. They are challenging in that they inevitably arise in complex geometries where there is associated flow separation, an inducing main stream flow, turbulence momentum transfer through a shear layer and region of reattachment. The application areas to which they apply are diverse, e.g. environmental flows in a complex estuary or around a breakwater, flows in complex geometries as might be found in industrial plant or over complex aerodynamic shapes as encountered in the aircraft industry. Additionally, there is beginning to be amassed a large body of experimental data for test cases (see proceedings, Stanford Conference, 1980-81) and hence such flows are beginning to find popularity as a testing ground for advanced computational techniques.

The prototype problem can be formulated as follows.

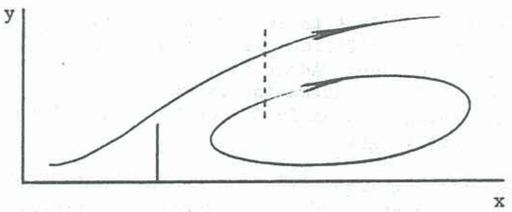

Figure 2 Prototype Recirculating Flow

Consider flow past a barrier and a particle executing mean streamline circulation. In the event of losing energy to the boundary friction of the containing vessel and to smaller scales of motion, the motion of that particular particle would die out unless there is a sustaining energy transferred into the recirculating zone from outside the region and necessarily across mean streamlines. Such is the job of the turbulence model; to effect turbulence momentum transfer as a diffusion process which means setting the eddy viscosity or turbulence diffusion coefficient to achieve a net effect on the mean flow reasonably consistent with the non-linear energy cascade represented in the Navier-Stokes equations. The job of the numerics is to implement the physics as intended by the derived differential equation set without the introduction of any significant numerical mixing.

6.1 Flow Past a Breakwater

The example of depth averaged flow past a breakwater is used to illustrate numerical dispersion and the consequence of execessive diffusion giving an overdamped solution.

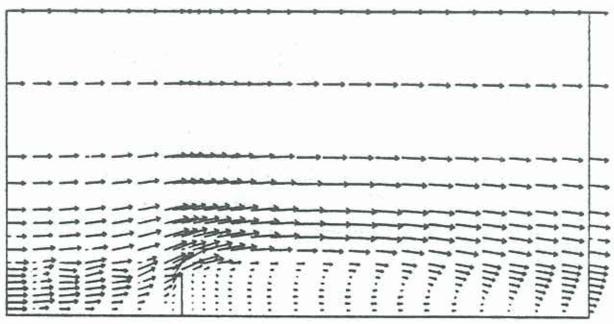

Figure 3a $\nu_t = 0.005 m^2/s$.

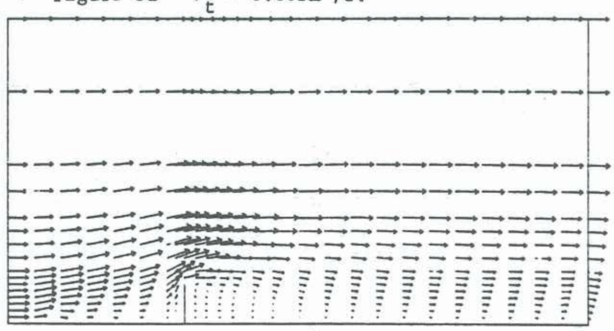

Figure 3b $\nu_t = 0.05 m^2/s$.

In Fig.3a the effect of numerical dispersion, thought of as the spatial spreading of component modes, is evident in the oscillatory nature of the velocity vector pattern upstream of the breakwater tip. This is the effect of 3rd and higher order odd derivative error terms which become significant through the gradients associated with the step change in the longitudinal velocity component which is seen to exist in moving from the near wall to the free-stream side of the breakwater tip.

In Fig.3b the effect is seen of arbitrarily increasing the diffusion coefficient as a blanket value by an order of magnitude. Admittedly the approach field is more realistic but attention is drawn to the heavily damped eddying zone as indicated by a hugh decrease in reattachment length.

The example highlights the above-mentioned minimum aims of turbulence modelling, accurate numerics and a turbulence model to represent the physics of turbulence momentum transfer as it varies over the flow field.

6.2 The Backward Facing Step

Flow past a backward facing step or sudden expansion has come to be a classical example of recirculating flow. Results, using the algorithm of Fig.1, are given here in terms of mean flow profiles, turbulence kinetic energy and Reynolds stress at approximately mid-recirculation zone downstream of the step face, at $x/h = 3$, where h is the height of the step.

The results are compared with the pulsed-wire experimental results of Baker (1977) and are seen to be in encouraging agreement. Details of the simulation have been reported in Tong (1982)[2,3] and the computing requirement to reach convergence on a finite element mesh of 96 quadratic quadrilateral elements (427 nodes) was approximately 6 minutes CPU time on the CDC 7600 of the Manchester Computing Centre.

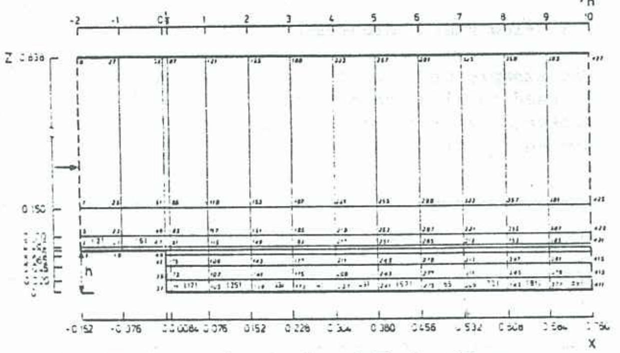

Figure 4 Mesh - Backward Facing Step Experimental Rig Baker (1977)

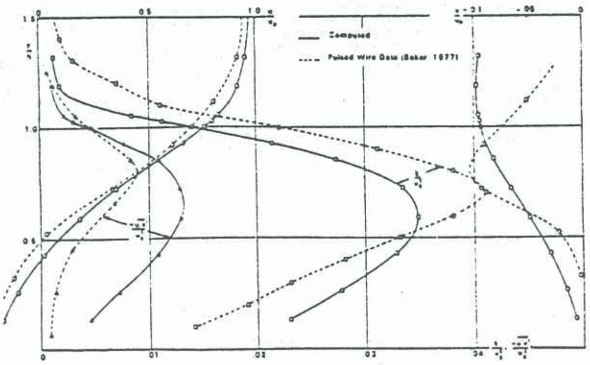

Figure 5 Results at $x/h = 3$ - Backward Facing Step

7. CONCLUDING REMARKS

Major difficulties in accurately modelling high Reynolds number, incompressible flows have been presented. These fall broadly onto the areas of first deriving an appropriate mathematical description of the physics and then finding a discrete (numerical) solution of that representative physics without undue introduction of spurious numerical effects.

Progress has been made towards the computational flume or wind tunnel in that turbulence quantities, comparable in credibility with experimental data, can be computed for complex flows. The basic nature of the problem, which this paper has sought to address, is so demanding that one must conclude that the strategy of formulation, numerical solution and verification against results from an on-going experimental programme will prevail for some time. Factors such as compressibility and buoyancy add further complication.

On the formulation side, the large eddy direct simulation approach of Stanford University must be seen as one of great potential given the projected role of hardware development while the demands on simulation of the profound differences between two- and three-dimensional inertial characteristics is suggested as an outstanding area for investigation (Tong, 1982[3]).

8. REFERENCES

BAKER,S. (1977) Regions of Recirculating Flow Associated with Two-Dimensional Steps. Ph.D. Thesis, University of Surrey.

BRADSHAW,P. (1976)(editor) Turbulence, vol.12. Topics in Applied Physics. Springer-Verlag, Berlin, p.8.

FERZIGER,J.H. (1977) Large Eddy Numerical Simulations of Turbulent Flows, AIAA Journal, vol.15, 9, pp.1261-1267.

HINZE,J.O. (1959) Turbulence, McGraw-Hill,New York,p.6.

LAUNDER,B.E. & SPALDING,D.B. (1974) The Numerical Computation of Turbulent Flows. Computer Methods in Applied Mechanics and Engineering, 3, pp.269-289.

LEONARD,A. (1974) Energy Cascade in Large Eddy Simulations of Turbulent Fluid Flows. In: Advances in Geo-Physics, vol.18A (editors) F.N.Frenkiel and R.E.Munn. Academic Press, pp.237-248.

RUBESIN,M.W. (1975) Subgrid - or Reynolds Stress - Modelling for Three-Dimensional Turbulence Computations. Aerodynamic Analysis Requiring Advanced Computers-Part I. NASA Report SP-347, pp.317-339.

STANFORD CONFERENCE (1980-81) Proceedings of the (1980-81) AFOSR-HTTM-Stanford Conference on Complex Turbulent Flows, published 1983.

TONG,G.D. (1980) Environmental Hydrodynamic Modelling - Problem Identification and a Strategy to Model Assessment. Chapt.25 of Industrialised Embayments and their Environmental Problems (eds.Collins,M.B. et.al.), Pergamon Press, Oxford, pp.383-392.

TONG,G.D. (1982)[1] Computation of Turbulent Recirculating Flow. Ph.D. Thesis, University of Wales.

TONG,G.D. (1982)[2] A Treatment of Wall Boundaries for (k-ε) Turbulence Modelling Within an Integral (Finite Element) Formulation. Proceedings: Fourth International Symposium, Finite Elements in Flow Problems, Tokyo, July, 1982.

TONG,G.D. (1982)[3] Computation of Recirculating Flows in Two-Dimensions Using Finite Elements and the k-ε Model. Proceedings: IAHR Symposium on Refined Modelling of Flows, Paris, September, 1982, pp.343-353.

9. ACKNOWLEDGEMENTS

The computational results presented herein were obtained as part of a research contract supported by Hydraulics Research Station, Wallingford, and carried out in the Department of Civil Engineering, University of Wales, Swansea, U.K.