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ABSTRACT

This paper discusses the extension of the FLOW3D code to handle flows in complex geometries using Body–Fitted Coordinates. The code uses a new algorithm, that of Rhie and Chow, to deal with the problems in a simple and efficient manner using non-staggered grids. This technique is briefly explained and its implementation in the code outlined. Other enhancements to the code are also described. Finally, the code is applied to a number of test problems. These are the laminar flow in a curved duct, for which accurate finite element results are available, and the turbulent flow in a rectangular box. A variety of grid distributions are used in the latter case and the results are compared with FLOW3D results using the standard algorithm. The results are in good agreement with the benchmark cases and they clearly demonstrate the ability of the code to handle problems in complex geometries.

1 INTRODUCTION

Details of the first release of the FLOW3D code for the prediction of laminar and turbulent flow have been presented by Jones, Kightley, Thompson and Wilkes (1985). This code has the aim of being used both for the prediction of realistic flows and as a vehicle for the development of physical models and advanced numerical methods. The code and its use are extensively documented in the user manuals, Jones et al (1986), Jones and Hanson (1986), and some applications of the production version of the code are described by Wilkes (1985a), McPherson (1985), and Burns and Jones (1986). Many other practical problems have been solved using the code, although the results have not yet appeared in the open literature. The code has also been used to investigate more advanced turbulence models and Wilkes (1986) has introduced an algebraic stress model into an experimental version of the code. This has been applied to several problems with strong curvature of the stream-lines, for which the standard turbulence model in the code, the $k - \varepsilon$ model, is known to have certain deficiencies.

This paper discusses enhancements to FLOW3D that have taken place, particularly the extension to deal with complex geometries using Body–Fitted Coordinates.

2 BODY-FITTED COORDINATES

There have been a number of different ways to extend the use of finite difference codes to the case of complex geometries. Most of these transform the coordinate system into one which matches the geometry, hence the term Body–Fitted Coordinates. Another approach has been to partially block off bounding cells. This, however, does not lead to a rational implementation of the no-slip condition and it is not always clear exactly where the boundary is located. Orthogonal grid systems are fairly straightforward to implement and several codes have been written for turbulent flow prediction using orthogonal grids, see for example Wilkes (1985b). In two-dimensions it is reasonably straightforward to generate orthogonal coordinates for any geometry, for example by conformal mapping. In three-dimensions it is not obvious how to generate orthogonal grids and indeed, it may not always be possible. Furthermore, it is desirable to have additional flexibility in choosing a grid to concentrate grid lines where the flow is changing rapidly. Great emphasis has been placed, therefore, on the use of grids which are non-orthogonal. Researchers have, however, experienced considerable difficulties with the use of non-orthogonal grids for incompressible flow predictions. The principal technique that has been adopted is to use staggered grids and velocity components perpendicular to the surfaces defined by grid lines. These are often referred to as the 'contravariant' velocity components. This configuration is sketched in Figure 1a. The approach leads to systems of equations which are more complicated than the standard form which uses Cartesian velocity components. Early attempts to use systems based upon non-staggered grids were not successful and led to 'chequerboard' oscillations in the pressure field. This made it difficult to implement non-orthogonal grid systems with the momentum equations based upon Cartesian velocity components. In particular, there were difficulties satisfying the mass conservation equation accurately, and many treatments instead used a Poisson equation to determine the pressure.

A remarkable breakthrough in the treatment of body-fitted coordinates for incompressible flow problems has been recently published by Rhie and Chow (1983). These authors have devised a successful method to use both non-staggered grids and Cartesian velocity components without encountering chequerboard oscillations. The paper which describes the technique really concentrates on the application of the method to the flow over an airfoil and its significance might easily have been lost. A.D. Gosman and co-workers, however, realised the potential of the method and have extensively applied it to a series of challenging problems, see for example Peric (1985). Their results have amply demonstrated the success of the technique.

Whilst the technique is based upon non-staggered grids, there still remains an underlying staggered grid and the concept of a mass control volume in which there is a discrete conservation of mass. The success of the algorithm is due to a method for relating the Cartesian velocity components at the centre of the mass control volume to the velocity components normal to the faces of the mass control volume. This is illustrated in Figure 1b. The exact details of the interpolation are beyond the scope of this paper. They may be found instead in Rhie and Chow (1983), Rhie (1981) or in Burns and Wilkes (1986).

The difference equations for the remaining terms in the governing equations may be obtained in two different ways. The first method is a coordinate transformation method. The physical coordinates are transformed to ones where the boundaries of the domain lie along coordinate directions. A uniform grid in the transformed coordinates is then adopted.

In the second method a grid consisting of distorted rectangles in two dimensions or distorted 'bricks' in three-dimensions is superimposed upon the computational domain. The grid is chosen so that grid lines lie along the boundaries of the problem. It is usual, although not necessary, to restrict the grid to be 'topologically cuboidal'. That is, it can be distorted, without tearing, into a conventional finite-difference grid. This assumption has many advantages for the numerical treatment. These advantages are discussed later in this paper.

The relevant difference equations are obtained in both cases by integrating the differential equations over each mass control volume, ensuring discrete conservation of momentum and energy. This is a much simpler process than that for staggered grids since the same control volume is used for each of the equations. The two procedures for obtaining the difference equations are very closely related. The main difference arises from the methods used to interpolate quantities to points other than at grid nodes. FLOW3D uses weight factors based upon the physical distances between points and does not assume that the points are uniformly spaced in a transformed coordinate. This should give better accuracy when the grid is highly distorted.

It should be noted that the Cartesian velocity components which are obtained do not satisfy a discrete mass conservation relationship. Instead they satisfy the mass conservation equation to third order in the local step size. The normal velocity components to the faces of the mass control volumes may be easily obtained however and thes do satisfy discrete mass conservation.

3 IMPLEMENTATION IN FLOW3D

The production version of FLOW3D has been restructured internally in order to increase the flexibility of the code and to pave the way for further new features. Care has been taken, however, to ensure that the code can tackle the problems solved by Release 1 in an efficient manner. For example, body-fitted coordinate systems require significantly greater amounts of memory to handle the non-orthogonal nature of the grid. The code has been structured, therefore, only to use this additional memory when the grid is non-orthogonal. Hence problems on Cartesian grids take considerably less memory than those using full body-fitted grids. The additional memory requirements should not prove to be a problem on most computer systems because of the use of virtual memory and the availability of much larger real memory on supercomputers such as the Cray XMP and the Cray 2. For a problem on a Cartesian grid there should also not be a penalty in CPU time due to the algorithm of Rhie and Chow.

At the same time, the treatment of the boundary conditions for inflow and outflow are being enhanced. For example, it should be possible to specify a pressure drop across the system and for the code to compute the relevant flow rates. It is also possible to approximate a fully developed profile at an inlet without doing a preliminary calculation to obtain the profiles of the variables across the inlet. These facilities improve the ability of FLOW3D to compute realistic engineering flows.

Because of the separation of the user's input from the solution process by means of the frontend a large degree of upward compatibility can be maintained between Release 1 and Release 2. Different input modules have been written, however, to allow the full power of the code to be used. Users who specify their input through the high level Command Language Frontend should experience no difficulties whatsoever in converting their input to Release 2.

There have also been many internal improvements in the software in order to improve its flexibility and speed. For example, the Frontend module has been speeded up considerably through a combination of improved searching techniques and simplifications due to the use of non-staggered grids. Optimisation of the internal data structures may also be applied in order to obtain greater gain from particular facets of the computer architecture.

The basic numerical algorithms used to solve the system of discrete equations are essentially unchanged, although there have been some improvements over those described in Jones et al (1985). For example, the SIMPLEC algorithm has been implemented in both Release 1 and Release 2. This gives a greater degree of reliability and robustness over the original algorithm. For example, the CPU times reported in Jones et al (1985) have now been halved with Release 1 through modifications to the solution strategy, see Kightley (1985). When the grid is non-orthogonal the difference molecules are no longer of the seven point form found with orthogonal grids in three dimensions. Instead they may have up to nineteen points present. The solution techniques employed for the difference equations have been enhanced to deal with these extended difference molecules. The linear algebra and the coding are considerably simplified by restricting the grid to be topologically cuboidal. Furthermore, it enables much more efficient techniques to be adopted and permits a greater degree of vectorisation on supercomputers.

A comprehensive library of physical properties has been introduced. This includes common fluids such as air and water, and also fluids which are of particular interest in nuclear energy applications, for example, liquid sodium, argon and carbon dioxide. This library has been written such that the bulk of it vectorises, and hence it is efficient to use variable physical properties in calculations.

At the time of writing, the code only handles incompressible flows, but it is anticipated that variable density and full compressibility will be available shortly. This is a necessary step for the implementation of combustion models.

Users of Release 1 have found the ability to treat combined conduction in solids and convection in fluids to be very useful and the code is being extensively used on many problems involving conduction-only regions. Furthermore, the conducting medium may have different thermal conductivities in each of the different coordinate directions and also have discontinuous thermal properties at the edges of mass control volumes. These facilities are being carried over to Release 2.

As FLOW3D has used a finite element graphics package, OUTPROC, see Winters and Jackson (1986), the graphics carries over virtually unchanged from Release 1. Many enhancements have, however, been introduced into OUTPROC and its flexibility increased. In particular, there is now a neutral plot file facility which enables interfaces to be written for other graphics packages. For example, IBM GDDM mainframe graphics and IBM PC graphics are now available.

4 GRID GENERATION

Grid generation is a severe problem for any code which can handle complex boundary shapes, particularly in three-dimensions. Only minimal grid generation facilities have been included within FLOW3D. The aim, instead, is to provide an easy interface to outside packages and preprocessors which can provide suitable grids. The main reason behind the decision to provide only limited facilities within FLOW3D for grid generation is the widespread availability of commercial packages for finite element and finite difference grid generation. These may be found in codes such as the Harwell finite element package TGIN, Winters and Jackson (1984), and in the well known TOMCAT package for two-dimensional grids, Thompson et al (1977). Most large laboratories also have access to computer aided design packages which can be used for generating suitable grids. Further details of techniques used for grid generation may be found in Thompson (1982) and Thompson, Warsi and Mastin (1982).

A separate grid-generation preprocessing package is being constructed specifically for use by FLOW3D. The principal technique adopted by this package is based upon the concept of 'transfinite interpolation', Gordon and Hall (1973). This enables grids to be determined fairly easily for a wide variety of boundary shapes. The user can also grid different parts of the computational domain separately and join them across interfaces. These grids may then be smoothed to eliminate slope discontinuities across the interfaces. Further flexibility is obtained through the use of dummy grid nodes inside solid regions. This enables multiply connected regions to be handled easily. Figure 2 shows a grid obtained for a sector of an annular region which contains a circular solid region. It is, in fact, a horizontal section through a model of a fast reactor pool where the circular region represents a pump. The grid was obtained by transfinite interpolation followed by some smoothing. The circular region inside the grid is treated as a solid by the code and the grid nodes within this circle are ignored. Alternatively, they may be used for conduction calculations within the solid.

5 EXAMPLE OF USE

At the time of writing, the production version of the code is being tested and validated on laminar and turbulent flow problems for which the solutions are known.

Accurate results for the two-dimensional laminar flow in a curved duct have been obtained by Cliffe et al (1982) using the Harwell finite element package TGSL. These were taken as the benchmark for a recent comparison exercise for flows in complex geometries, see Napolitano and Orlandi (1985). These results have also been used to validate FLOW3D. Figures 3a-c show the configurations and a 22 × 22 body-fitted grid for each of the three test problems. Figures 4,5 and 6 show a comparison between FLOW3D results using three different grids and the finite element code results for the wall vorticity and the wall pressure on the curved wall. The agreement is very good in all these cases and the results show the right trends as the grid is refined. The treatment of the pressure field at a solid boundary is different from that adopted in the earlier release of FLOW3D. It is pleasing to note that the treatment of the pressure at the boundary gives good results with no trace of any chequerboard oscillations.

Turbulent flows have been tested by solving many problems within a rectangular exterior boundary but with a non-orthogonal grid in the interior. The results have been compared with FLOW3D Release 1 results using a Cartesian grid. The grid configurations that were used for one particular case, the flow over a backward facing step, are shown in Figure 7. These include one rectangular grid and two non-orthogonal grids with differing degrees of non-orthogonality. Figures 8 give a comparison between the results for the streamwise component of the velocity at different downstream locations for this particular case. The agreement between the results is very good. In Figures 9 the turbulent kinetic energy at different downstream locations is compared. This is a quantity which is very sensitive to differences in numerical treatment. The agreement between the Release 2 results with the different grids is good but there are small systematic differences between these results and the Release 1 results. Bearing in mind the coarse nature of the grid the differences are still small and may be due to the different treatments of the grid staggering.

Further computations are being carried out and more detailed results, and comparisons with experiments, will be presented at the 1986 HTFS Research Symposium.

6 FUTURE DEVELOPMENTS

Compressible flows have a high priority in the development programme of FLOW3D and a compressible version of the code will soon be available. Combustion models will be incorporated into FLOW3D shortly after this.

More speculative developments are being carried out in conjunction with Dr. S. Flood of the Dept. of Metallurgy and Science of Materials at the University of Oxford to predict free surfaces and solidification fronts. The application here is to metal casting and other metallurgical problems. The treatment adopted is to move the grid adaptively with the free surface and the solidification front in order to give a sharp representation of the interfaces. The same treatment should also be applicable to adaptive gridding. This time the aim is to concentrate the grid lines in regions where the errors are largest.

7 CONCLUDING REMARKS

The algorithm of Rhie and Chow has provided, in the authors' opinion, a remarkable breakthrough in the treatment of flow problems in complex geometries. This has enabled FLOW3D to have a reasonable compromise between the geometric capability of finite element methods and the speed and efficiency of finite difference methods, particularly in three-dimensions. It also opens up the way forward to many new applications and to give improved accuracy through the use of adaptive gridding. There will, of course, be problems along the way but there is an exciting time ahead as new and challenging problems can now be solved through the combination of new algorithms, reduced computing costs, large computer memories and new computer architectures.

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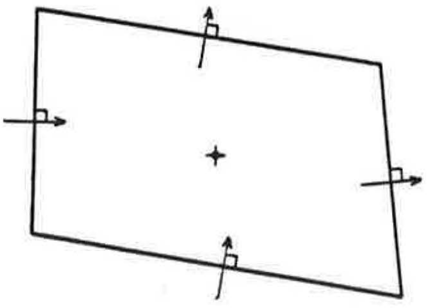


Fig. 1a. Mass control volume illustrating the use of velocity components normal to the faces of the mass control volume, and the scalar quantities at the centre of the mass control volume.

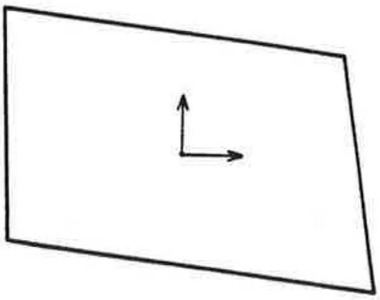


Fig. 1b. Mass control volume illustrating the use of Cartesian velocity components and scalar quantities all located at the centre of the mass control volume.

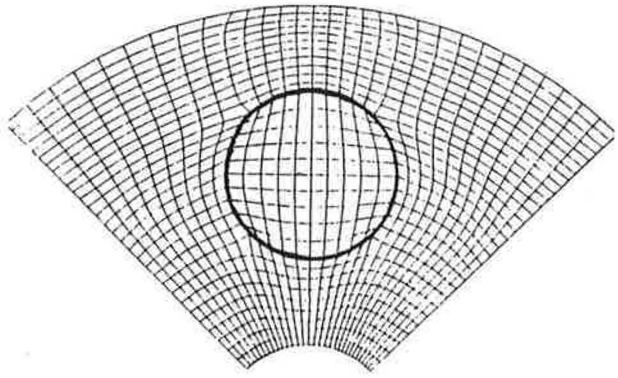


Fig. 2. Grid obtained in the sector of an annular region containing a circular solid region.

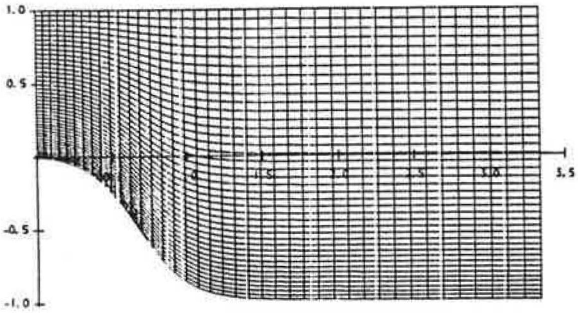


Fig. 3a. Geometry and grid, curved duct problem 1.

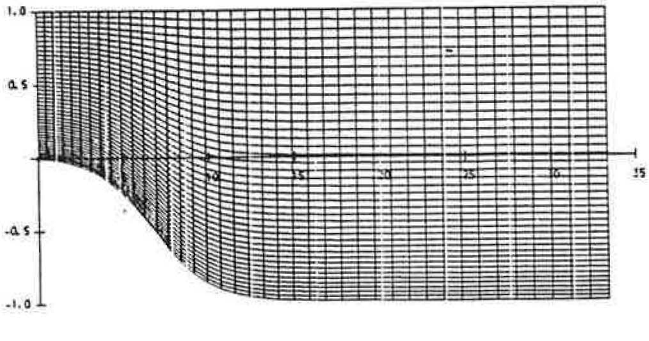


Fig. 3b. Geometry and grid, curved duct problem 2.

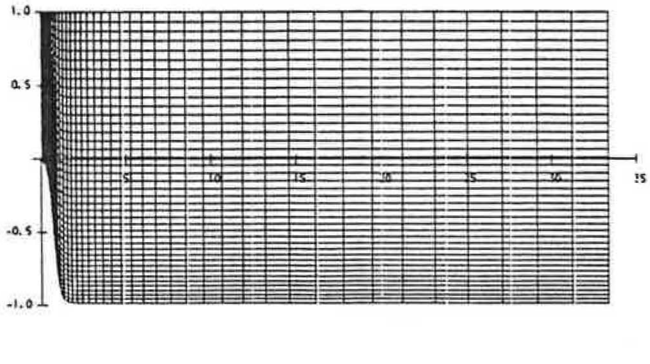
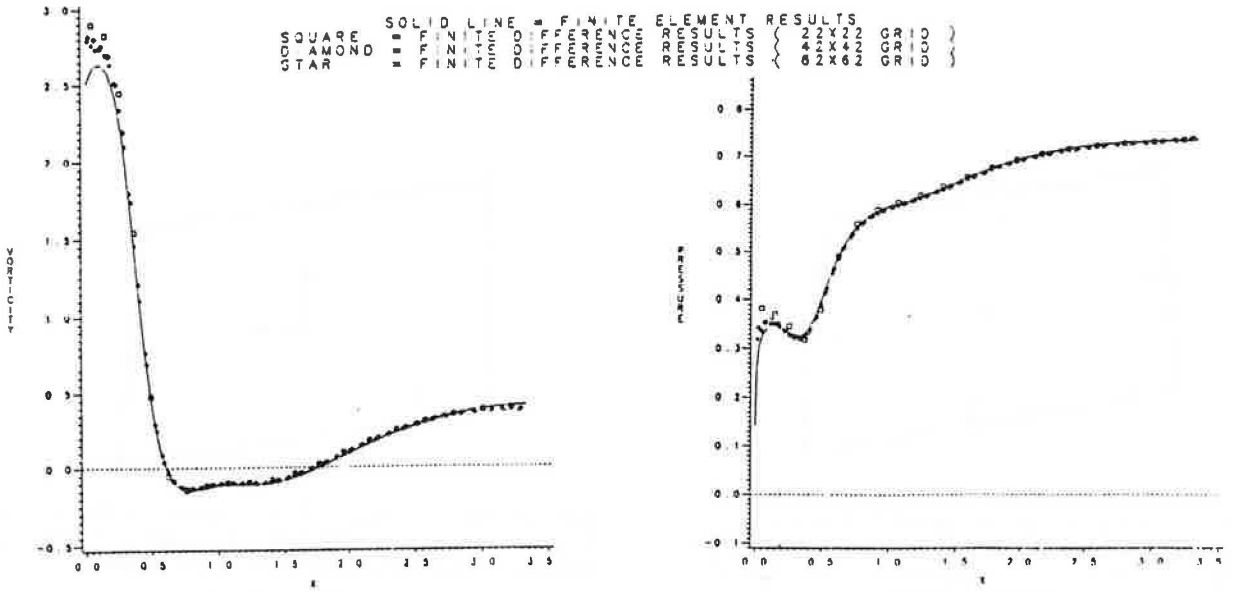


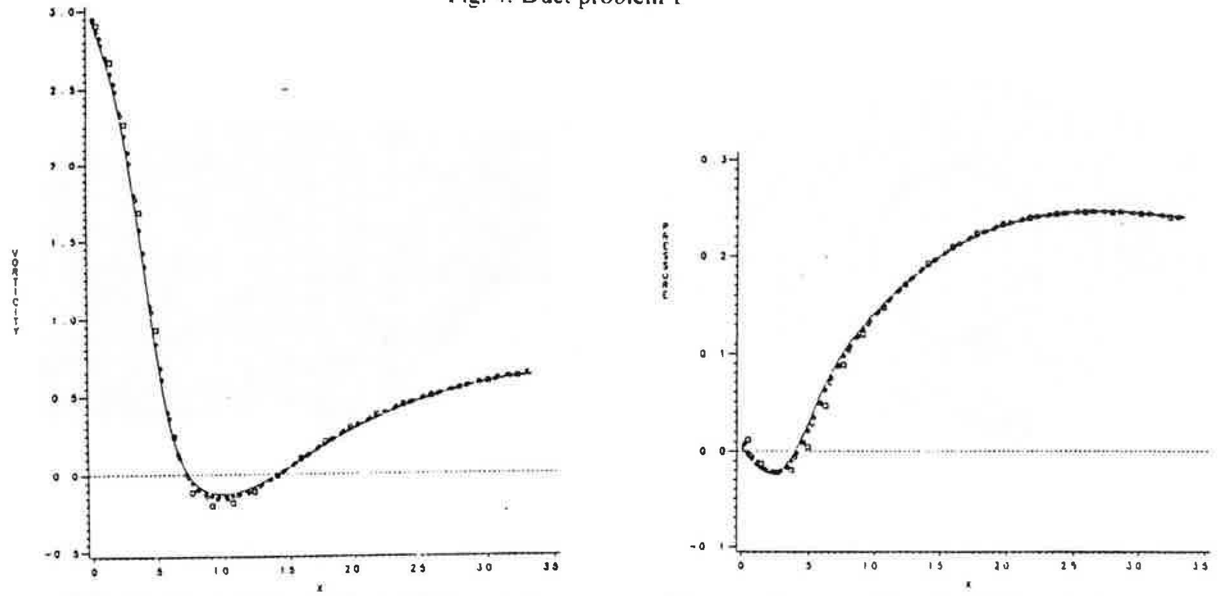
Fig. 3c. Geometry and grid, curved duct problem 3.



a) wall vorticity

b) wall pressure

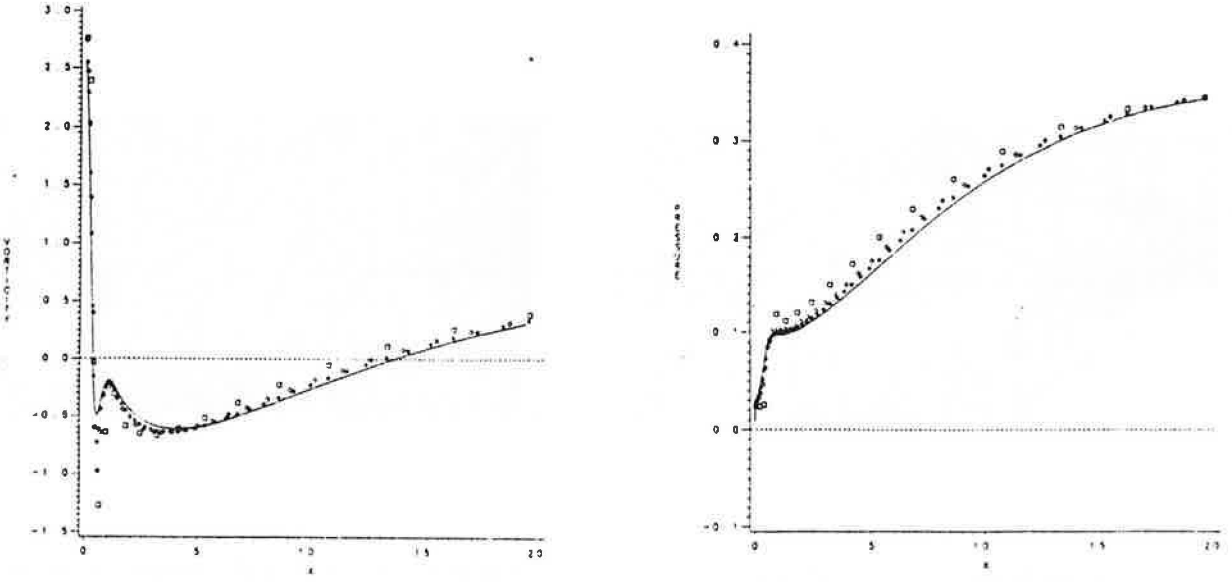
Fig. 4. Duct problem 1



a) wall vorticity

b) wall pressure

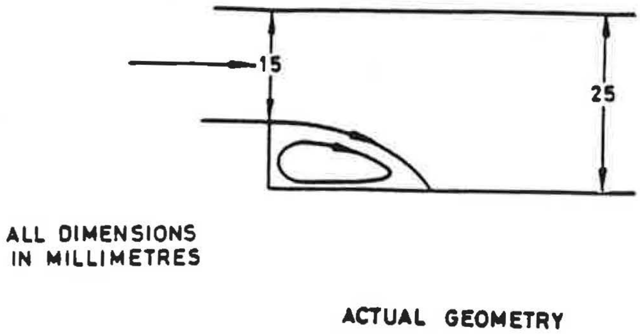
Fig. 5. Duct problem 2

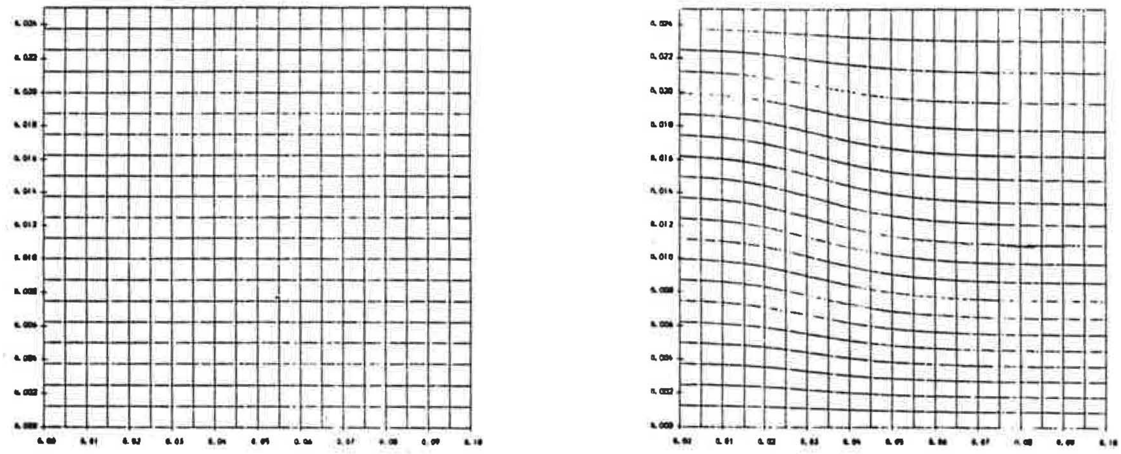


a) wall vorticity

b) wall pressure

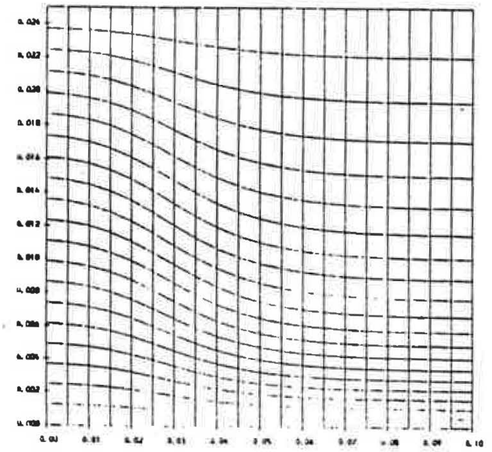
Fig. 6. Duct problem 3





a) grid stretching factor 0.0
(Cartesian grid)

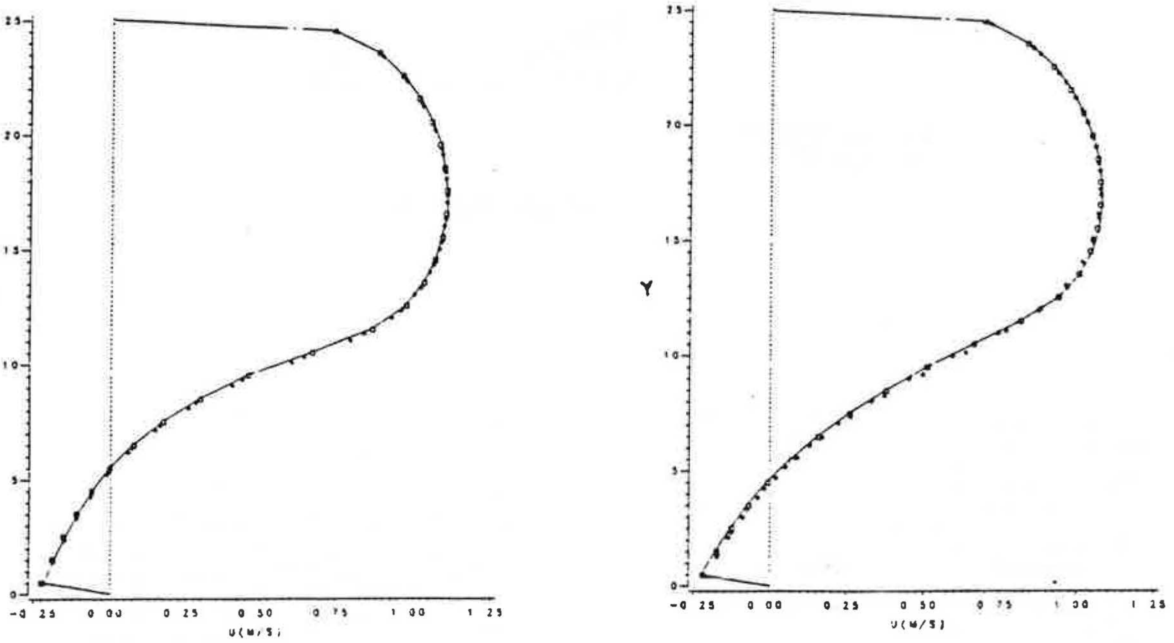
b) grid stretching factor 1.5



c) grid stretching factor 2.5

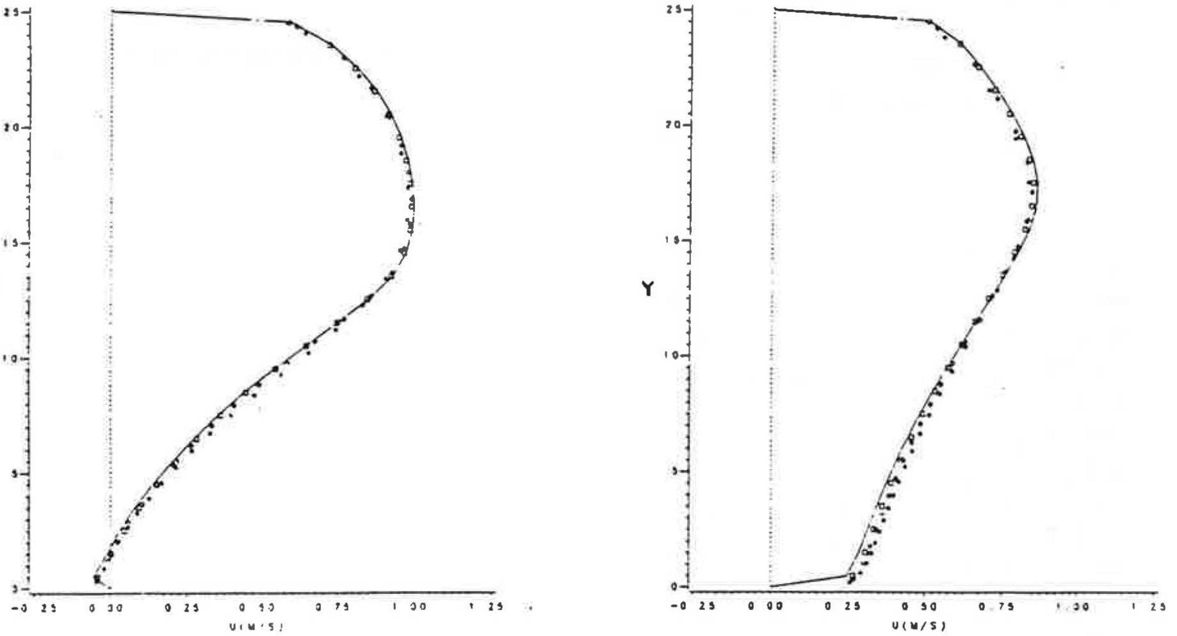
Fig. 7. Grid configuration, flow over a backward facing step.

SOLID LINE = FLOW3D RELEASE 1 RESULTS
SQUARE = FLOW3D RELEASE 2 RESULTS (STRETCH FACTOR = 0.0)
DIAMOND = FLOW3D RELEASE 2 RESULTS (STRETCH FACTOR = 1.5)
STAR = FLOW3D RELEASE 2 RESULTS (STRETCH FACTOR = 2.5)



a) x = 10mm

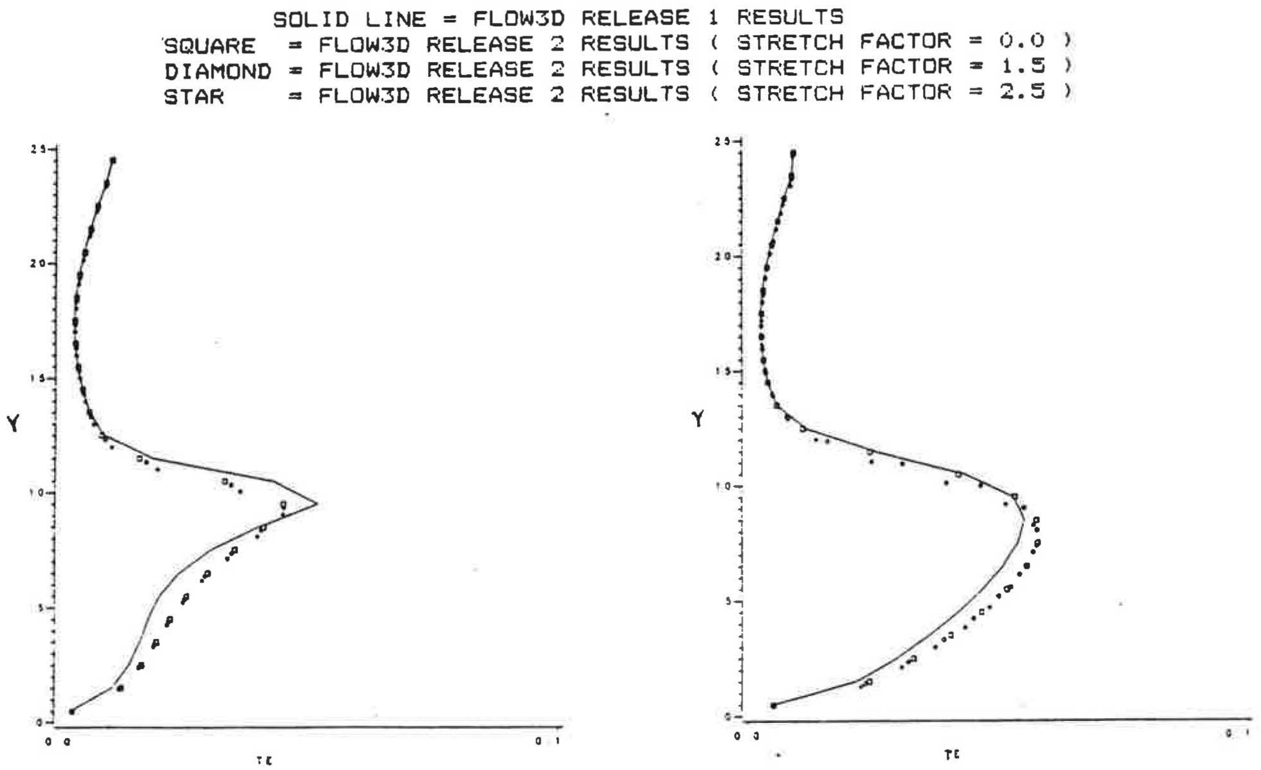
b) x = 20mm



c) x = 40mm

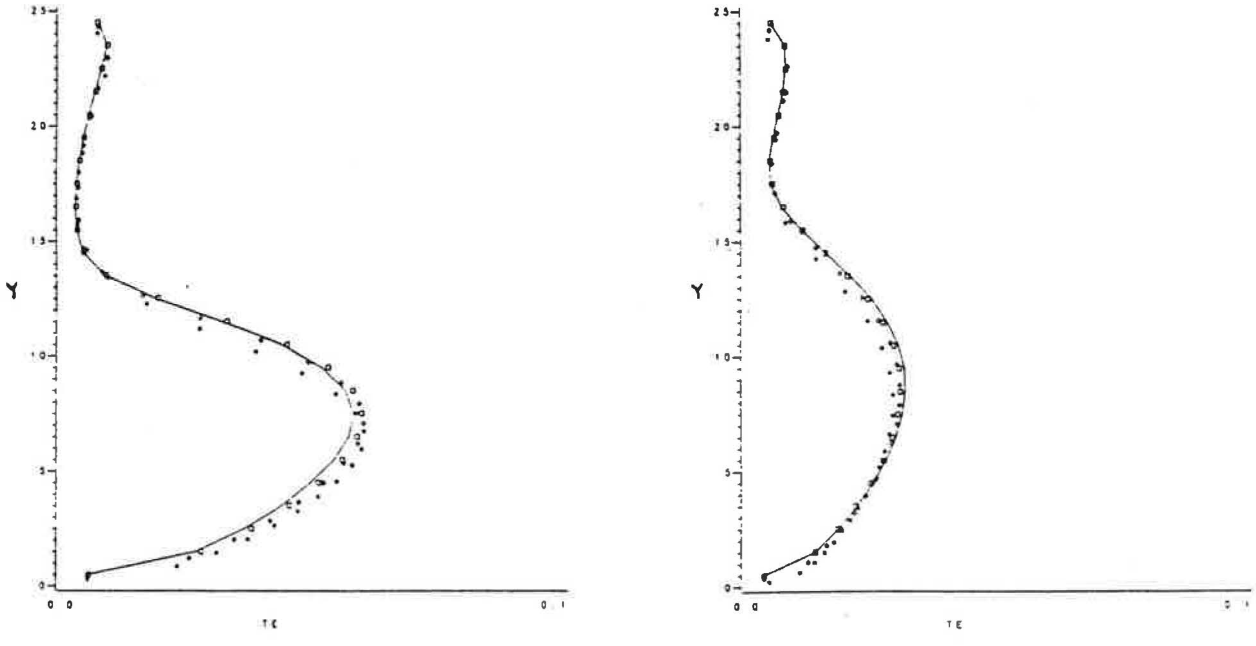
d) x = 100mm

Fig. 8. Streamwise velocity components at different downstream locations, flow over a backstep.



a) x = 10mm

b) x = 20mm



c) x = 40mm

d) x = 100mm

Fig. 9. Turbulent kinetic energy at different downstream locations, flow over a backstep.

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