

**Prediction of Turbulent Flow of
Inelastic Shear-Thinning Fluids
in Ducts and Mixing Vessels**

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Abstract

This study describes and assesses a computational procedure for the prediction of laminar and turbulent flows of inelastic shear-thinning fluids in ducts and agitated mixing vessels.

Closure of the governing momentum and mass conservation equation set is effected by a version of the $k-\epsilon$ model of turbulence, modified to account for shear-thinning fluid behaviour. Wall boundary conditions are handled using conventional ‘wall functions’, also modified to reflect shear-thinning fluid flow phenomena.

The partial differential equations are discretised by the finite volume method. A novel higher-order differencing scheme for the convection terms in the momentum equations is implemented. The PISO algorithm is employed in the solution of the coupled equations.

The substantial savings in computing effort and storage in obtaining solutions of a given accuracy, afforded by the new differencing scheme, are demonstrated firstly in a laminar flow. Predictions for turbulent Newtonian fluid flow in a mixing vessel at $Re = 48,000$ are for the most part near grid-independent, and show the quicker approach to grid independence achievable with the new differencing scheme. Assessment by reference to a comprehensive set of experimental data shows quantitative agreement for the mean axial and radial velocities; poorer qualitative as well as quantitative agreement for the mean swirl velocities. Turbulence energy is underpredicted in regions removed from the impeller.

Predictions for fully-developed turbulent pipe flow of shear-thinning fluids are shown to be of comparable accuracy to those for Newtonian fluids in the absence of rheological mechanisms other than shear-thinning; less accurate where drag-reduction is involved. Predictions for flow in a pipe with an axially-mounted baffle are of comparable accuracy for Newtonian and shear-thinning fluids; shear-thinning effects are manifest as a greater range of Kolmogorov scales in the latter cases. Predictions of mixing vessel flow of Newtonian and shear-thinning fluids at $Re = 9,600$ again demonstrate shear-thinning effects at the level of the Kolmogorov scales. Agreement with experiment is qualitatively satisfactory; quantitative discrepancies are attributed to underprediction of turbulence in the shear-thinning case, due to turbulence model and boundary condition inadequacies.

The turbulence model, the wall boundary conditions and the impeller model are identified as the aspects of the methodology in need of refinement.

Preface

This thesis represents the main result of the research which I carried out as part of BRITE project RIIB.0085.UK(H), a collaborative project between Imperial College, London, ICI Chemicals and Polymers, Runcorn, and Unilever Research, Vlaardingen. The project aims were the “provision of tested predictive design methods for process equipment, particularly stirred vessels and tubes, in which fluid mechanics and rheology influence process result”. The novel tasks undertaken were the modelling of certain multi-phase and non-Newtonian phenomena, and their influence on turbulence. While my activities in the period October 1986 – April 1990 included the contribution to the development and testing of the computer codes written to embody all aspects of the modelling and methodology, the greater part of my work was concerned with the non-Newtonian element of the project. The specific form of non-Newtonian behaviour for the flows of which it was our remit to develop a predictive methodology was shear-thinning, and this represents a pioneering effort to model the effects of this phenomenon in turbulent flow.

It is inevitable that if ambitious goals are set for a project, some will be more completely fulfilled than others; the wisdom of hindsight provides tomorrow’s targets. That many of these goals were reached reflects a generous spirit of co-operation on the part of a number of individuals whose contributions it gives me pleasure to acknowledge.

My grateful thanks go to my supervisor Prof. A. David Gosman, for coupling expert guidance with a judicious blend of constructive criticism and encouragement throughout.

It has been a privilege to have worked with Dr. Spyros Politis, whose thoroughness of method has been so instructive, and whose invariable willingness to help was so important in reaching both understanding and goals. Additionally and specifically, the modifications to the $k - \epsilon$ model of turbulence published herein are his.

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Mr. Randal Hockey and Mr. Fernando de Pinho provided the experimental data essential for this study.

The perception of Prof. Alan Chesters of Unilever Research finds expression in the approach adopted to the determination of the viscosity of a shear-thinning

fluid in turbulent flow; specifically, the arguments in sections 3.7.1 and 3.7.2 are largely his.

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1. Introduction

The range of geometries in which the flow of fluids has been studied is wide; analytical approaches are being supplanted by increasingly sophisticated techniques of experimental measurement such as laser-Doppler anemometry, and of computer-based computational methods such as finite volume analysis. The fluids of interest in most such studies, however, exhibit the type of flow behaviour characteristic of one particular class of fluids only, those generally referred to as Newtonian.

The increasing interest in the flow behaviour of certain classes of those fluids not exhibiting Newtonian behaviour is occasioned in particular by their importance in the processing industries. Virtually all polymers, suspensions and emulsions are non-Newtonian substances; the industries in which they are encountered include food processing, paint, soap and detergent, plastics and synthetic fibres among many others.

The questions of interest in fluid flow from the standpoint of design of processing plant include such global characteristics as pressure drop in ducts and impeller power dissipation in mixing vessels, and such local characteristics as rates of heat transfer, mixing and reaction, with a view to the selection of plant operating conditions and pumps, impellers *etc.* of the appropriate type and size to yield maximum production rate with desired product properties at minimum capital and operating cost. The traditional approach to such problems, of 'scale-up' on the basis of various dimensionless parameters, is frequently associated with the necessity to build full-scale pilot plant and some degree of trial and error, because of the difficulty in identifying the relevant scaling criteria and the incompatibilities among them. Scaling up is yet more unreliable as a basis for prediction of plant performance if the fluids in question are not Newtonian, as differences in fluid behaviour necessitate consideration of still more dimensionless parameters. The review of problems in stirring technology of Kipke (1982) identifies the processing of non-Newtonian fluids in particular as meriting further research, and exemplifies a growing awareness that empirical methods serve still less well as design tools when employed with such fluids.

Furthermore, scaling up can offer guidance related to the aforementioned global characteristics only; evaluation of the efficacy of mixing processes requires knowledge of local flow patterns which empirical techniques cannot provide. Thus the need arises for techniques for the prediction of the flow field as a whole, and in recent years numerical methodologies have reached the stage of development, in

the discipline of Computational Fluid Dynamics (CFD), at which they represent practicable design tools. Thus the work of Perić (1985) exemplifies recent developments of computational methodologies to handle the flow of Newtonian fluids in complex geometries, while Issa and Gosman (1981), Bolour-Froushan (1986) and Politis (1989) have developed related techniques for the prediction of single-phase Newtonian and two-phase flows in mixing vessels.

1.1 The problem and objectives

The aim of this study is to refine the aforementioned computational methodologies for the prediction of single-phase turbulent flows of Newtonian fluids in ducts and mixing vessels, in terms of accuracy and economy, and to broaden their scope to handle such flows of certain classes of non-Newtonian fluids also. Non-Newtonian fluids form an extremely wide class of different materials, with little in common except fluidity and non-conformity to the Newtonian model. This study limits consideration to the specific class of fluids described as shear-thinning, and the fluids of interest will be referred to as such from hereon; definition of the term will be made in the following chapter.

Numerical accuracy, the degree to which the solution of discretised algebraic equations satisfies the original differential equation, is a primary interest in this work, with improvement of the accuracy of the methodology sought through the employment of a novel differencing scheme and investigation of the improvement in accuracy to be gained with grid refinement. Physical accuracy is the degree to which the differential equations represent the reality of the problem under consideration, and depends on the validity of the assumptions underlying the modelling incorporated in these equations. Turbulence must be modelled, as the limitations on computing resources, in terms of both memory and processor time, do not permit the solution of the Navier-Stokes equations for turbulent flow due to the degree of temporal and spatial resolution which would be required. The shear-thinning behaviour of the fluid must now also be modelled. The accuracy of the modelling is therefore also an issue of primary importance here, and is assessed by reference to experimental data.

Some effort is explicitly directed to improving economy, using an improved equation set solver. Reducing computing resource requirements, in terms of both processor time and memory, is also a chief motive for the development and im-

plementation of an improved differencing scheme, however, insofar as predictions of a given accuracy for a lower expenditure of such resources are an anticipated outcome of the use of a better scheme.

1.2 Present contributions

This study makes the following contributions :

- Implementation and assessment of a version of the $k - \epsilon$ model of turbulence modified to account for the flow of shear-thinning fluids.
- Use of ‘wall functions’, with values of the empirical coefficients modified on the basis of experimental data, to handle wall boundary conditions in turbulent flow of shear-thinning fluids.
- Implementation of a conjugate gradient solver for the pressure correction equation set.
- Implementation of the Self Filtered Central Differencing scheme of Ziman (1990).
- Prediction and detailed analysis of the turbulent flow of a Newtonian fluid in a mixing vessel and of shear-thinning fluids in straight pipes, pipes with an axially-mounted baffle, and in a mixing vessel.
- Assessment of the predictions by comparison with experimental data.

1.3 The thesis outline

Previous studies of the flow of shear-thinning fluids are reviewed in chapter two. The nature of the fluids of interest is described, constitutive equations by which they may be characterised are considered, and the validity of dimensional analysis as applied to flows of shear-thinning fluids investigated. Experimental, empirical/analytical and computational work relating to turbulent pipe flow of these fluids is summarised, and such few investigations of mixing vessel flow as have been conducted are subsequently outlined; conclusions follow.

The partial differential equations by which turbulent flow of Newtonian and shear-thinning fluids may be described are presented in chapter three. Proceeding from the exact, but as-yet-in-practice insoluble Navier-Stokes equations, the rationale behind, and usual approaches to, turbulence modelling are discussed. A model for the evaluation of the molecular viscosity of shear-thinning fluids, in

turbulent flow, is described. The $k - \epsilon$ model of turbulence used in this study is set forth in a form extended to model flows of shear-thinning fluids, and finally, boundary conditions for the equation sets are described.

The method of solution of the equation set is described in chapter four. Discretisation, *ie.* the replacement of the (continuous) partial differential equations by algebraic equations for discrete values of the unknowns at a finite number of points, using the finite volume method, is outlined first. The relative merits of the principal differencing schemes *ie.* methods of interpolation between these points, are briefly discussed, and the new scheme selected for this study is described. The staggered and co-located computational grid arrangements used are discussed, and numerical considerations in the handling of boundary conditions are addressed. The iterative solution algorithm for the coupled equation sets is detailed before solution algorithms for the individual equation sets are discussed.

The complete methodology having thus been described, the remaining chapters are concerned with the results of a number of test cases.

In chapter five the quality of predictions obtainable with the new differencing scheme is considered for the case of laminar flow in a duct with a step contraction, and thus in the absence of the uncertainties associated with turbulence modelling. Detailed analysis of predictions of a Newtonian fluid mixing vessel flow using the new differencing scheme, comparison with experiment and evaluation of differencing scheme performance by comparison with predictions obtained using an alternative differencing scheme, are presented.

In chapter six, analysis of predictions for turbulent flow of shear-thinning fluids in straight pipes, in a pipe with an axially-mounted baffle, and in a mixing vessel are in turn analysed and compared with experimental data.

Chapter seven summarises findings of the study and the conclusions drawn therefrom, and makes recommendations for future work.

2 Literature survey

2.1 Introduction

Previous studies of turbulent flows of inelastic shear-thinning fluids in pipes and mixing vessels are reviewed. An insight into the effects of shear-thinning behaviour on flow patterns is sought, particularly in the region of low turbulence intensity near solid boundaries where such effects would be expected to manifest themselves. This is of importance in establishing boundary conditions for the flow model to be presented later, and specifically whether the approach to boundary condition prescription widely used for flows of Newtonian fluids may be used for those of shear-thinning fluids also.

The nature of the fluids of interest is outlined in section 2.2, and constitutive equations by which they may be characterised are briefly discussed in section 2.3. The question of dimensional analysis and scaling is addressed in section 2.4. Studies of turbulent flow of shear-thinning fluids in pipes are discussed in section 2.5, those concerned with the agitation of shear-thinning fluids in mixing vessels are considered in section 2.6. Most of the studies nominally address themselves to non-Newtonian fluid flows. Most are however limited to consideration of purely viscous fluids, and the term shear-thinning has been substituted where necessary to emphasise that only one particular class of non-Newtonian behaviour is being examined. Finally, conclusions are presented in section 2.7.

2.2 The fluids of interest

There is no clear line of demarcation between solids and fluids. The Hooke theory of elasticity and the Newtonian theory of viscosity represent opposite ends of a continuous spectrum of material behaviour – see for example Walters (1980) – and may be characterised by the Deborah number, defined as

$$De = \frac{\Lambda}{t} \quad (2.2.1)$$

The characteristic time of a flow process t is the time (measured from some material point) for a non-negligible change in kinematic conditions. The characteristic time of a material, Λ , is in some sense the length of memory of the fluid, and would in principle be zero for a purely viscous fluid and infinite for an ideal elastic solid, since elasticity connotes ability to recover from deformation. A precise definition

for Λ for intermediate materials is elusive – that of Astarita and Marucci (1974) extracts it from the apparent viscosity curve of the material. High De corresponds to solid-like behaviour, low De to fluid-like behaviour. In practice the value of Λ for water of 10^{-13} sec. is sufficiently small for elastic effects to be ignored, but for polymer melts, generally thought of as fluids, Λ can be of the order of seconds.

Nonzero normal stresses seem characteristic of fluids with elasticity in the sense that fluid memory of past behaviour is important in determining rheological response (Schowalter, 1978). Having noted that no fluid is truly inelastic, *ie.* that all will exhibit normal stresses in shear flow, interest will be from hereon confined to those fluids for which elasticity effects are negligible *ie.* to ‘purely viscous fluids’. Such fluids are generally classified as Newtonian and viscous non-Newtonian. The former exhibit a linear relationship between shear stress and strain rate while the latter are characterised by a constitutive equation of the general form

$$\tau_{ij} = \mu(I_{\dot{\gamma}}, II_{\dot{\gamma}}, III_{\dot{\gamma}})\dot{\gamma}_{ij} \quad (2.2.2)$$

where τ_{ij} is the stress tensor, μ is a decreasing function of the invariants $I_{\dot{\gamma}}$, $II_{\dot{\gamma}}$, and $III_{\dot{\gamma}}$ of the strain tensor $\dot{\gamma}_{ij}$ for shear-thinning (pseudoplastic) fluids and an increasing function of these invariants for shear-thickening (dilatant) fluids. The invariants are the three independent scalars which can be formed by taking the trace, *ie.* summing the diagonal elements, of $\dot{\gamma}_{ij}$, $\dot{\gamma}_{ij}^2$ and $\dot{\gamma}_{ij}^3$, so called because their values are independent of the choice of co-ordinate system to which the components of $\dot{\gamma}_{ij}$ are referred; they are listed in Appendix A. (It is noted in passing that (2.2.2) may also be written with μ as a function of the invariants of τ_{ij} ; several of the specific forms of (2.2.2) proposed in the literature are so expressed.) For the flow of incompressible fluids $I_{\dot{\gamma}}$ becomes zero. For viscometric flows (unidirectional shear flows for which the shear rate $\dot{\gamma}$ is independent of time at a given particle) $III_{\dot{\gamma}}$ is zero, and limited experimental evidence (Slattery and Bird, 1961, Bird *et al*, 1977) appears to justify the common practice of assuming $III_{\dot{\gamma}}$ to be unimportant for non-viscometric flows also. Accordingly for present purposes (2.2.2) is written

$$\tau_{ij} = \mu(II_{\dot{\gamma}})\dot{\gamma}_{ij} \quad (2.2.3)$$

Only shear-thinning fluids are of interest in this study – these display the shear stress-strain rate relationship shown in figure 2.1, and accordingly the relationship between molecular viscosity and strain rate shown in figure 2.2.

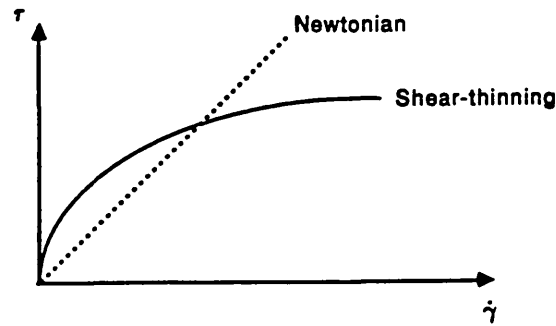


Figure 2.1 Shear stress – strain rate relationship for Newtonian and shear-thinning fluids

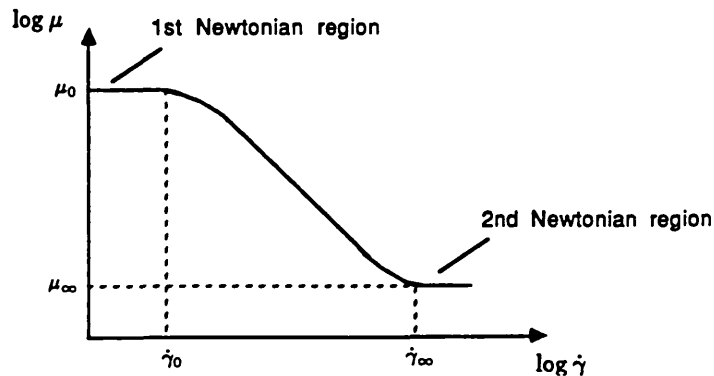


Figure 2.2 Molecular viscosity – strain rate relationship for shear-thinning fluids

2.3 Constitutive equations for shear-thinning fluids

A number of forms of (2.2.3) have been proposed in the literature – see, for instance, Bird *et al*, 1977) – varying in complexity depending on the range of the molecular viscosity-strain rate curve which they reproduce and the accuracy with which they do so.

2.3.1 The ‘power law’ model

The section of the curve in Fig. 2.2 between shear rates $\dot{\gamma}_0$ and $\dot{\gamma}_\infty$ may be approximated by

$$\mu = K \left(\frac{1}{2} II_{\dot{\gamma}} \right)^{(n-1)/2} \quad (2.3.1)$$

where the parameters K and n are constant for a given fluid, with K representing

fluid consistency and n the degree of departure from Newtonian behaviour. This is the so-called ‘power law’, accurate for many fluids within the range $\dot{\gamma}_0$ to $\dot{\gamma}_\infty$ but incorrectly giving infinite and zero viscosities in the lower and upper strain rate limits, respectively.

2.3.2 The Carreau model

The Carreau model gives μ as a continuous function of $\dot{\gamma}$ over the complete range of $\dot{\gamma}$ from zero to infinity, of the form

$$\frac{\tilde{\mu} - \mu_\infty}{\mu_0 - \mu_\infty} = \left[1 + \lambda^2 \frac{1}{2} II_{\dot{\gamma}} \right]^{\frac{n-1}{2}} \quad (2.3.2)$$

where λ is a time constant with the dimension of seconds, and μ_0 , μ_∞ are the limiting viscosities in the lower and upper strain rate limits, respectively.

The simplified (two rather than three parameter) form of the model as given by

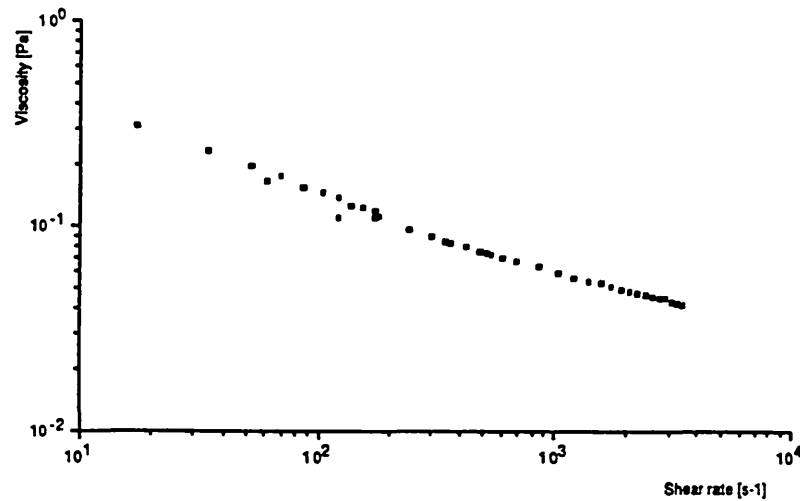
$$\frac{\mu}{\mu_0} = \left[1 + \lambda^2 \frac{1}{2} II_{\dot{\gamma}} \right]^{(n-1)/2} \quad (2.3.3)$$

reproduces the shape of the shear stress-strain rate curve in the shear rate range zero to $\dot{\gamma}_\infty$.

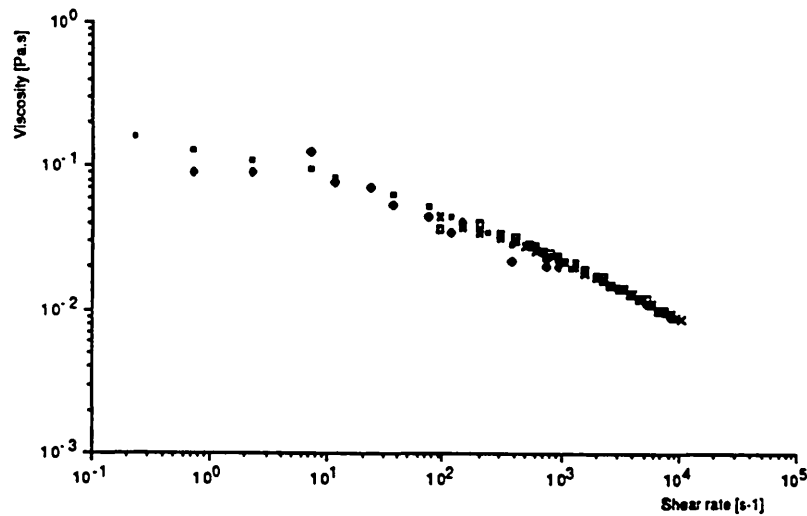
2.3.3 Choice of constitutive equation

In the mathematical modelling of fluid flow to be considered in the following chapter the relationship between shear stress and strain rate must be prescribed; the choice of constitutive equation is made here.

While mean strain rates in turbulent flow may be comparatively low, shear rates at the dissipative eddy level at which viscous mechanisms operate are several orders of magnitude greater (*cf.* later discussion in section 3.7.2); hence the inaccuracy of the ‘power law’ at low strain rates is not a restriction on its use in such flows. The question indeed arises as to whether these strain rates are greater than $\dot{\gamma}_\infty$, and accordingly whether shear-thinning fluids exhibit sensibly Newtonian behaviour in viscous dissipation of turbulent energy. All that may be said at present is that for the range of shear rates generally achievable in a viscometer ($< 20 \times 10^3 \text{ s}^{-1}$) ‘power law’ behaviour is exhibited by aqueous solutions of both Carbopol and Carboxymethylcellulose (CMC) – figure 2.3 – and that if the limiting value of the viscosity, μ_∞ , may be expected to be that of the pure solvent



Viscometric viscosity of a three month old 0.35 % Carbopol sample.



Viscometric viscosity of CMC at 25° C.

Figure 2.3 Molecular viscosity – strain rate relationship for aqueous solutions of Carbopol and CMC. Data of de Pinho (1990)

the ‘power law’ curve must be extrapolated to strain rates of the order of 10^4 s^{-1} before this is attained.

Accordingly the ‘power law’ will be employed in the turbulence modelling to be presented in sections 3.7 and 3.8, where it will become apparent that its simplicity is also necessary in keeping the analysis tractable.

In laminar flows the inaccuracy of the ‘power law’ in the lower strain rate limit is sufficient to warrant the use of (2.3.3). The unavailability of high strain

rate viscometric data precludes the determination of μ_∞ in (2.3.2), and indicates that such strain rates do not occur in laminar flow in any case. A method for the determination of the parameters in (2.3.3) is outlined in appendix B.

2.4 Scaling with non-Newtonian fluids

2.4.1 Scope and limitations

Dimensional analysis, and the use of dimensionless groups of parameters, is a firmly established procedure in the analysis of Newtonian fluid flows. It is accepted, for example, that in Newtonian fluid flow, the forced convection flow regime in a pipe or mixing vessel may be characterised as laminar or turbulent on the basis of a Reynolds number, irrespective of the scale of the geometry or the particular fluid involved. Likewise it is commonplace to compare the results of various forced convection studies, experimental and computational, on the basis of a Reynolds number, again irrespective of the geometry or fluid for which they were conducted. It is important to establish from the outset whether or not this is possible in studies of shear-thinning fluid flows, particularly in assessing previous work, since so much of it is predicated by the assumption that the Newtonian approaches are still valid.

To scale up the results of experimental work on a small model to a large-scale prototype and to achieve the same kind of flow pattern in the geometries on the two scales it is necessary to ensure geometric, kinematic and dynamic similarity between the model and prototype.

Geometric similarity exists between two geometrical figures if the ratio of all corresponding length dimensions is constant, and it is a prerequisite of kinematic and dynamic similarity in order to ensure that corresponding positions in the two systems exist. Kinematic similarity exists in two such systems if the ratios of all corresponding velocities at corresponding positions are constant. Dynamic similarity exists in two such systems if the ratios of all corresponding forces at corresponding positions are constant. Because of the frequent difficulty in enforcing the latter requirement for each and every force acting in the flow, the constant ratio is usually sought only for the most important forces, these being established by an order of magnitude analysis.

Astarita (1978) concluded that a non-trivial scaling law, in the sense of permitting scale-up outside the range of experimental data, cannot be established for non-Newtonian fluids. The fact that only one dimensional parameter is required for

the Newtonian constitutive equation, and hence that only one dimensionless group is relevant for scaling purposes, hinges on the assumed linearity of the stress-strain relationship. Two dimensional parameters arise from the non-linear stress-strain relationship for a shear-thinning fluid (2.2.3), however, a characteristic viscosity μ_{char} and a characteristic time Λ . In addition two fluids characterised by the same values of both μ_{char} and Λ will not necessarily have the same constitutive equation, and if a specific constitutive equation, valid for all shear rate ranges, is adopted the number of parameters will exceed two. These may be expressed in terms of μ_{char} , Λ and a set of dimensionless parameters. Assuming inertial and viscous forces to be dominant in the pipe and mixing flows of interest *ie.* assuming elastic, gravitational and surface tension forces to be negligible, a scaling law requires equality of a dimensionless group based on the characteristic viscosity, *ie.* a Reynolds number

$$Re = \frac{LU\rho}{\mu_{\text{char}}} \quad (2.4.1)$$

and of a dimensionless group based on the characteristic time, *ie.* a Weissenberg number

$$We = \frac{\Lambda U}{L} \quad (2.4.2)$$

in addition to equality of all dimensionless rheological parameters at both levels. It follows from the latter requirement that the same material must be used at both levels, in view of the virtual impossibility of finding two different materials with equal values of all parameters. But the dimensionless group Re/We contains only the linear dimension L in addition to fluid properties, and thus L must be the same at model and prototype levels.

The above point may perhaps be seen more clearly by examining the transport equations in non-dimensional form. In the following L and U represent a characteristic length and velocity, respectively, so that $u_i = Uu_i^*$, $x_i = Lx_i^*$ and $p = \rho U^2 p^*$, where the superscript $*$ denotes a dimensionless quantity. Taking the case of steady state, incompressible, laminar pipe flow for clarity, the instantaneous momentum equation reads

$$\rho \frac{\partial}{\partial x_j} (u_j u_i) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu (II_{\dot{\gamma}}) \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] \quad (2.4.3)$$

Two constitutive equations will be considered, namely the ‘power law’ (2.3.1) and simplified Carreau (2.3.3) models. Equation (2.4.3) then reads, in non-dimensional

form

$$\frac{\partial}{\partial x_j^*}(u_j^* u_i^*) = -\frac{\partial p^*}{\partial x_i^*} + \frac{KU^{n-2}}{\rho L^n} \frac{\partial}{\partial x_j^*} \left\{ \left[\frac{1}{2} \left(\frac{\partial u_i^*}{\partial x_j^*} \frac{\partial u_j^*}{\partial x_i^*} + \left(\frac{\partial u_j^*}{\partial x_i^*} \right)^2 \right) \right]^{n-1} \left(\frac{\partial u_i^*}{\partial x_j^*} + \frac{\partial u_j^*}{\partial x_i^*} \right) \right\} \quad (2.4.4)$$

for the ‘power law’ and

$$\frac{\partial}{\partial x_j^*}(u_j^* u_i^*) = -\frac{\partial p^*}{\partial x_i^*} + \frac{\mu_0}{\rho U L} \frac{\partial}{\partial x_j^*} \left\{ \left[1 + \left(\frac{\lambda U}{L} \right)^2 \left[\frac{1}{2} \left(\frac{\partial u_i^*}{\partial x_j^*} \frac{\partial u_j^*}{\partial x_i^*} + \left(\frac{\partial u_j^*}{\partial x_i^*} \right)^2 \right) \right]^{\frac{n-1}{2}} \left(\frac{\partial u_i^*}{\partial x_j^*} + \frac{\partial u_j^*}{\partial x_i^*} \right) \right\} \quad (2.4.5)$$

for the Carreau model. Here subscripts $i, j = 1, 2, 3$ (with implicit summation over repeated indices). Scaling theory *requires that the non-dimensional index n must equate at model and prototype levels*, and in addition that the group

$$Re = \frac{KU^{n-2}}{\rho L^n} \quad (2.4.6)$$

equate at the two levels for the case of the ‘power law’ or that the groups

$$Re = \frac{\rho U L}{\mu_0} \quad We = \frac{\lambda U}{L} \quad (2.4.7)$$

equate at the two levels for the case of the Carreau model. The Reynolds number equality for the ‘power law’ case, *for any particular index n* , may be readily achieved – Newtonian fluids are one such case. Astarita (1978) contended that if the limitation of ‘power law’ validity to a certain shear rate range was accepted, the resulting requirement that the shear rate range be equal at model and prototype levels was equivalent to introducing a second dimensional parameter, thus making scaling impossible. This appears erroneous insofar as shear rate range equality is ensured if kinematic similarity obtains. What can be concluded is that the more dissimilar the rheological properties of two fluids the flows of which are being compared, the less reliable is the characterisation and comparison of the flows on the basis of Reynolds number alone. The greatest caution in the application of the traditional scaling methods must be exercised when constitutive equations requiring two or more dimensional parameters are necessary to characterise the fluids, or, in the case of the ‘power law’ being a sufficiently accurate characterisation, when the shear-thinning indices are very different.

2.4.2 Reynolds number for pipe flow

Metzner and Reed (1955) defined a Reynolds number for laminar pipe flow (as summarised in appendix C)

$$Re_{\text{gen}} = \frac{\rho V^{2-n'} D^{n'}}{K' 8^{n'-1}} \quad (2.4.8)$$

based on the following relationship

$$\tau_w = K' \left(\frac{8V}{D} \right)^{n'} \quad (2.4.9)$$

for the general case of the flow of a fluid for which K' and n' are constants over small ranges of shear stress only, defined as (see appendix C)

$$K' = \frac{D \Delta P}{4L} \left(\frac{8V}{D} \right)^{n'} \quad (2.4.10)$$

and

$$n' = \frac{d \ln(D \Delta P / 4L)}{d \ln(8V/D)} \quad (2.4.11)$$

They thus represent fluid consistency and shear-thinning index for piecewise ‘power law’ approximations to the constitutive equation (2.2.3). Equation (2.4.8) is not a basis for scaling, however, since K' and n' are pipe diameter dependent, and a scaling theory allowing scale-up outside the range of experimental data is in principle impossible for a correlation between dimensionless groups, such as (2.4.8). In the specific case where the ‘power law’ with a single set of parameters is sufficiently accurate over the full range of strain rates of interest, however, (2.4.8) takes the form (details in appendix C)

$$Re_{\text{pl}} = \frac{\rho V^{2-n} D^n}{K 8^{n-1} \left(\frac{3n+1}{4n} \right)} \quad (2.4.12)$$

and this is a basis for the comparison for the comparison of the flows of ‘power law’ fluids of equal n .

An alternative approach is to define a Reynolds number in terms of the apparent viscosity at the wall, μ_w – Eissenberg and Bogue (1964):

$$Re_{\mu_w} = \frac{\rho U D}{\mu_w} \quad (2.4.13)$$

The calculation of μ_w will be addressed in section 2.5 – taking μ_w as a characteristic viscosity of the flow acknowledges the fact that viscous effects in high-Reynolds number turbulent pipe flow are important in the near-wall region only.

2.4.3 Reynolds number for mixing vessel flow

For the flow of Newtonian fluids in Rushton-turbine-agitated mixing vessels a bulk Reynolds number may be defined as

$$Re_{mv} = \frac{D_{imp}^2 N \rho}{\mu} \quad (2.4.14)$$

in which D_{imp} is the impeller diameter and N is the impeller rotational speed, and a power number N_P as

$$N_P = \frac{P}{\rho N^3 D^5} \quad (2.4.15)$$

where P is the input power – see, for example, Uhl and Gray (1966). The $N_P - Re_{mv}$ correlation is then found to take the form illustrated in figure 2.4; the laminar regime extends to $Re_{mv} \approx 10$ and the invariance of N_P with Re_{mv} characteristic of full turbulence is seen to obtain above $Re_{mv} \approx 10^4$.

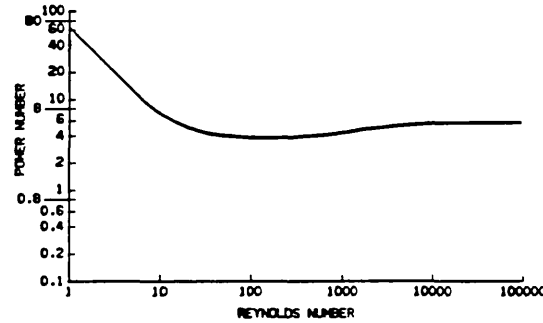


Figure 2.4 Power number – Reynolds number correlation, flow of Newtonian fluids in Rushton-turbine-agitated mixing vessels, from Oldshue (1983)

Metzner and Otto (1957) put forward the concept of an apparent average viscosity for a shear-thinning fluid in a mixing vessel. This would be defined by considering two identical sets of equipment, one containing a Newtonian and the other a shear-thinning fluid, and when the viscosity of the former is such that the power measured at each impeller is the same the average viscosities could be said to be the same in both. They then defined a bulk Reynolds number for mixing vessel flow of shear-thinning fluids in terms of this apparent average viscosity, μ_{av} :

$$Re_{mv,st} = \frac{D_{imp}^2 N \rho}{\mu_{av}} \quad (2.4.16)$$

They further assumed that the fluid motion in the general region of the impeller can be characterised by an average shear rate which is linearly related to the

rotational speed of the impeller, *viz.*

$$\left(\frac{du}{dr}\right)_{\text{average}} = cN \quad (2.4.17)$$

For a given impeller rotational speed (2.4.16) would then permit the calculation of the average shear rate and hence, from viscometric data, μ_{av} .

Metzner and Otto suggested that the value of the constant c in (2.4.16) be established by the reverse procedure, considering power- and speed-matched flows of Newtonian and shear-thinning fluids. Since the viscosity of the Newtonian fluid can be established by reference to the $N_P - Re_{\text{mv}}$ curve, and since, according to the above arguments, this is equal to the apparent average viscosity of the shear-thinning fluid, the average shear rate in the flow of the shear-thinning fluid may be found from viscometric data. Metzner and Otto (1957) made power consumption measurements for a number of shear-thinning fluids (solutions of CMC, Carbopol and Attasol) with several impeller/tank diameter ratios and impeller rotational speeds, and using the above procedure they established a 'best' value of c of 13. Metzner et al (1961) presented measurements, again in the same vessel, in support of (2.4.17). Chen and Hashimoto (1979) made power consumption measurements for flows of shear-thinning slurries in mixing vessels of similar configuration; for a Rushton turbine they obtained a value for c of 10.3 using this procedure. The significance of such a discrepancy in the value of c is limited: a difference of a factor of 2 produces a difference in μ_{av} , and hence $Re_{\text{mv,st}}$, of a factor of 1.6 for a shear-thinning fluid of index 0.7, and a difference of a factor of 5 in c produces a difference in μ_{av} of 3 for the same fluid.

Metzner and Otto (1957), Metzner et al (1961) and Chen and Hashimoto (1979) then found the correlations of their $N_P - Re_{\text{mv}}$ data to be close to that for Newtonian fluids in the laminar and fully-turbulent regimes, with some discrepancies in the transition region; their results are reproduced as figure 2.5. These results would seem to indicate that the use of the correlation, as a design tool in indicating impeller power requirements, may be extended to the flow of shear-thinning fluids as a qualitative guide, but the caution necessary in using Reynolds-number-based correlations for flows of such fluids is yet greater here, given the tenuousness of the average viscosity concept. For the purposes of this study interest in the $N_P - Re_{\text{mv}}$ correlation is limited to the indication it can offer of the flow regime obtaining in the vessel for a given N_P or Re_{mv} .

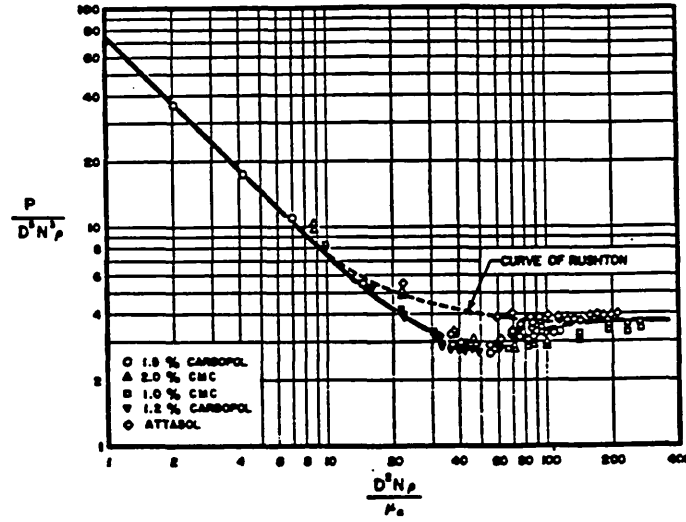


Figure 2.5 Power number – Reynolds number data of Metzner & Otto, flow shear-thinning fluids in Rushton-turbine-agitated mixing vessels, compared with correlation for Newtonian fluids

2.5 Flow of shear-thinning fluids in pipes

The turbulent fully-developed flow of Newtonian fluids in pipes is often analysed in terms of a laminar sublayer adjacent to the wall and a fully turbulent core (Schlichting, 1960). Fully developed pipe flow may be characterised by a non-dimensional semi-logarithmic expression for the velocity profile

$$u^+ = A \ln y^+ + B \quad (2.5.1)$$

in the turbulent core and a linear expression in the laminar sublayer

$$u^+ = y^+ \quad (2.5.2)$$

– figure 2.6, where

$$u^+ = \frac{u}{u_*} \quad (2.5.3)$$

$$u_* = \sqrt{\frac{\tau_w}{\rho}} \quad (2.5.4)$$

The dimensionless distance from the wall, y^+ , is given by

$$y^+ = \frac{y u_* \rho}{\mu} \quad (2.5.5)$$

for a Newtonian fluid.

In consequence of the near-uniformity of the shear stress in the viscous sub-layer μ may be replaced in (2.5.5), for a shear-thinning fluid, by the wall viscosity, μ_w ; for the same reason μ_w may be expressed in terms of the wall shear stress:

$$\mu_w = \frac{\tau_w}{(du/dy)_w} \quad (2.5.6)$$

The ‘power law’ constitutive equation (2.3.1) is accurate in the high-strain-rate regime obtaining in the viscous sublayer, and thus

$$\mu_w = \tau_w^{(n-1)/n} K^{1/n} \quad (2.5.7)$$

from which

$$y^+ = \frac{yu_*\rho}{\mu_w} = y \left(\frac{\rho u_*^{2-n}}{K} \right)^{1/n} \quad (2.5.8)$$

Equation (2.5.1) may be determined from Prandtl’s mixing length hypothesis – Schlichting (1960); A then represents the inverse of the von Karman mixing length coefficient κ . Experiment indicates $\kappa \approx 0.4$ for flows of Newtonian fluids, and this value would be expected to obtain also for the flows of those non-Newtonian fluids in which fluid rheology does not interfere with the inertially-dominated mechanism of turbulence (*cf.* later discussion in section 3.5). The constant B must also be determined from experiment; it determines the value of y^+ at which (2.5.1) and (2.5.2) intersect, y_{it}^+ *ie.* the thickness of the laminar sublayer in dimensionless terms. For Newtonian fluids the accepted value of B is ≈ 5.5 and hence $y_{it}^+ \approx 11.62$.

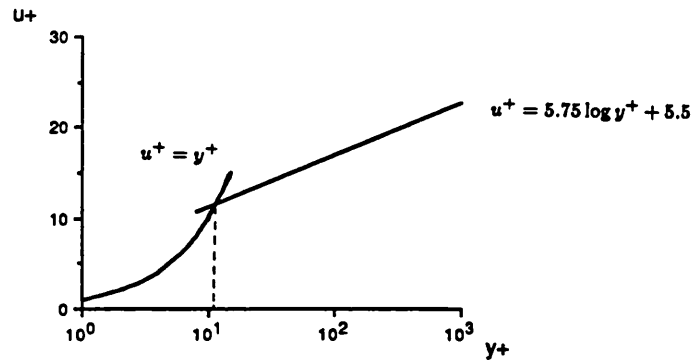


Figure 2.6 $u^+ - y^+$ velocity profile representation for the fully developed turbulent pipeflow of a Newtonian fluid

Equation (2.5.1) may be integrated across the cross-sectional area (see appendix D) to obtain a relationship between the Fanning friction factor

$$f = \frac{\tau_w}{\rho V^2/2} \quad (2.5.9)$$

and Reynolds number of the form

$$\frac{1}{\sqrt{f}} = \frac{A}{\sqrt{2}} \log(Re\sqrt{f}) + \frac{1}{\sqrt{2}}(B - 6.35) \quad (2.5.10)$$

ie.

$$\frac{1}{\sqrt{f}} = \frac{A}{\sqrt{2}} \log(Re\sqrt{f}) - 0.6 \quad (2.5.11)$$

for a Newtonian fluid. The expression

$$\frac{1}{\sqrt{f}} = 4 \log(Re\sqrt{f}) - 0.4 \quad (2.5.12)$$

is found to agree well with experiment, the discrepancy in the value of the last term in (2.5.11) and in (2.5.12) being attributable to the inaccuracy of (2.5.1) near the pipe centreline.

The validity of this approach for shear-thinning fluid flow will be examined in the following section.

2.5.1 Experimental studies

Bogue and Metzner (1963) obtained Pitot tube measurements of fully developed velocity profiles for the turbulent flow of shear-thinning fluids – in this case, aqueous solutions of Carbopol, of four different concentrations, in the turbulent core region (they did not have sufficient confidence in the reliability of their near wall data to present it). Hoyt (1972), among others, has observed that Pitot tube measurements of velocity in such fluids are prone to error, due to the presence of polymer molecules, but the good agreement (within 3.5%) obtained by Bogue and Metzner between the mean flow velocity obtained by integrating their velocity profiles, and that obtained from flowmeter measurements, would appear to permit some confidence to be placed in their data. In addition their viscometry measurements were made in the same range of mean shear stresses as in the pipe, and importantly, only runs during which there was no significant change of rheological properties are presented (many shear-thinning polymer solutions degrade rapidly, often under moderate conditions of shear).

Bogue's velocity profile data for the Carbopol solutions have been reinterpreted and presented here on a $u^+ - y^+$ basis – figure 2.7.

The behaviour of the 0.1% solution appears sensibly Newtonian in that it is fitted by equation (2.5.1) with a Newtonian value of A and near-Newtonian

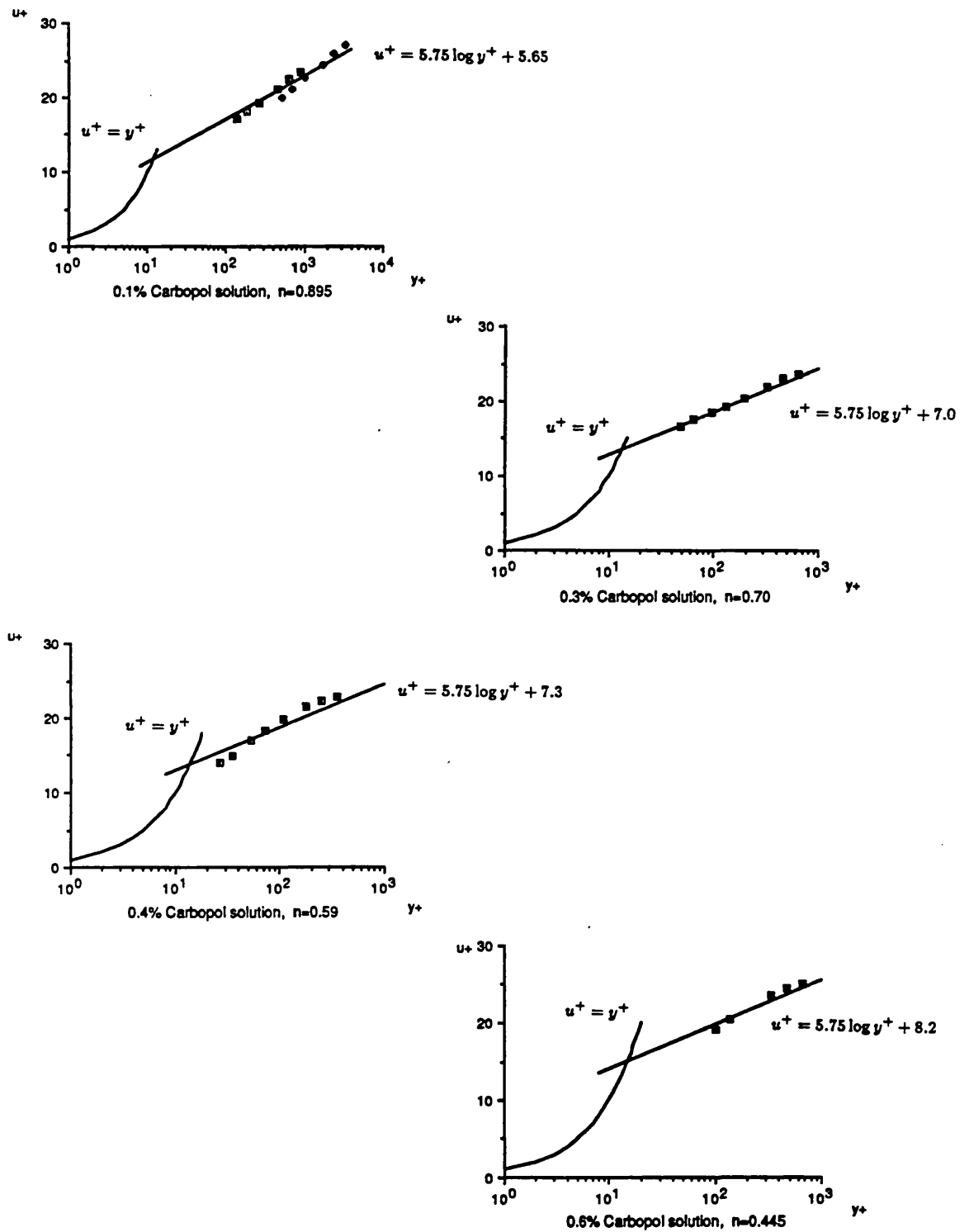


Figure 2.7 Velocity profiles for fully developed turbulent pipeflow of aqueous solutions of Carbopol. Data of Bogue (1961)

Solution	n	B	y_{lt}^+	Re_{μ_w}	$f(\text{exp})$	$f(2.5.13)$
0.1%	0.895	5.65	11.82	33,400	5.82×10^{-3}	5.82×10^{-3}
				150,263	4.14×10^{-3}	4.14×10^{-3}
0.3%	0.700	7.00	13.50	24,800	5.48×10^{-3}	5.47×10^{-3}
0.4%	0.590	7.30	13.87	12,807	6.23×10^{-3}	6.21×10^{-3}
0.6%	0.445	8.20	14.96	27,850	4.75×10^{-3}	4.79×10^{-3}

Table 2.1. Comparison of friction factors obtained from pressure drop data of Bogue (1961), for turbulent pipe flow of Carbopol solutions, with predictions of (2.5.13). Value of B obtained from velocity profile data of Bogue (1961) – figure 2.7.

value of B . However, with increasing concentration and decreasing n there is an upward and apparently parallel shift of the dimensionless profile, suggesting that the rheology affects the dimensionless sublayer thickness but not the behaviour in the fully-turbulent regime, as might be expected (*cf.* discussion in section 3.5). This judgement is subject to the qualification that the number of data points is extremely limited, more particularly as several in each case are at or near the pipe centreline, and accordingly would lie outside the logarithmic region if the fluid were Newtonian, as noted earlier. Furthermore, there must be some doubt in the case of the 0.4% solution as to whether the flow is fully turbulent. While bearing the uncertainty regarding Reynolds numbers in mind, that for the flow of the 0.4% solution is particularly low, and a ‘log law’ region of Newtonian or other slope is difficult to identify; rather the profile is characteristic of a transitional flow. Nevertheless, it appears that (2.5.1) represents the fully developed profile for the Carbopol solution also, with A equal to the Newtonian value of 5.75, and B incremented to an increasing degree as n decreases – table 2.1. A higher value of y_{lt}^+ is implied – table 2.1 – and hence a thicker laminar sublayer in dimensionless terms.

As before, the velocity profile may be integrated across the cross-sectional area (appendix D), as in the Newtonian case, to obtain the correlation

$$\frac{1}{\sqrt{f}} = 4 \log(Re_{\mu_w} \sqrt{f}) + \frac{1}{\sqrt{2}}(B - 6.35) \quad (2.5.13)$$

Equation (2.5.13) may be recast as

$$B = \frac{2}{\sqrt{f}} - 5.66 \log(Re_{\mu_w} \sqrt{f}) + 6.35 \quad (2.5.14)$$

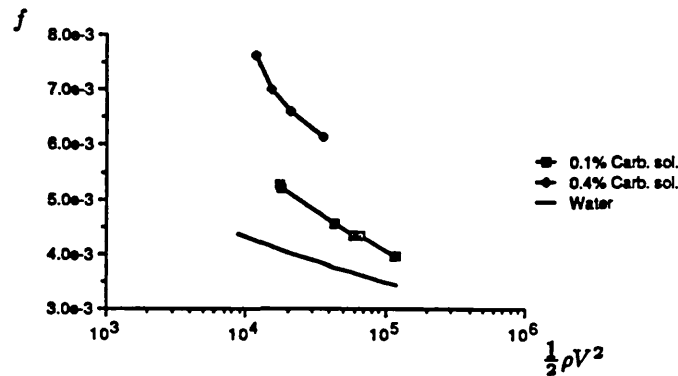


Figure 2.8 Comparison of pressure drop, in pipe flow, of aqueous solutions of Carbopol and of water. Data of Bogue (1961)

and thus B may be obtained from pressure drop data where velocity data is unavailable. This is of some value given that the flows of many shear-thinning fluids (slurries, suspensions, some polymer solutions) are not amenable to optical measuring techniques while the reservations expressed in the literature regarding Pitot tube measurements of the flows of such fluids have been alluded to already.

Bogue also obtained pressure drop measurements for the flow of the Carbopol solutions, indicating a greater pressure drop for the solution than for the same mass flow rate of solvent – figure 2.8. The friction factor obtained from (2.5.13) is compared with these measured values in table 2.1, using the values of B deduced from the velocity profile fits. Given the limited extent of the velocity data, and consequent uncertainty surrounding the B values, the agreement is good.

Shaver and Merrill (1959) obtained pressure drop and velocity profile data, and dye injection photographs, for the turbulent flow of aqueous solutions of CMC, alginate and Carbopol. The manner in which their data is presented does not allow for friction factor comparisons on a mass flow rate equality basis, however, nor for reinterpretation of their velocity data – their comparisons were made on a Re_{pl} basis. Their velocity profile measurement technique is not stated, and they characterised the fluids using the ‘power law’ but with different parameters for different shear rate ranges. Their photographs illustrate a thicker laminar sublayer for the polymer solutions than for the pure solvent at the same mass flow rate, and a progressively lower turbulence intensity with decreasing shear-thinning index – the latter may, however, be attributable to increasing fluid consistency. It

is not clear whether these photographs are unique, or representative of a range of bulk flow velocity cases, for each fluid. Definitive conclusions could only be drawn if the latter were the case.

2.5.2 Drag reduction

Drag reduction, a phenomenon whereby the pressure loss in the turbulent flow of a fluid is dramatically reduced by the addition of small concentrations of certain high molecular weight polymers, is defined as

$$\% \text{ drag reduction} = \frac{\Delta P_s - \Delta P_p}{\Delta P_s} \times 100 \quad (2.5.15)$$

where ΔP represents pressure loss due to friction, and the subscripts s and p refer to the pure solvent and the polymer solution, respectively. Comprehensive reviews of drag reduction studies have been presented by Hoyt (1972) and Virk (1975). They concluded that the mechanism of drag reduction remains obscure, but that the balance of the evidence indicates that viscoelastic effects are responsible, a view shared by Lumley (1969): "all of the polymer solvent combinations that display drag reduction also display, in higher concentrations, viscoelastic effects, although such effects are imperceptible at the concentrations usually involved in drag reduction". Its significance in the present context is that several of the solutions commonly used in shear-thinning fluid studies exhibit drag reduction.

Much confusion is frequently occasioned in the literature by the failure to make explicit the basis of comparison in discussing drag-reducing flows. The potential for confusion will be apparent from the pressure drop data of Dodge (1957) for aqueous solutions of CMC and Carbopol, with similar viscometric characteristics on the basis of the 'power law' (0.3% CMC: $n = 0.62, K = 1.9 \times 10^{-1} \text{ kg/ms}^{2-n}$, 0.3% Carbopol: $n = 0.617, K = 5.22 \times 10^{-1} \text{ kg/ms}^{2-n}$). These are presented on a mass flow rate comparison basis in figure 2.9, in which the CMC solution is seen to be drag-reducing and the Carbopol solution drag-increasing.

The difference in behaviour of two apparently similar solutions makes clear that one or other of the solutions cannot be characterised by a constitutive equation of the form of (2.2.3) alone.

Ernst (1966,1967) obtained velocity profile data at various flow rates for the fully developed turbulent flow of 0.05% aqueous solutions of CMC ($n = 0.92$) and representative profiles are reproduced as figure 2.10. The profiles are plotted

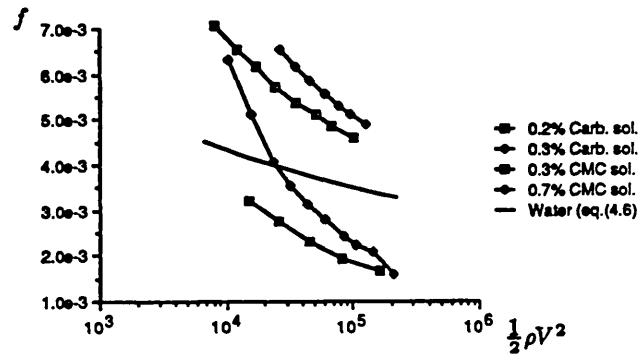


Figure 2.9 Comparison of pressure drop, in pipe flow, of aqueous solutions of Carbopol and of CMC. Data of Dodge (1957)

on a $u^+ - \log y^+$ basis, with Re_{μ_w} as parameter, and demonstrate an upward and parallel shift to the Newtonian profile (2.5.1), superimposed for reference. It appears that the shift is a function of Re_{μ_w} . (Whether this would be so for Carbopol solutions also is important to establish; Bogue's data for the Carbopol solutions was unfortunately obtained for one flow rate only in each case, with the exception of the near-Newtonian behaving 0.1% solution.) Ernst found that the CMC solution exhibited substantial drag reduction, and, consistent with the findings of other investigators of the phenomenon, as summarised by Virk (1975), that it is only exhibited above a certain flow rate, below which the drag is actually greater than that associated with the flow of the pure solvent.

While lack of data prevents the conclusion that the degree of upward shift ΔB in the 'log law' profile for the flow of a shear-thinning fluid of a given shear-thinning index n is independent of Re_{μ_w} , there is extensive experimental evidence that ΔB is a function of Re in the flow of drag-reducing *constant viscosity* fluids, of which that of Mizushima and Usui (1977), and Allan *et al* (1984) may be cited as representative. Given the limited degree of shear-thinning exhibited by the CMC solutions used by Ernst, it is probable that the greater part of the upward shift illustrated in figure 2.10 is associated rather with drag reduction. This illustrates the importance of identifying the particular non-Newtonian mechanism governing a particular flow structure, and the confusion which may be occasioned if more

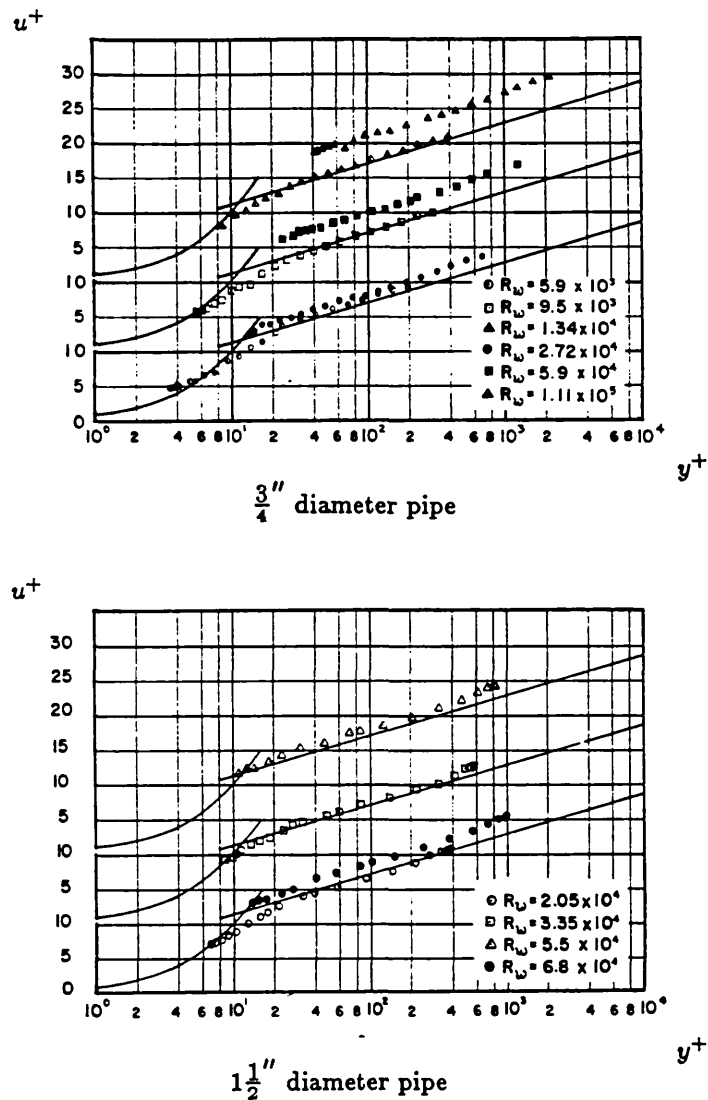


Figure 2.10 Velocity profiles for fully developed turbulent pipe flow of a 0.05% aqueous solution of CMC. Data of Ernst (1967)

than one such mechanism is operative, given the difficulty of distinguishing the effect and relative importance of each.

2.5.3 Analytical studies

A number of analytical approaches to turbulent pipeflow of shear-thinning fluids have appeared in the literature.

Based on the data of Dodge (1957), Dodge and Metzner (1959) derived the following relationship (as summarised in Appendix D)

$$\frac{1}{\sqrt{f}} = A_{1n} \log [Re_{pl}(f)^{1-n'/2}] + C'_{2n} \quad (2.5.17)$$

where A_{1n} and C'_{2n} are functions of n . To determine A_{1n} and C'_{2n} Dodge and Metzner plotted $1/\sqrt{f}$ against $\log[Re_{pl}(f)^{1-n'/2}]$, as presented for one value of n' in figure 2.11b. The slope of this curve is A_{1n} , and from a plot of A_{1n} against n' , figure 2.11c, they determined that

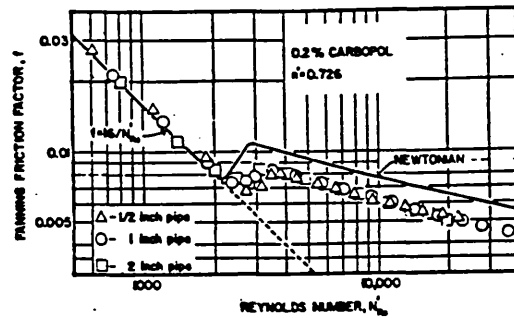
$$A_{1n} = \frac{4}{(n')^{0.75}} \quad (2.5.18)$$

$$C'_{2n} = \frac{-0.4}{(n')^{1.2}} \quad (2.5.19)$$

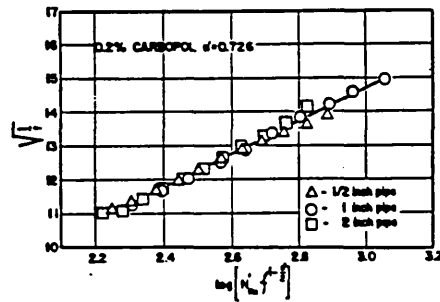
Dodge and Metzner's plot of their experimentally obtained friction factors against the predictions of (2.5.17), figure 2.11d, for n ranging from 0.36 to 0.73 and Re_{pl} ranging from 2,900 to 36,000, shows a mean absolute deviation of experimental from predicted values of f of 1.9%, and a maximum of 8.5%.

Dodge and Metzner, in establishing the parametric dependence of the velocity defect (D.5), point out that it is independent of the viscosity for Newtonian fluids, and claim that the equivalent assumption for 'power law' fluids is that the defect is independent of K . This is not obvious: the dimensions of K are not those of viscosity, but rather $\text{kg}/\text{ms}^{2-n}$. A velocity defect dependence on K would make (2.5.17) functionally dependent on K also. Further doubt is cast on (2.5.17) by the variation noted by Dodge and Metzner themselves in the values of the coefficient A_{1n} with pipe diameter, evident from figure 2.11c. Their interpretation is unconvincing: "since it is well established for Newtonian fluids that no extraneous diameter effects exist, it is concluded that the indicated non-Newtonian diameter discrepancies in A_{1n} do not constitute a real effect".

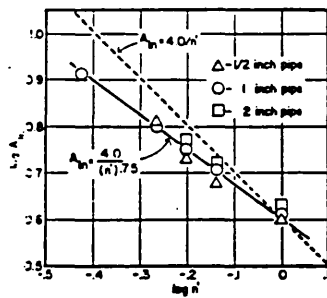
A further reservation concerning Dodge and Metzner's work is the question of scaling. If the fluid may be characterised by the 'power law', the friction factor – Reynolds number relationship is, according to Dodge and Metzner, unique for any given shear thinning index n , and scale up by an arbitrary amount is permissible. If however, the fluid does not obey the 'power law', the relationship is not



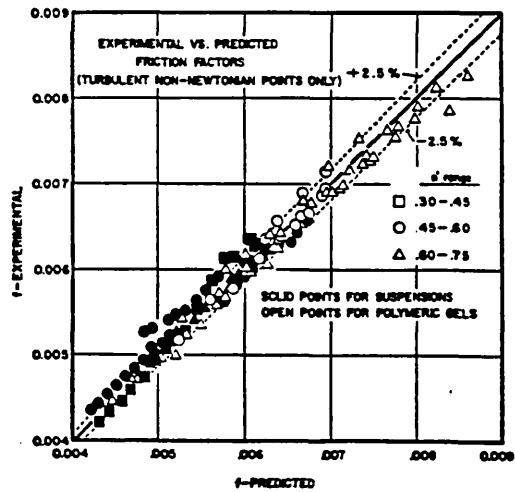
a. Typical non-Newtonian friction factor results



b. Turbulent data from figure a plotted in terms of the correlation variables



c. The A_{1n} function: variance with the flow behaviour index n'



d. Comparison of experimental friction factors with those predicted

Figure 2.11 Data of Dodge and Metzner (1959) used in establishing (2.5.17)

unique, since K' and n' are pipe diameter dependant – and, as noted earlier, in principle a scaling theory allowing scale up outside the range of experimental data is impossible for an empirical correlation between dimensionless groups, such as (2.5.17).

The approach of Pai, in using a single polynomial expression for the complete turbulent flow velocity distribution, was extended by Brodkey, Lee and Chase (1961) to include the ‘power law’ model. The velocity across the pipe is assumed to be represented by a three term power series

$$\frac{u}{u_{\max}} = 1 + a_1 \left(\frac{r}{R}\right)^{(n+1)/n} + a_2 \left(\frac{r}{R}\right)^{2m} \quad (2.5.20)$$

where the series is limited by the number of known boundary conditions, these being just sufficient to evaluate the coefficients in a three term expression. The expression is held to be valid from wall to centreline, and as such provides a more accurate integrand than (2.5.1) to obtain an expression for the friction factor. The value of the empirical integer constant m must be established experimentally for each Reynolds number considered, however. Comparison with the experimental data of Shaver and Merrill (1959) for the turbulent flow of aqueous solutions of CMC and alginate, appeared to indicate satisfactory agreement with the former, less so with the latter. However the obvious limitation of the approach is the lack of knowledge of the parametric dependance of m (if such there is). Brodkey (1963) proposed a correlation of m with Reynolds number for Newtonian fluids, but his tentative extension of this to fluids characterised by the ‘power law’ is unlikely to be a fruitful approach, since such a correlation would be required for each flow index n of interest.

Edwards and Smith (1980b) reviewed the numerous expressions proposed in the literature to describe the eddy viscosity in fully developed turbulent Newtonian pipe flow. These, in combination with the assumption that shear stress varies linearly with radial distance, give fully developed turbulent velocity profiles of which the proposal of Spalding (1961) is representative:

$$y^+ = u^+ + \exp\left(\frac{-B}{A}\right) \left[\exp\left(\frac{u^+}{A}\right) - 1 - \left(\frac{u^+}{A}\right) - \frac{1}{2!} \left(\frac{u^+}{A}\right)^2 - \frac{1}{3!} \left(\frac{u^+}{A}\right)^3 \right] \quad (2.5.21)$$

The velocity profiles predicted by a number of these proposals are in good agreement with experimental measurements for fully developed turbulent Newtonian pipe flow. Edwards and Smith suggested that the use of velocity profile expressions derived from eddy viscosity expressions, such as (2.5.21), may be extended

to shear-thinning flows if μ is replaced by μ_w as a characteristic viscosity for the flow. The proposal has again served to highlight the lack of experimental data to establish correlations between Reynolds numbers of a given index and the friction velocity, since knowledge of the pressure drop is necessary to establish velocity distributions on this basis.

Wilson and Thomas (1985) assumed that the rate of energy dissipation of a turbulent eddy is represented by the integral of the shear stress-strain rate curve. The value of the integral for a shear-thinning fluid is greater than that for a Newtonian fluid with a viscosity equal to the viscosity at the wall for the shear-thinning fluid. This represents not a greater rate of energy dissipation (this being dictated by the cascade mechanism) but a greater apparent viscosity, and consequently greater length scale, at the dissipative eddy level. They further assumed that the length scales and characteristic velocities of the largest and smallest eddies coincide at the intersection of the laminar sublayer and turbulent core. This implies a thicker laminar sublayer; they suggested that the dissipative eddy length scale, and accordingly sublayer thickness and y_{lt}^+ , are greater for the shear-thinning solution by a factor equal to the ratio of the 'energy' integral. This was used as the basis for a correlation between the 'power law' index and the upward shift in the 'log law', ΔB , and hence for an $f - Re$ relationship. "Significant agreement" was claimed with the Dodge and Metzner relationship (2.5.16), on the basis of Re_{pl} ; and "essential agreement" with measured pressure drop in flows of several shear-thinning fluids, comparing on the basis of Re_{μ_w} .

The hypothesis is based, however, on the mean strain rate as the upper limit for the integral – but in turbulent flow the shear rate fluctuates widely, typically being several orders of magnitude greater than the mean strain rate at the dissipative level, as will be demonstrated in section 3.7.2.

The attempt of Brewster and Irvine (1987) exemplifies the continuing attempts appearing in the literature to refine the $f - Re_{pl}$ 'relationship', which make no acknowledgement of the uncertainties associated with flow characterisation on the basis of a Reynolds number alone – they use a 'modified power law model', but as this inevitably requires a second dimensional parameter (a characteristic viscosity in this case) the approach is erroneous for the reasons discussed in section 2.4.

2.6 Agitation of shear-thinning fluids in mixing vessels

Experimental investigation of mixing vessel flow of shear-thinning fluids has been almost exclusively limited to establishment/confirmation of $N_P - Re$ correlations as discussed briefly in section 2.4.3. Metzner and Taylor (1960) conducted a streak photography study of flow patterns of CMC in a mixing vessel, and observed that the mixing process consisted of highly turbulent mixing confined to the impeller region, with fluid motion elsewhere in the tank serving primarily to bring fresh fluid into this region, and that impeller jet velocities increase exponentially with increasing impeller speed due to shear-thinning. No detailed characterisations of such flows *ie.* mean and r.m.s. velocity measurements, have been identified in the literature.

2.7 Conclusions

It is clear from the discussion on scaling procedures that unless the ‘power law’ model is accepted as a sufficiently accurate characterisation of the fluid, the flow of every shear-thinning fluid in every geometry is dynamically unique, and that comparisons of flow characteristics on the basis of a Reynolds number, or any other single parameter, are not reliable. Moreover, in the case of ‘power law’ fluids, only comparisons between flow regimes involving fluids of the same index n are valid – kinematic similarity is not obtainable between the flow of a shear-thinning fluid and that of water, for example.

Such a conclusion represents a strong argument in favour of computational methods for the analysis of the flow of shear-thinning fluids. Quite apart from fluid properties, however, certain flow field-dependent empirical constants required by these methods must be obtained from experimental data. The number of such experimental cases must of necessity be limited. Thus these empirical constants must be used in the numerical analysis of flow cases dynamically dissimilar to those for which they were obtained, unlike in the prediction of Newtonian flows, and the uncertainty with respect to their accuracy will accordingly be greater.

Such data as is available appears to indicate that the ‘law of the wall’, (2.5.1), for velocity distribution in fully-developed turbulent pipe flow, is valid for shear-thinning fluids also. It has been indicated how the parameter B may be obtained from pressure drop data (2.5.14) – this frequently being easier to obtain and involving less experimental uncertainty with regard to experimental accuracy than velocity profile data, for shear-thinning fluids. Much more experimental data than

has been published to date is required for a range of flow rates for each of a range of shear-thinning indices, to establish with confidence whether the upward shift in the semi-logarithmic velocity profile is always parallel for inelastic fluids, and to determine the degree of that shift *ie.* the value of B .

This upward shift relative to the profile for Newtonian fluids corresponds to a thicker laminar sublayer in dimensionless terms. This result on a $y^+ = y\rho u_* / \mu_w$ basis of comparison is qualitatively, and to the limited extent permitted by the experimental data, quantitatively consistent with the observed reduction in pressure drop in flows of shear-thinning fluids relative to that in flows of Newtonian fluids when these are compared on a Re_{μ_w} basis. The caution necessary in drawing conclusions from such comparisons is again borne out, however, by the very different flow behaviour of apparently similar (on the basis of the 'power law') solutions, more readily apparent when comparison is made on mass flow rate basis. There is clearly a rheological mechanism other than shear-thinning responsible for such differences; no study to date has definitively identified this mechanism, still less separated its effects from those attributable to shear-thinning.

3 The governing equations

3.1 Introduction

Fluid flow is fully represented by the Navier-Stokes equations for mass and momentum conservation, irrespective of the geometric complexity involved; these are set out in section 3.2. The small time and length scales associated with the dissipative eddies of turbulent flows, however, render solution of these equations impracticable with the numerical methods and computing resources available at present and for the foreseeable future. The averaging procedure used to circumvent this difficulty is presented in section 3.3. The closure problem arising in turn is addressed by turbulence modelling; this is considered in section 3.4. Current thinking on the nature of turbulence processes is briefly discussed in section 3.5, as a preamble to consideration of turbulence models, which address the closure problem, in section 3.6. Section 3.7 is concerned with the evaluation of strain-rate dependent molecular viscosity in turbulent flow. The $k - \epsilon$ model of turbulence used in this study, in a form extended to model the flow of shear-thinning fluids, is described in section 3.8. The complete set of partial differential equations to be solved is presented in section 3.9. Finally the handling of the various boundary conditions arising in the geometries of interest is discussed in section 3.10.

3.2 Instantaneous equations

The instantaneous equations for mass and momentum conservation are well established – see, for instance, Bird, Stewart and Lightfoot (1960). Using Cartesian tensor notation for compactness, and denoting instantaneous quantities by the superscript $\hat{}$, the equation for mass conservation, or continuity is given by

$$\frac{\partial \hat{u}_i}{\partial x_i} = 0 \quad (3.2.1)$$

and those for momentum conservation by

$$\frac{\partial}{\partial x_j} (\rho \hat{u}_j \hat{u}_i) = -\frac{\partial \hat{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \hat{\tau}_{ij} \quad (3.2.2)$$

for the steady-state flow of a homogeneous fluid of constant density. Here subscripts $i, j = 1, 2, 3$ (with implicit summation over repeated indices), u_i is the velocity component in the i direction, ρ denotes density, p pressure and τ_{ij} the deviatoric stress tensor. The relationship between the deviatoric stress components

and the corresponding rates of strain has been discussed in the previous chapter. The gravitational force is treated as negligible and omitted from (3.2.2).

3.3 Time-averaged equations

The time and length scales associated with the dissipative eddies in turbulent flow are such that solution of (3.2.1) and (3.2.2) using current numerical methods and computing resources is not feasible. Some form of statistical averaging must be employed to render these tractable, and that most commonly used is Reynolds' decomposition of an instantaneous quantity $\hat{\phi}$ into its mean, $\bar{\phi}$, and fluctuating, ϕ' , components – see, for instance, Hinze (1975):

$$\hat{\phi} = \bar{\phi} + \phi' \quad (3.3.1)$$

For unsteady flows the mean quantity may only be meaningfully interpreted as the average of the quantity over a number of identically defined flow cases, at the same temporal and spatial locations. For the steady flows of interest in this study, however, the mean may be interpreted as a time average over a finite time interval – see, for instance, Bradshaw (1978):

$$\bar{\phi} = \lim_{t \rightarrow \infty} \frac{1}{t} \int_{t_0}^{t_0+t} \hat{\phi} \, dt \quad (3.3.2)$$

and

$$\phi' = \lim_{t \rightarrow \infty} \frac{1}{t} \int_{t_0}^{t_0+t} (\hat{\phi} - \bar{\phi}) \, dt \quad (3.3.3)$$

since, for the steady state, $\partial \bar{\phi} / \partial t = 0$, and accordingly the integrals are independent of t_0 .

Substituting $\bar{\phi} + \phi'$ for $\hat{\phi}$ in (3.2.1) and time averaging yields

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0 \quad (3.3.4)$$

and subtracting (3.3.4) from (3.2.1) gives

$$\frac{\partial u'_i}{\partial x_i} = 0 \quad (3.3.5)$$

Writing (3.2.2) in terms of decomposed quantities and time averaging yields

$$\rho \frac{\partial}{\partial x_j} (\bar{u}_j \bar{u}_i) + \rho \frac{\partial}{\partial x_j} (\overline{u'_j u'_i}) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \bar{\tau}_{ij} \quad (3.3.6)$$

– where it may be shown that the divergence of the fluctuating stress tensor, $\partial(p' + \tau'_{ij})/\partial x_j$, vanishes. Thus one additional term arises in (3.3.6), the second on the left hand side, and from (3.3.5)

$$\overline{\frac{\partial}{\partial x_j}(u'_j u'_i)} = \frac{\partial}{\partial x_j} \overline{(u'_i u'_j)} \quad (3.3.7)$$

This represents mean transport of fluctuating momentum by velocity fluctuations, and is thus the divergence of a momentum flux. It may therefore be interpreted as the divergence of the additional stresses arising in the fluid as a result of turbulence, and when thus interpreted, as is usual, the terms $\overline{\rho u'_i u'_j}$ are referred to as the Reynolds stresses. As an apparent stress relative to the mean flow, it is grouped with the deviatoric stress, such that the momentum conservation equation is written as

$$\rho \frac{\partial}{\partial x_j} (\bar{u}_j \bar{u}_i) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} (\bar{\tau}_{ij} - \overline{\rho u'_i u'_j}) \quad (3.3.8)$$

Because of the presence of the Reynolds stress term, the time-averaged conservation equations, (3.3.4) and (3.3.8), do not constitute a closed set, unlike the instantaneous equations, (3.2.1) and (3.2.2). This closure problem is addressed next.

3.4 The Reynolds stress transport equation

A transport equation for the Reynolds stresses may be derived by multiplying the instantaneous momentum equation for the i direction by u'_j , that for the j direction by u'_i , adding the two and time averaging. Using the continuity relationships (3.3.4) and (3.3.5) the Reynolds stress transport equation may then be expressed as

$$\begin{aligned} \rho \frac{\partial}{\partial x_k} \bar{u}_k \overline{(u'_i u'_j)} = & - \underbrace{\left\{ \overline{u'_j u'_k} \frac{\partial \bar{u}_i}{\partial x_k} + \overline{u'_i u'_k} \frac{\partial \bar{u}_j}{\partial x_k} \right\}}_{\text{generation}} - \\ & \underbrace{\mu \left[\left(\frac{\partial u'_i}{\partial x_k} + \frac{\partial u'_k}{\partial x_i} \right) \frac{\partial u'_j}{\partial x_k} + \left(\frac{\partial u'_j}{\partial x_k} + \frac{\partial u'_k}{\partial x_j} \right) \frac{\partial u'_i}{\partial x_k} \right]}_{\text{dissipation}} + \underbrace{p' \left(\frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right)}_{\text{pressure-strain}} - \\ & \underbrace{\frac{\partial}{\partial x_k} \left\{ \overline{\rho u'_i u'_j u'_k} - \mu \left(\frac{\partial}{\partial x_k} \overline{(u'_i u'_j)} + u'_j \frac{\partial u'_k}{\partial x_i} + u'_i \frac{\partial u'_k}{\partial x_j} \right) + \overline{p'(\delta_{jk} u'_i + \delta_{ik} u'_j)} \right\}}_{\text{diffusion}} \end{aligned} \quad (3.4.1)$$

The closure problem manifests itself in the form of a number of unknown fluctuating velocity and velocity gradient correlations. The derivation of (3.4.1) does not therefore immediately solve the difficulty of arriving at a closed set of simultaneous equations which mathematically model the random process. By expressing the Reynolds stresses in terms amenable to physical interpretation it does, however, lend itself to the approximate modelling required to dispose of the need for transport equations for higher-order correlations.

Equation (3.4.1) expresses the net rate of increase of $\overline{u'_i u'_j}$ in an identifiable volume of fluid in terms of a) generation by mean strain b) redistribution by pressure-strain interaction c) redistribution by viscous diffusion, negligible in relative magnitude at high Reynolds numbers (*cf.* discussion in following section), and d) viscous dissipation, non-negligible since a function of fluctuating velocity derivatives. For a detailed discussion of the above see Launder (1984a).

The dissipation terms may be expressed as a function of the scalar quantity $\bar{\epsilon}$, the mean rate of viscous dissipation (Launder, 1984a):

$$\mu \left[\left(\frac{\partial u'_i}{\partial x_k} + \frac{\partial u'_k}{\partial x_i} \right) \frac{\partial u'_j}{\partial x_k} + \left(\frac{\partial u'_j}{\partial x_k} + \frac{\partial u'_k}{\partial x_j} \right) \frac{\partial u'_i}{\partial x_k} \right] = \frac{2}{3} \rho \bar{\epsilon} \delta_{ij} \quad (3.4.2)$$

in the case of isotropic, high-Reynolds-number turbulence. This definition will be useful presently.

3.5 Turbulence processes

Turbulence is, in the conventional wisdom – see, for instance, Bradshaw (1978), conceived of as an inertially-governed process of energy transfer through successively smaller spatial scales, with viscous stresses providing the eventual sink. Based on the random walk theorem, by which the distance between two randomly disturbed particles will, on the average, increase, the length of a vortex element, which may be conceived of as a vortex line or as an eddy, will increase. The diameter of such an element will accordingly decrease; by conservation of angular momentum its angular velocity will increase. Interaction of vortex elements maintains the random fluctuations while angular velocity is transferred to smaller length scales. The influence of the mean velocity field is exerted on the largest vortex elements, which in turn stretch the next smallest. If angular momentum is conserved while vortex radii are reduced, it follows that the kinetic energy of the

vortex increases, this being at the expense of the kinetic energy of the mean field. Within the smallest vortices strain rates are sufficiently large that viscous stresses predominate. While molecular viscosity provides the dissipation mechanism, it does not influence the rate at which energy is transferred through the ‘cascade’. This is the high-Reynolds-number hypothesis, underpinning most approaches to turbulence modelling, including that to be adopted here. Thus its validity is crucial to this study; any uncertainty as to how well grounded it is in relation to the turbulent flow of shear-thinning fluids derives from the very high consistencies associated with such fluids.

The high-Reynolds-number hypothesis implies that the rheological behaviour of the fluid will have little if any influence on the bulk flow parameters, the large scale interactions in a turbulent flow being inertia dominated and essentially independent of the details of the mechanism of momentum transport. However, viscosity *does* govern the time and length scales associated with the dissipative vortices, as these must adjust themselves to dissipate all of the energy which they receive. These scales are of crucial importance in determining reaction rates and other micromixing processes in mixing vessels – Oldshue (1983), and as such are variables of primary interest. As the only field variables expected to reflect shear-thinning behaviour in regions removed from solid boundaries, their prediction for such fluids is a central goal of this study. Viscosity is of course a prime determinant of near-wall flow structures – the extent to which rheological effects manifest themselves thereby has been made clear in the foregoing chapter.

3.6 Turbulence models

The models proposed in response to the closure problem may broadly be classified as those based on the notion of an effective turbulent transport coefficient, considered in section 3.6.1, and those based on the solution of approximated equations for the Reynolds stresses, considered in section 3.6.2.

3.6.1 Turbulent viscosity models

The Reynolds stresses in (3.3.8) may be conceived of as directly proportional to the gradients of the mean velocities, in a like manner to the viscous stresses – the Boussinesq model – see, for instance, Hinze (1975). The coefficient of proportion-

ality in such a relationship is variously described as an apparent, eddy or turbulent viscosity, and denoting this by μ_t , the Reynolds stresses are modelled as

$$-\rho \overline{u'_i u'_j} = \mu_t \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \rho k = \mu_t \bar{\gamma}_{ij} - \frac{2}{3} \delta_{ij} \rho k \quad (3.6.1)$$

where the term in the time-averaged turbulence kinetic energy k

$$k = \frac{1}{2} \sum_{j=1,3} \overline{v_j'^2} \quad (3.6.2)$$

ensures equation balance when $i = j$ and the equation is summed. This term may be interpreted (Launder, 1973) as an effective increase in the static pressure by two thirds of the turbulence energy due to the turbulent agitation.

Any quantity relating the second order tensors $\overline{u'_i u'_j}$ and $\bar{\gamma}_{ij}$ must be a tensor of zero, second, fourth or higher order, and the complexities associated with all but the first, a scalar, mean that it is generally adopted. The limitations implied (the not-always-realistic disregard of transport and history effects on the Reynolds stresses, and the requirement that the principal axes of the Reynolds stresses and of the mean strain be coincident) are discussed by Hanjalić and Launder (1972) and Castro and Bradshaw (1976).

All models based on the turbulent viscosity concept assume a direct proportionality between μ_t and a mixing length l and a velocity scale, v , after Prandtl (1925):

$$\mu_t \propto l v \quad (3.6.3)$$

Prandtl suggested a direct proportionality between l and distance from solid boundaries in the case of confined flows; other forms of empirical prescription are required in free flows. Prandtl also hypothesised that the mixing velocity v is proportional to the product of the mixing length and transverse mean velocity gradient, $l du/dy$, from considerations of transverse momentum exchange, achieved through collisions of fluid parcels of different velocity u over distance l .

It will be apparent that an approach using empirical relationships for both mixing length and mixing velocity lacks universality. The mixing length relationship is geometry dependent, while in regions of low velocity gradients (recirculation zones, velocity maxima etc.) the mixing velocity, and hence μ_t , vanish, in contradiction of experimentally observed patterns of turbulence.

As a first improvement on the Prandtl hypothesis Kolmogorov (1942) proposed a relationship between the mixing velocity and the turbulence kinetic energy,

k :

$$\mu_t = C_\mu \sqrt{k} l \quad (3.6.4)$$

where C_μ is a constant and the value of k is determined from a differential transport equation in which k is the dependent variable.

This type of model has the advantage over the mixing length model that in pipes or annuli having regions of low velocity gradient the k equation enables account to be taken of the influence of neighbouring regions on the local turbulence energy (Launder and Spalding, 1972). A model taking similar account of neighbouring regions on the turbulence length scale requires a transport equation for that quantity also, however. In fact, as pointed out by Launder and Spalding (1972), any variable $z = k^m l^n$, with m and n constants, would suffice as the dependent variable for the second equation. They surveyed the variables used, which have included $k^{1/2}/l$ (a turbulent frequency), $k^{3/2}/l$ (the turbulence kinetic energy dissipation rate), l itself, kl , and k/l^2 , the time-average square of the vorticity fluctuations, or square of the frequency of the turbulent eddies. While the transport equation for z is similar in form irrespective of the particular variable chosen, including terms representing convection, diffusion, turbulent interactions with the mean flow and other turbulent motion, the dissipation rate $k^{3/2}/l = \epsilon$ has been the predominant choice of those using two-equation turbulence models. This is in large measure due to the conclusion of Launder and Spalding (1974) that in contrast to the equations for kl and k/l^2 , that for ϵ does not require adjustment of 'constants' with distance from solid boundaries in order to fit experimental data. l is an unattractive choice as it does not diffuse at a rate proportional to the spatial gradients of l (Launder and Spalding, 1972), and third order correlations appearing in the transport equations must be represented by way of spatial gradients of the dependent variable of the relevant equation (Launder and Spalding, 1974).

The $k - \epsilon$ model of turbulence, as it is generally referred to, is that used in this study. Brief mention will first be made, however, of alternatives to turbulent viscosity models of turbulence.

3.6.2 Reynolds and algebraic stress models

An alternative approach is that based on the solution of approximated equations for the Reynolds stresses, in which the dissipative, diffusive and redistributive processes embodied by the exact equations (3.4.1) for the Reynolds stresses are simulated. The approximations involve a length scale for which a transport equa-

tion is also required. Hanjalić and Launder (1972) and Launder, Reece and Rodi (1975), whose proposals are representative of these Reynolds stress models, used ϵ as the length scale. Reynolds stress models offer improved accuracy in avoiding the assumption of a scalar turbulent viscosity, an assumption contradicted by experimental evidence for all but the simplest shear flows. That they have not replaced turbulent viscosity models is due to the computational expense of the solution of the equations for the various components of $\overline{u'_i u'_j}$ – in complex flows where the Reynolds stress model is most justified, all six components must be calculated.

Rodi (1976) proposed a compromise between the economy of the turbulent viscosity approach and the apparent universality of Reynolds stress models. The convection and diffusion of $\overline{u'_i u'_j}$ are assumed proportional to k , and the differential equation for $\overline{u'_i u'_j}$ thus simplified to an algebraic expression. Transport equations are required for k and a length scale, in addition to the algebraic equation set for $\overline{u'_i u'_j}$, but the approach acknowledges the anisotropic nature of turbulent diffusion. The algebraic equations are, however, non-linear, and consequent numerical instabilities and non-uniqueness of solution have been reported.

It must be borne in mind in considering the potential advantages of Reynolds and algebraic stress models, that closure still requires the prescription or solution of a transport equation for a length scale-related quantity, and this is widely recognised – see, for instance, Launder (1984a) – as being largely responsible for the inability of any turbulence model to make accurate predictions for a broad range of flow types with only one set of empirical coefficients.

3.7 The mean molecular viscosity

The decomposition of instantaneous quantities into mean and fluctuating components, (3.3.1), means that when instantaneous deviatoric stress tensor, $\hat{\tau}_{ij}$, in (3.2.2)

$$\hat{\tau}_{ij} = \hat{\mu} \hat{\gamma}_{ij} \quad (3.7.1)$$

is time-averaged, the relationship

$$\overline{\tau}_{ij} = \overline{\mu \dot{\gamma}_{ij}} + \overline{\mu' \dot{\gamma}'_{ij}} \quad (3.7.2)$$

is obtained. It is then apparent that knowledge of $\overline{\mu}$ is required for closure. In addition, whether modelling of the correlation $\overline{\mu' \dot{\gamma}'_{ij}}$ is required depends on its

magnitude relative to the term $\overline{\mu' \dot{\gamma}_{ij}}$; this question is addressed first in section (3.7.1). Determination of strain-rate dependent molecular viscosity necessitates determination of the relevant strain rate from the range of shear rates obtaining in turbulent flow; this is considered in section (3.7.2). Finally the calculation of molecular viscosity from the p.d.f. of the dissipation rate is described in section 3.7.3.

3.7.1 Relative magnitude of viscosity-strain correlations

The magnitude of $\overline{\mu' \dot{\gamma}_{ij}}$ relative to $\overline{\mu \dot{\gamma}_{ij}}$ depends on the response time of the fluid *ie.* whether (2.3.1) is obeyed instantaneously, or whether the characteristic timescale of the Kolmogorov eddies is so small compared to the response time that such obedience is not possible. The case of faithful material response to all fluctuations will be taken first.

$$\begin{aligned}\hat{\mu} &= f(\hat{I} \hat{I}_{\dot{\gamma}}) \\ &= f(\hat{\dot{\gamma}}_{ij} : \hat{\dot{\gamma}}_{ij}) \\ &= f(\overline{\dot{\gamma}_{ij}} : \overline{\dot{\gamma}_{ij}} + 2\overline{\dot{\gamma}_{ij}} : \dot{\gamma}'_{ij} + \dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}) \\ &= f\left[\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij} \left(1 + 2\frac{\overline{\dot{\gamma}_{ij}} : \dot{\gamma}'_{ij}}{\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}} + \frac{\overline{\dot{\gamma}_{ij}} : \overline{\dot{\gamma}_{ij}}}{\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}}\right)\right]\end{aligned}\quad (3.7.3)$$

Since in general $\overline{\dot{\gamma}_{ij}} \ll \dot{\gamma}'_{ij}$, the last term in (3.7.3), which is second order in $\overline{\dot{\gamma}_{ij}}/\dot{\gamma}'_{ij}$, may be considered negligible. By a binomial expansion of (3.7.3), therefore

$$\hat{\mu} = f(\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}) + f'(\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}) 2\overline{\dot{\gamma}_{ij}} : \dot{\gamma}'_{ij} + \dots \quad (3.7.4)$$

Hence the first term in (3.7.2) becomes

$$\overline{\mu \dot{\gamma}_{ij}} = \left\{ f(\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}) + 2\overline{\dot{\gamma}_{ij}} : \overline{f'(\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}) \dot{\gamma}'_{ij}} \right\} \overline{\dot{\gamma}_{ij}} \quad (3.7.5)$$

The first of the r.h.s. terms in (3.7.5), and accordingly its p.d.f., is an even function of $\dot{\gamma}'_{ij}$, the second, and in consequence its p.d.f., an odd function of $\dot{\gamma}'_{ij}$.^{*} The mean value of the latter is therefore zero *ie.*

$$\overline{\mu \dot{\gamma}_{ij}} = \overline{f(\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij})} \overline{\dot{\gamma}_{ij}} \quad (3.7.6)$$

Likewise the second term in (3.7.2) becomes

$$\begin{aligned}\overline{\mu' \dot{\gamma}_{ij}} &= \overline{(\hat{\mu} - \overline{\mu}) \dot{\gamma}'_{ij}} \\ &= \overline{f(\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}) \dot{\gamma}'_{ij}} + 2\overline{\dot{\gamma}_{ij}} : \overline{f'(\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}) \dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}} \\ &= 2\overline{\dot{\gamma}_{ij}} : \overline{f'(\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}) \dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}} + \dots\end{aligned}\quad (3.7.7)$$

^{*}where a non-skewed distribution of $\dot{\gamma}_{ij}$ has been assumed

Consequently the ratio of the second to the first term in (3.7.2) is

$$\frac{\overline{\mu' \dot{\gamma}'_{ij}}}{\overline{\mu \dot{\gamma}_{ij}}} = \frac{2f'(\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}) \dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}}{f(\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij})} \quad (3.7.8)$$

For shear-thinning fluids $f'(\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}) < 0$ for all $\dot{\gamma}_{ij}$, and thus $\overline{\mu' \dot{\gamma}'_{ij}}$ and $\overline{\mu \dot{\gamma}_{ij}}$ are of opposite sign. Taking the 'power law' (2.3.1) for f , viz.

$$f = K(\frac{1}{2})^{(n-1)/2} (\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij})^{(n-1)/2} \quad (3.7.9)$$

gives

$$f' = K(\frac{1}{2})^{(n-1)/2} (\frac{n-1}{2}) (\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij})^{(n-3)/2} \quad (3.7.10)$$

(3.7.8) then has the value $n - 1$, independent of the range of values which $\dot{\gamma}'_{ij}$ can assume at a given point, provided that these are in the range for which the 'power law' is applicable. If a significant proportion of the values of $\dot{\gamma}'_{ij}$ are above the limiting value of 'power law' applicability *ie.* in the 2nd Newtonian range (*cf.* figure 2.2), (3.7.8) will depend on the range of values of $\dot{\gamma}'_{ij}$ obtaining, and will in general be *smaller* in magnitude than $n - 1$. Thus $n - 1$ is the *maximum* value of $\overline{\mu' \dot{\gamma}'_{ij}} / \overline{\mu \dot{\gamma}_{ij}}$ *ie.*

$$-1 < \frac{\overline{\mu' \dot{\gamma}'_{ij}}}{\overline{\mu \dot{\gamma}_{ij}}} < 0 \quad (3.7.11)$$

In other words the correlation $\overline{\mu' \dot{\gamma}'_{ij}}$ reduces the magnitude of $\overline{\tau_{ij}}$, for a given $\overline{\mu}$ and $\overline{\dot{\gamma}_{ij}}$, by a factor not greater than the 'power law' index n *ie.* (3.7.2) becomes

$$\begin{aligned} \overline{\tau_{ij}} &= \overline{\mu \dot{\gamma}_{ij}} \left(1 + \frac{\overline{\mu' \dot{\gamma}'_{ij}}}{\overline{\mu \dot{\gamma}_{ij}}} \right) \\ &= n \overline{\mu \dot{\gamma}_{ij}} \end{aligned} \quad (3.7.12)$$

Turning to the case where the material response is such that μ cannot follow $\overline{\dot{\gamma}_{ij}}$, the second term $\overline{\mu' \dot{\gamma}'_{ij}}$ in (3.7.2) is zero, and the first term $\overline{\mu \dot{\gamma}_{ij}}$ is of the form of (3.7.6), though probably with a somewhat different absolute value, related to that in the case of faithful material response by a factor $C_{\text{slow resp.}}$, *viz.*

$$\overline{\mu \dot{\gamma}_{ij}} = C_{\text{slow resp.}} f(\overline{\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}}) \quad \overline{\dot{\gamma}_{ij}} \quad (3.7.13)$$

Thus the influence of material response on the effective value of μ is

$$\frac{\mu_{\text{slow resp.}}}{\mu_{\text{fast resp.}}} = \frac{C_{\text{slow resp.}} f(\overline{\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}})}{n f(\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij})} \quad (3.7.14)$$

The exact value of the ratio $\overline{f(\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij})} / \overline{f(\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij})}$ can be obtained only from the p.d.f. for $\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}$ but its value will increase (from unity for $n = 1$) with decreasing n , counteracting the effect of shear-thinning on the value of μ . Given that response time is not a measurable quantity, it is not obvious how $C_{\text{slow resp.}}$ might be estimated; it seems reasonable, however, that it would be of order unity.

Since the correlation $\overline{\mu' \dot{\gamma}'_{ij}}$ is at most $n - 1$ times $\overline{\mu \dot{\gamma}_{ij}}$, since further n is almost invariably in the range 0.5 – 1.0, and since failure of the fluid to respond to variations in strain rate would reduce its relative magnitude yet further, it will not be modelled here; rather the viscous stress $\overline{\tau}_{ij}$ is taken as

$$\overline{\tau}_{ij} = \overline{\mu \dot{\gamma}_{ij}} \quad (3.7.15)$$

3.7.2 The relevant strain rate

The use of any of the constitutive relationships in $\dot{\gamma}_{ij}$ presented in section 2.3 requires determination of the dominant strain rate from the range of strain rates obtaining in turbulent flow, from that characteristic of the bulk flow, $\dot{\gamma}_B$, to that characteristic of the Kolmogorov eddies, $\dot{\gamma}_K$.

The characteristic velocity of a turbulent eddy of length scale l is given by

$$u_l \propto (\overline{\epsilon} l)^{1/3} \quad (3.7.16)$$

and the related strain rate by

$$\dot{\gamma}_l \propto \frac{u_l}{l} \propto \left(\frac{\overline{\epsilon}}{l^2} \right)^{1/3} \quad (3.7.17)$$

ϵ may be considered independent of l (cf. discussion in section 3.5) and (3.7.17) then indicates that the maximum strain rate is that associated with the Kolmogorov eddies.

The characteristic length scale of the Kolmogorov eddies, η , is given by

$$\eta = \left(\frac{\mu^3}{\rho^3 \overline{\epsilon}} \right)^{1/4} \quad (3.7.18)$$

and the characteristic velocity by

$$u_K = \left(\frac{\mu_K \overline{\epsilon}}{\rho} \right)^{1/4} \quad (3.7.19)$$

from which

$$\dot{\gamma}_K = \left(\frac{\bar{\epsilon}\rho}{\mu_K} \right)^{1/2} \quad (3.7.20)$$

In the above, μ_K is the molecular viscosity obtaining in the Kolmogorov eddies, the molecular viscosity of interest (*cf.* section 3.5). The characteristic strain rate associated with the bulk flow is given by

$$\dot{\gamma}_B \propto \frac{U}{L} \quad (3.7.21)$$

where the velocity U and length scale L are characteristic of the large-scale motions in the flow. The relative magnitudes of the characteristic bulk flow and Kolmogorov eddy strain rates are then given by

$$\frac{\dot{\gamma}_K}{\dot{\gamma}_B} = \left(\frac{\bar{\epsilon}\rho}{\mu_K} \right)^{1/2} \left(\frac{L}{U} \right) \quad (3.7.22)$$

and since

$$\bar{\epsilon} = C \frac{U^3}{L} \quad (3.7.23)$$

where the spatially-varying constant of proportionality C typically ranges in value from 10^{-2} to 1, (3.7.21) may be written as

$$\frac{\dot{\gamma}_K}{\dot{\gamma}_B} = \left(C \frac{\rho U L}{\mu_K} \right)^{1/2} = (C Re)^{1/2} \quad (3.7.24)$$

Since Re is of the order of 10^4 or greater for fully turbulent flows, (3.7.24) indicates that $\dot{\gamma}_K$ is at least one, and typically two or more, orders of magnitude greater than $\dot{\gamma}_B$.

3.7.3 The p.d.f. approach

The instantaneous rate of viscous dissipation of turbulence kinetic energy is defined by the non-averaged form of (3.4.2) as

$$\hat{\epsilon} = \frac{\hat{\mu}}{\rho} \left(\frac{1}{2} \dot{\gamma}'_{ij} : \dot{\gamma}'_{ij} \right) \quad (3.7.25)$$

Now, selecting the ‘power law’ (2.3.1) on the basis of its simplicity and likely validity at Kolmogorov eddy strain rates, and decomposing $I\hat{I}_{\dot{\gamma}}$ into $\overline{I\hat{I}_{\dot{\gamma}}} + I\hat{I}'_{\dot{\gamma}}$, $\hat{\mu}$ is given by

$$\hat{\mu} = K \left[\frac{1}{2} (\bar{\dot{\gamma}}_{ij} : \bar{\dot{\gamma}}_{ij} + \dot{\gamma}'_{ij} : \dot{\gamma}'_{ij} + 2\bar{\dot{\gamma}}_{ij} : \dot{\gamma}'_{ij}) \right]^{(n-1)/2} \quad (3.7.26)$$

Since in general $\overline{\dot{\gamma}_{ij}} \ll \dot{\gamma}'_{ij}$, the instantaneous molecular viscosity is expressed as

$$\hat{\mu} = K[\frac{1}{2}\dot{\gamma}'_{ij} : \dot{\gamma}'_{ij}]^{(n-1)/2} \quad (3.7.27)$$

Hence the $\hat{\mu} - \hat{\epsilon}$ relationship may be written as

$$\hat{\mu} = K^{2/(n+1)}(\rho\hat{\epsilon})^{(n-1)/(n+1)} = A\hat{\epsilon}^m \quad (3.7.28)$$

where

$$A = \rho^m K^{2/(n+1)} \quad (3.7.29)$$

and

$$m = \left(\frac{n-1}{n+1}\right) \quad (3.7.30)$$

The time-average of $\hat{\mu}$ is then defined as

$$\bar{\mu} = A \int_0^\infty \hat{\epsilon}^m P(\hat{\epsilon}) d\hat{\epsilon} \quad (3.7.31)$$

where $P(\hat{\epsilon})$ is the p.d.f. of the instantaneous rate of viscous dissipation $\hat{\epsilon}$.

Using the concept of progressive subdivision of a domain of interest, and employing the central limit theorem, Gurvich and Yaglom (1967) examined the ratio of dissipation rates in a given volume and the immediately larger volume in which it is located. They were thus able to lend weight to the Kolmogorov (1962) hypothesis that a non-negative quantity associated with the microscales of turbulence has a log-normal distribution at high Reynolds numbers, and to offer the following relationship for the variance of the distribution:

$$\sigma^2 = A_1 + A_2 \ln\left(\frac{L}{\eta}\right) \quad (3.7.32)$$

where the constant A_1 is a function of the macrostructure of the flow and A_2 is a universal constant.

Monin and Yaglom (1975) have reviewed the arguments for the high-Reynolds-number log-normal distribution, and instance the experimental findings of Stewart *et al* (1970) and Kuo and Corrsin (1971) in its support. In the absence of reported measurements for flows of shear-thinning fluids it is assumed here that $P(\hat{\epsilon})$ for such flows is log-normal also *ie*.

$$P(\hat{\epsilon}) = \frac{1}{\hat{\epsilon}\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{\ln\hat{\epsilon}-M}{\sigma}\right)^2} \quad (3.7.33)$$

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where M is the mean and σ the standard variation of the distribution. Using (3.7.33) the integrated form of (3.7.31) reads

$$\bar{\mu} = Ae^{(Mm+m^2\sigma^2/2)} \quad (3.7.34)$$

$\bar{\epsilon}$ is given by (3.7.33) as

$$\bar{\epsilon} = e^{(M+\sigma^2/2)} \quad (3.7.35)$$

Thus from (3.7.34) and (3.7.35) $\bar{\mu}$ may be written in terms of $\bar{\epsilon}$:

$$\bar{\mu} = A\bar{\epsilon}^m e^{m(m-1)\sigma^2/2} \quad (3.7.36)$$

With A and m functions of fluid properties only, given by (3.7.29) and (3.7.30), and $\bar{\epsilon}$ determined from its own transport equation as described in section 3.8.2, σ^2 is the quantity remaining to be determined.

Based on a range of data Monin and Yaglom (1975) recommend a value of $\sim 0.4 - 0.5$ for the quantity A_2 in (3.7.32); this is adopted here for shear-thinning fluids also. In the absence of guidance as to an appropriate value for A_1 in the same expression it must be taken equal to zero. Thus the following approximation to (3.7.32) is obtained:

$$\sigma^2 \approx 0.45 \ln\left(\frac{L}{\eta}\right) \quad (3.7.37)$$

L is defined as

$$L = \frac{C_\mu^{3/4} k^{3/2}}{\epsilon} \quad (3.7.38)$$

where the quantity C_μ will be formally introduced in section 3.8, and η is given by (3.7.18).

3.8 The $k - \epsilon$ model of turbulence

The $k - \epsilon$ model employs the Kolmogorov relationship (3.6.3) for the determination of μ_t , with ϵ as the length scale parameter. From dimensional considerations

$$\bar{\epsilon} = \frac{k^{3/2}}{l} \quad (3.8.1)$$

and hence

$$\mu_t = \frac{C_\mu \rho k^2}{\bar{\epsilon}} \quad (3.8.2)$$

where C_μ is an empirical coefficient, the value of which will be discussed in section 3.8.4.

Here k and $\bar{\epsilon}$ are determined from differential transport equations, the derivations of which are outlined in section 3.8.1 and 3.8.2, respectively. Consideration of μ as a field variable results in extra terms in the transport equation for $\bar{\epsilon}$; the relative significance of these is assessed in section 3.8.3. Modelling of these extra terms is presented in section 3.8.4. Finally, the determination of the values of the empirical coefficients used in the model is reviewed in section (3.8.5), in the light of its extension to flows of shear-thinning fluids.

3.8.1 The k transport equation

k is defined by (3.6.4) and its transport equation may accordingly be obtained by multiplying the equation of motion for u'_i by u'_i , summing for all three normal stress components and time-averaging, *ie.* by contracting the indices in (3.4.1), *viz.*

$$\rho \frac{\partial}{\partial x_j} (\bar{u}_j k) = - \frac{\partial}{\partial x_j} (\overline{\rho u'_j k'} + \overline{u'_j p'}) - \overline{\rho u'_i u'_j} \frac{\partial \bar{u}_i}{\partial x_j} - \mu \left(\frac{\partial u'_i}{\partial x_j} \frac{\partial u'_i}{\partial x_j} \right) \quad (3.8.3)$$

Equation (3.8.3) states that the net transport of turbulence energy into the domain of interest by convection and diffusion is equal to turbulence energy generation by the working of Reynolds stresses against mean gradients and energy dissipation by viscous mechanisms, where diffusive transport is caused by gradients in triple velocity correlations and in $\overline{u'_j p'}$. Here k' stands for $u'_i u'_i / 2$.

Equation (3.8.3) is rendered soluble by replacing fluctuating quantity correlations by approximate modelling.

The practice in modelling the diffusion term has been to treat the fluctuating spatial pressure gradients as negligible and to assume the fluctuating spatial velocity gradient term proportional to the mean spatial kinetic energy gradient, in a like manner to momentum diffusion, thus:

$$-\overline{\rho u_j k'} = \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_j} \quad (3.8.4)$$

where σ_k is the effective turbulent Prandtl number, with an expected value of order unity (Launder, 1973a).

No new assumptions or approximations are required in replacing the Reynolds stresses in the generation term by the product of turbulent viscosity and mean strain rate*, thus:

$$-\overline{\rho u'_i u'_j} = \mu_t \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \quad (3.8.5)$$

Evaluation of the dissipation of energy term is deferred by writing it as

$$\mu \left(\frac{\partial u'_i}{\partial x_j} \frac{\partial u'_i}{\partial x_j} \right) = \rho \bar{\epsilon} \quad (3.8.6)$$

The modelled form of the transport equation for k is thus

$$\rho \frac{\partial}{\partial x_j} (\bar{u}_j k) = \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_j} \right) + \mu_t \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \frac{\partial \bar{u}_i}{\partial x_j} - \rho \bar{\epsilon} \quad (3.8.7)$$

3.8.2 The ϵ transport equation

The time-averaged exact form of the transport equation for $\bar{\epsilon}$, with μ a field variable, is given by (details of derivation in appendix F)

$$\begin{aligned} \underbrace{\frac{\partial(\rho \bar{u}_j \bar{\epsilon})}{\partial x_j}}_A = & \underbrace{-\frac{\partial}{\partial x_j} \left(-\frac{\partial \overline{\mu \epsilon'}}{\partial x_j} + \overline{u'_j \epsilon'} + 2\nu \frac{\partial u'_i}{\partial x_l} \frac{\partial p'}{\partial x_l} \right)}_B - \underbrace{2\mu \frac{\partial u'_i}{\partial x_l} \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_j}{\partial x_l}}_C - \\ & \underbrace{2 \left(\frac{\partial}{\partial x_j} \left(\mu \frac{\partial u'_i}{\partial x_l} \right) \right)^2}_D - \underbrace{2\mu u'_j \frac{\partial u'_i}{\partial x_l} \frac{\partial^2 \bar{u}_i}{\partial x_l \partial x_j}}_E + \underbrace{\bar{u}_j \frac{\partial u'_i}{\partial x_l} \frac{\partial u'_i}{\partial x_l} \frac{\partial \mu}{\partial x_j}}_F + \quad (3.8.8) \\ & \underbrace{u'_j \frac{\partial u'_i}{\partial x_l} \frac{\partial u'_i}{\partial x_l} \frac{\partial \mu}{\partial x_j}}_G + \underbrace{2\mu \frac{\partial u'_i}{\partial x_l} \frac{\partial^2 u'_i u'_j}{\partial x_l \partial x_j}}_H + \underbrace{2 \frac{\partial p'}{\partial x_l} \frac{\partial u'_i}{\partial x_l} \frac{\partial \mu}{\partial x_j}}_I \end{aligned}$$

Equation (3.8.8) equates the convective transport of $\bar{\epsilon}$ to diffusion-like terms B, tending to smooth spatial variations in $\bar{\epsilon}$; a vortex-stretching term C, a mechanism augmentative of turbulence energy and hence negative here, a viscous sink D and mean velocity gradient – dissipation component interactions E which also augment turbulence energy. Terms F – I are the terms additional to the standard form of (3.8.8) for Newtonian flows, resulting from consideration of μ as a field variable.

* It should be noted that the isotropic component in δ_{ij} vanishes by continuity

3.8.3 Order-of-magnitude analysis of the ϵ equation

In order to assess the significance of the extra terms in (3.8.8) arising from consideration of μ as a field variable, an order-of-magnitude analysis of (3.8.8) is presented here.

The approach is that described by Launder (1984a): $k^{1/2}$ is taken as representative of fluctuating velocities not appearing under derivative operators, while $\partial u'_i/\partial x_j$ is taken as proportional to the strain rate characteristic of the Kolmogorov eddies, (3.7.20). For products of the form $u'_k \partial u'_i/\partial x_j$, the order of the resultant averaged product is reduced by a decorrelation factor $Re_t^{1/2}$ where

$$Re_t = \frac{\rho k^{1/2} L}{\mu} \quad (3.8.9)$$

in order that its magnitude be the same as that of $\partial k/\partial x_j$, to which it is formally identical.* The standard terms in (3.8.8) then scale, on a per unit mass basis, as follows:

$$A \quad \frac{\partial}{\partial x_j} (\bar{u}_j \bar{\epsilon}) \propto \frac{U \bar{\epsilon}}{L}$$

$$B \quad \frac{\partial}{\partial x_j} \left\{ -\frac{\partial}{\partial x_j} \overline{\nu \epsilon'} + \frac{\overline{u'_j \epsilon'}}{\rho} + 2 \frac{\overline{\nu \partial u'_i}{\partial x_l} \frac{\partial p'}{\partial x_l}}{\rho} \right\} \propto \frac{k^{1/2} \bar{\epsilon}}{L} Re_t^{-1/2}$$

$$C \quad \overline{2\nu \frac{\partial u'_i}{\partial x_l} \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_j}{\partial x_l}} \propto \frac{k^{1/2} \bar{\epsilon}}{L} Re_t^{1/2}$$

$$D \quad \overline{2 \left(\frac{\partial}{\partial x_l} \left(\nu \frac{\partial u'_i}{\partial x_j} \right) \right)^2} \propto \frac{k^{1/2} \bar{\epsilon}}{L} Re_t^{1/2}$$

$$E \quad \overline{2u'_j \nu \frac{\partial u'_i}{\partial x_l} \frac{\partial^2 \bar{u}_i}{\partial x_l \partial x_j}} \propto \frac{U \bar{\epsilon}}{L} Re_t^{-1}$$

Estimation of the magnitudes of terms F - I is performed along the lines of the above: scaling of the gradient $\partial \nu/\partial x_j$ is now required. An initial assumption that the Kolmogorov scales are the relevant quantity implies, from (3.7.18), that $\partial \nu/\partial x_j$ scales as $(\nu \epsilon)^{1/4}$. Thus term F would scale as

$$F \quad \overline{\bar{u} \frac{\partial u'_i}{\partial x_l} \frac{\partial u'_i}{\partial x_l} \frac{\partial \nu}{\partial x_l}} \propto \frac{U \epsilon}{L} Re^{3/4}$$

*when $k=i$

This indicates that the order of magnitude of term F exceeds those of all other terms. Since F represents interaction of the high frequencies of small-scale motion with convective transport of a small quantity, ν , it is unlikely that the above estimate of the viscosity gradient is correct. Thus it is assumed here that $\partial\nu/\partial x_j$ scales with ν/L . Hence

$$\text{F} \quad \overline{u_j \frac{\partial u'_i}{\partial x_l} \frac{\partial u'_i}{\partial x_l} \frac{\partial \nu}{\partial x_l}} \propto \frac{U\bar{\epsilon}}{L}$$

$$\text{G} \quad \overline{u'_j \frac{\partial u'_i}{\partial x_l} \frac{\partial u'_i}{\partial x_l} \frac{\partial \nu}{\partial x_j}} \propto \frac{k^{1/2}\bar{\epsilon}}{L} Re_t^{1/4}$$

$$\text{H} \quad \frac{2\nu}{\partial x_l} \frac{\partial u'_i}{\partial x_l} \frac{\partial^2 \overline{u'_i u'_j}}{\partial x_l \partial x_j} \propto \frac{k^{1/2}\bar{\epsilon}}{L} Re_t^{-1/2}$$

Implicit in the estimate for the diffusion-like term B is the assumption that the term in the fluctuating gradient $\partial p'/\partial x_i$ is of the same magnitude as the term in the fluctuating velocity derivative correlation. Based on this assumption the order of magnitude of term I is given by

$$\text{I} \quad 2 \frac{\partial p'}{\partial x_l} \frac{\partial u'_i}{\partial x_l} \frac{\partial \nu}{\partial x_l} \propto \rho \left(\frac{k}{L} \right)^2 Re_t^{-1/2}$$

The order of magnitude of the various terms may then be listed relative to that of the convective term A:

A	B	C	D	E	F	G	H	I
1	$\frac{k^{1/2}}{U} \frac{1}{Re_t^{1/2}}$	$\frac{k^{1/2}}{U} Re_t^{1/2}$	$\frac{k^{1/2}}{U} Re_t^{1/2}$	$\frac{1}{Re_t}$	1	$\frac{k^{1/2}}{U} \frac{1}{Re_t^{1/4}}$	$\frac{k^{1/2}}{U} \frac{1}{Re_t^{1/2}}$	$\frac{\rho k^{1/2}}{U} \frac{1}{Re_t^{1/2}}$

Thus of the 4 additional terms F - I arising from consideration of μ as a field variable, only F and G would be expected to be non-negligible, relative to the standard terms. On the basis of this analysis only terms F and G are retained in the modelled form of the transport equation for $\bar{\epsilon}$.

3.8.4 Modelled form of the ϵ equation

The derivation of the modelled form of the transport equation for $\bar{\epsilon}$ presented in this section formally involves approximations to each of the terms in (3.8.8). It

owes at least as much, however, to dimensional analysis, analogy, and attempts, in assigning values to empirical coefficients, to reproduce the features of certain well-characterised flows; this applies equally to the treatment of the terms in $\partial\mu/\partial x_i$ in (3.8.8).

The diffusive term B, by analogy with the momentum equations, is modelled by the gradient diffusion assumption, viz.:

$$-\frac{\partial}{\partial x_j} \overline{\rho \epsilon' u'_k} = \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_\epsilon} \frac{\partial \bar{\epsilon}}{\partial x_j} \right) \quad (3.8.10)$$

where the fluctuating pressure term is treated as negligible.

The above order-of-magnitude analysis has shown that while the terms C and D become indefinitely large by comparison with the other terms in the ϵ equation as the turbulence Reynolds number increases, the difference between them remains finite (the terms are of opposite sign), and must be comparable in magnitude to the other terms, in order to satisfy the equation. The difference is assumed (Launder, 1973b) proportional to the dissipation rate divided by the decay time of the turbulence, thus:

$$2\mu \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_i}{\partial x_l} \frac{\partial u'_j}{\partial x_l} + 2\mu \left(\frac{\partial^2 u'_i}{\partial x_j \partial x_l} \right)^2 = \frac{C_2 \bar{\epsilon}^2}{k} \quad (3.8.11)$$

The dissipation components multiplying the mean velocity gradients in (3.8.8) are approximated as two terms proportional to $\bar{\epsilon}$, viz.:

$$2\mu \left(\frac{\partial u'_i}{\partial x_l} \frac{\partial u'_j}{\partial x_l} + \frac{\partial u'_l}{\partial x_i} \frac{\partial u'_l}{\partial x_j} \right) = \left(C_1 \rho \frac{\overline{u'_i u'_j}}{k} + \tilde{C}_1 \rho \delta_{ij} \right) \bar{\epsilon} \quad (3.8.12)$$

The latter term disappears by continuity. Term F is modelled as follows:

$$\begin{aligned} \bar{u}_j \frac{\partial u'_i}{\partial x_l} \frac{\partial u'_i}{\partial x_l} \frac{\partial \mu}{\partial x_j} &= \rho \bar{u}_j \frac{\epsilon'}{\mu} \frac{\partial \mu}{\partial x_j} \\ &= \rho \bar{u}_j \frac{\bar{\epsilon}}{\bar{\mu}} \frac{\partial \bar{\mu}}{\partial x_j} \end{aligned} \quad (3.8.13)$$

and term G as:

$$\begin{aligned} \overline{u'_j \frac{\partial u'_i}{\partial x_l} \frac{\partial u'_i}{\partial x_l} \frac{\partial \mu}{\partial x_j}} &= \overline{u'_j \frac{\rho \epsilon'}{\mu} \frac{\partial \mu}{\partial x_j}} \\ &= \rho \frac{\overline{u'_j \epsilon'}}{\mu} \frac{\partial \bar{\mu}}{\partial x_j} \\ &= -\frac{\mu_t}{\sigma_\epsilon \bar{\mu}} \frac{\partial \bar{\epsilon}}{\partial x_j} \frac{\partial \bar{\mu}}{\partial x_j} \end{aligned} \quad (3.8.14)$$

The modelling represented by (3.8.13) and (3.8.14) is such as to preserve the relative order of magnitude of the unmodelled forms of terms F and G.

The modelled form of the transport equation for ϵ is thus

$$\begin{aligned} \rho \frac{\partial}{\partial x_j} (\bar{u}_j \bar{\epsilon}) = & \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_\epsilon} \frac{\partial \bar{\epsilon}}{\partial x_j} \right) + C_1 \frac{\mu_t \bar{\epsilon}}{k} \frac{\partial \bar{u}_i}{\partial x_j}^2 - \\ & C_2 \frac{\rho \bar{\epsilon}^2}{k} + \rho \frac{\bar{\epsilon} \bar{u}_j}{\bar{\mu}} \frac{\partial \bar{\mu}}{\partial x_j} - \frac{\mu_t}{\sigma_\epsilon \bar{\mu}} \frac{\partial \bar{\epsilon}}{\partial x_j} \frac{\partial \bar{\mu}}{\partial x_j} \end{aligned} \quad (3.8.15)$$

3.8.5 The $k - \epsilon$ model empirical coefficients

(3.8.2), (3.8.7) and (3.8.15) constitute the complete model. It is seen that there are five empirical coefficients, $C_1, C_2, C_\mu, \sigma_k$ and σ_ϵ . Determination of the values of these is detailed in appendix G.

Briefly, C_2 is obtained from considerations of decay of grid turbulence. The diffusion and generation terms in both transport equations are negligible in such flows; C_2 may then be expressed in terms of decay of energy level with distance and this latter compared with experimental observations. In the near-wall region of a bounded flow transport of turbulence energy is negligible; equating turbulence energy production and dissipation then permits the expression of C_μ in terms of the ratio of the wall shear stress to turbulence energy.

Convection (but not diffusion) of ϵ may also reasonably be assumed negligible in near-wall flows. Substitution of the 'law of the wall' (2.5.1) in the ϵ equation then produces an algebraic relationship for C_1 in terms of $C_2, C_\mu, \sigma_\epsilon$ and κ .

From the foregoing it will be apparent that C_2 is determined from inertially-dominated flow data and should thus be invariant with fluid rheology. C_1 is dependent on κ alone of the 'law of the wall' parameters, and discussion in the foregoing chapter has reaffirmed that this quantity also is independent of shear-thinning behaviour. Furthermore, in the absence of turbulence distribution data for the flow of inelastic shear-thinning fluids no conclusions can be drawn as to whether alternative values of C_μ are appropriate in such flows. Accordingly, the values of the coefficients recommended by Launder and Spalding (1974), and listed in table 3.1, are retained here.

C_1	C_2	C_μ	σ_k	σ_ϵ
1.44	1.92	0.09	1.0	1.3

Table 3.1 $k - \epsilon$ model empirical coefficient values

3.9 Final form of the equations

The complete set of equations in the form solved is assembled here.

The equations, hitherto developed in Cartesian tensors are now expanded in the x, r, θ cylindrical polar coordinate system appropriate for the axisymmetric geometries of interest in this study. Overbars are omitted as all quantities are to be understood to be time-averaged from hereon. The transport equations then have the common form

$$\begin{aligned} \frac{\partial}{\partial x}(\rho u \phi) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v \phi) = & \frac{\partial}{\partial x} \left[\Gamma_\phi \left(\frac{\partial \phi}{\partial x} \right) \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[r \Gamma_\phi \left(\frac{\partial \phi}{\partial r} \right) \right] + \\ & \frac{1}{r} \frac{\partial}{\partial \theta} \left[\Gamma_\phi \left(\frac{\partial \phi}{\partial \theta} \right) \right] + S_\phi \end{aligned} \quad (3.9.1)$$

ϕ stands for the axial component of velocity u , the radial component v , the scalar product of radial distance and swirl component $r.w$, k and ϵ in turn. Γ_ϕ takes the form $\mu + \mu_t$ for $\phi = u, v$ and $r.w$, and the form μ_t/σ_ϕ for $\phi = k$ and ϵ . The terms S_ϕ take the form

$$S_u = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left((\mu + \mu_t) \frac{\partial u}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r(\mu + \mu_t) \frac{\partial v}{\partial x} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left[(\mu + \mu_t) \frac{\partial w}{\partial x} \right] \quad (3.9.2)$$

$$\begin{aligned} S_v = & -\frac{\partial p}{\partial r} + \frac{\partial}{\partial x} \left((\mu + \mu_t) \frac{\partial u}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r(\mu + \mu_t) \frac{\partial v}{\partial r} \right) + \\ & \frac{1}{r} \frac{\partial}{\partial \theta} \left[(\mu + \mu_t) \frac{\partial w}{\partial r} \right] - \frac{1}{r} \frac{\partial}{\partial \theta} \left[(\mu + \mu_t) \frac{w}{r} \right] - \\ & \frac{2(\mu + \mu_t)}{r^2} \frac{\partial w}{\partial \theta} + \frac{\rho w^2}{r} - \frac{2(\mu + \mu_t)v}{r^2} \end{aligned} \quad (3.9.3)$$

$$\begin{aligned} S_{r.w} = & r \frac{\partial}{\partial x} \left[\frac{(\mu + \mu_t)}{r} \frac{\partial u}{\partial \theta} \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[r(\mu + \mu_t) \frac{\partial v}{\partial \theta} \right] + \\ & \frac{1}{r} \frac{\partial}{\partial \theta} \left[\frac{(\mu + \mu_t)}{r} \frac{\partial(wr)}{\partial \theta} \right] - \frac{2}{r} \frac{\partial}{\partial r} \left((\mu + \mu_t) w r \right) + \\ & 2 \frac{\partial}{\partial \theta} \left(\frac{(\mu + \mu_t)v}{r} \right) \end{aligned} \quad (3.9.4)$$

$$S_k = G - \rho \epsilon \quad (3.9.5)$$

and

$$\begin{aligned} S_\epsilon = & C_1 G \frac{\epsilon}{k} - \frac{C_2 \rho \epsilon^2}{k} + \frac{\epsilon}{\nu} \left(u \frac{\partial \mu}{\partial x} + v \frac{\partial \mu}{\partial r} + \frac{w}{r} \frac{\partial \mu}{\partial \theta} \right) - \\ & \frac{\mu_t}{\mu \sigma_\epsilon} \left(\frac{\partial \epsilon}{\partial x} \frac{\partial \mu}{\partial x} + \frac{\partial \epsilon}{\partial r} \frac{\partial \mu}{\partial r} + \frac{1}{r^2} \frac{\partial \epsilon}{\partial \theta} \frac{\partial \mu}{\partial \theta} \right) \end{aligned} \quad (3.9.6)$$

with

$$G = \mu_t \left\{ 2 \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial r} \right)^2 + \left(\frac{1}{r} \frac{\partial w}{\partial \theta} \right)^2 + \left(\frac{v}{r} \right)^2 + \frac{2v}{r^2} \frac{\partial w}{\partial \theta} \right] + \left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x} \right)^2 + \left(\frac{1}{r} \frac{\partial u}{\partial \theta} + \frac{\partial w}{\partial x} \right)^2 + \left(r \frac{\partial}{\partial r} \frac{w}{r} + \frac{1}{r} \frac{\partial v}{\partial \theta} \right)^2 \right\} \quad (3.9.7)$$

The pipe flows analysed are all assumed axisymmetric, and accordingly all of the terms in circumferential gradients $\partial/\partial\theta$ are zero.

3.10 Boundary conditions

Four types of boundary conditions are associated with duct flow: solid boundaries (the duct wall and any internal obstacles), the duct axis, and the inlet and outlet planes of the duct section of interest. In agitated mixing vessels the specification of boundary conditions in the region of the impeller, and at the liquid surface if a lid is not used, is required in addition to solid boundary (wall, bottom, baffle and lid if used) and axis conditions. Furthermore, if baffles and/or other geometric features are equally spaced such that self-repeating sectors of the vessel may be identified, the solution domain may be restricted to such a sector to limit its size, as illustrated by figure 3.1; cyclic boundary conditions must then be imposed on the delimiting $x - r$ planes.

It is apparent from the discussion in the previous chapter that the treatment of solid boundaries is a central issue in the development of a model for the prediction of turbulent flows of shear-thinning fluids; this is accordingly addressed first, in section 3.10.1. Boundary conditions imposed in the impeller region are a key determinant of predicted flow patterns in mixing vessels and these are addressed next, in section 3.10.2. Description of the remaining boundary conditions follows in section 3.10.3.

3.10.1 Solid boundaries

Within the viscous sublayer and buffer zone present in turbulent flow adjacent to solid boundaries, the effective transport coefficients change by more than an order of magnitude as the local Reynolds number of turbulence $Re_t = k^2/\nu\epsilon$ decreases *ie.* as vigorous turbulent mixing is replaced by viscous mechanisms (these becoming

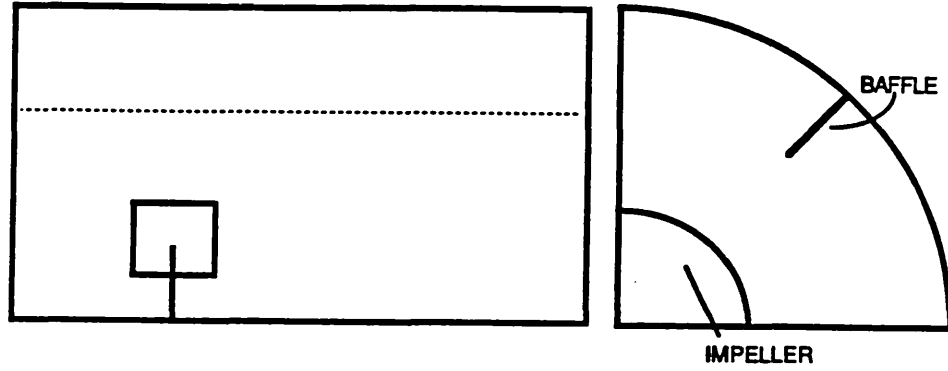


Figure 3.1 Solution domain, mixing vessel

important when Re_t goes below ≈ 150 (Launder, 1988)). Many turbulence models applied in this low-Reynolds-number region have been developed from some high-Reynolds-number closure by introducing various viscosity-dependent terms and/or making the coefficients of existing terms functions of a turbulence Reynolds number. An alternative, and more economical, approach (in terms of avoidance of near-wall grid refinement) involves the prescription of mean shear stress in terms of a normal distance Reynolds number, using the experimentally observed ‘law of the wall’ (2.5.1).

Low-Reynolds-number models

Jones and Launder (1972) were the first to extend the $k - \epsilon$ model to the low-Reynolds-number region allowing for calculation right through the viscous sublayer to the solid wall. This incorporates van Driest’s (1956) extension of Prandtl’s mixing length hypothesis (3.6.2) for applicability in the near-wall region

$$\kappa_{\text{mod}} = \kappa[1 - e^{-y/A_1}] \quad (3.10.1)$$

in which A_1 is an empirical constant. (3.8.2) is rewritten as

$$\mu_t = \frac{C_\mu f_\mu \rho k^2}{\epsilon} \quad (3.10.2)$$

where

$$f_\mu = e^{\frac{-A_2}{(1+Re_t/50)}} \quad (3.10.3)$$

A further sink term is added to the transport equation for k such that (3.9.5) reads

$$S_k = G - \rho\epsilon - 2\frac{\mu}{\rho}\left(\frac{\partial\sqrt{k}}{\partial y}\right)^2 \quad (3.10.4)$$

The term in ϵ , interpreted as the isotropic part of the energy dissipation, can then go to zero at the wall while the extra term represents non-isotropic dissipation in the viscous sublayer. Additional source terms are introduced into the dissipation rate equation such that the Newtonian form of (3.9.6) now reads

$$S_\epsilon = C_1 G \frac{\epsilon}{k} - C_2 f_2 \rho \frac{\epsilon^2}{k} + 2\frac{\mu\mu_t}{\rho^2}\left(\frac{\partial^2 u}{\partial y^2}\right)^2 \quad (3.10.5)$$

in which

$$f_2 = 1 - 0.3e^{-(Re_t)^2} \quad (3.10.6)$$

The final term in (3.10.5) was chosen simply to ensure otherwise-unobtainable agreement of near-wall turbulence kinetic energy levels with experimental values, and f_2 such that model predictions of grid turbulence accorded with experiment for both high and low turbulence intensities. A number of alternative proposals for the eddy viscosity function f_μ and for the source and sink terms in the k and ϵ transport equations have appeared in the literature – *eg.* those of Hassid and Poreh (1978), Lam and Bremhorst (1981) and Nagano and Hishida (1987) – with a view to improving prediction accuracy in the flow of Newtonian fluids. The low-Reynolds-number approach permits the prediction of mean and turbulence quantities right up to the wall, and excellent agreement with experimental data in a range of two-dimensional flows appears to be achievable with the more recent refinements (Nagano and Hishida, 1987). Considerable mesh refinement is however required, typically requiring five to ten grid points across the viscosity-affected zone, and this renders the approach impractical, in terms of computing resources, for three-dimensional flow analysis. Furthermore the superiority of low-Reynolds-number approaches over the ‘wall function’ approach in predicting flow separation and reattachment remains unproved.

It is also noted, however, that modifications to the Jones and Launder model to enable prediction for flows of drag-reducing fluids have been suggested by Durst and Rastogi (1977) and Hassid and Poreh (1978). In view firstly of the fact that some shear-thinning solutions also exhibit drag-reduction, and secondly of the widespread nonspecific use of the term non-Newtonian, without reference to the

particular mechanisms involved, brief consideration of these proposals is appropriate here.

Durst and Rastogi (1977) suggested that the higher damping of turbulence energy in the near-wall region in the flow of drag-reducing fluids, for which (very limited) experimental evidence is available, be modelled by increasing the value of the damping function f_μ *ie.* by increasing the value of the constant A_2 in (3.10.3) – this produces an upward shift in the log law, with velocity profiles approaching those associated with the maximum drag reduction asymptote. They wrote the value of the upward shift ΔB in the ‘log law’ profile as a function of the ratio of friction velocity to the friction velocity at onset of drag reduction, and of polymer concentration, molecular weight and number of backbone links in the molecular chain. The value of A_2 was then chosen according to the value of ΔB it produces. Good agreement with measured pressure drop in the flow of a drag-reducing but constant viscosity polymer solution, at the same Reynolds number, was obtained, and agreement with velocity distribution data in the flow of such a fluid was also satisfactory. Predictions of turbulence energy k showed augmentation of the order of 15% in the region $y^+ \approx 30$ but comparison with data was not made. Working independently Hassid and Poreh (1978) concluded that changes to the values of the empirical coefficients in the Jones and Launder model alone were insufficient to reproduce the turbulence energy distribution in drag-reducing fluid flow, and instead proposed different forms of the damping function f_μ and the additional source terms in (3.10.4) and (3.10.5). No attempt was made to relate values of the empirical coefficients to the fluid properties, rather they were obtained from friction factors measured at the Reynolds numbers of interest. Good agreement was obtained between predicted and measured velocity distributions, moderate agreement between predicted turbulence energy and measured streamwise velocity r.m.s. values.

These models may offer useful guidance in the development of models for flows of shear-thinning fluids in which drag reduction is *also* involved – the limitation of interest in these studies to constant-viscosity fluids is explicit, however, and they are not as such of immediate interest here.

Wall functions

The fundamental assumption of zero fluid slip at a rigid, impermeable boundary implies the disappearance of convective transport associated with motion parallel to the boundary in the limit as the boundary is approached. In a sufficiently thin

near-wall region, therefore, and where the flow remains attached, the distribution of flow field variables is simply a function of normal distance y from the wall, and in many cases such a region spans the complete low-Reynolds-number region.

Solution for flow field variables within the viscous sublayer adjacent to the wall may then be avoided by prescription of their values within the fully turbulent part of the low-Reynolds-number zone. Mean velocity is then prescribed using the 'law of the wall',

$$u^+ = A \ln y^+ + B \quad (2.5.1)$$

which, it has been concluded in the previous chapter, adequately characterises boundary-layer velocity distributions in the flow of shear-thinning fluids also. If the region of interest is within the sublayer, however, prescription is made according to

$$u^+ = y^+ \quad (2.5.2)$$

With the additional assumptions of local equilibrium, Couette flow in the laminar sublayer, and equality of Reynolds stresses with the viscous stresses in the sublayer, the turbulence energy may be prescribed as (see appendix G)

$$k = \frac{\tau_w}{\rho} \frac{1}{C_\mu^{1/2}} \quad (3.10.7)$$

and the dissipation rate as (see appendix G)

$$\epsilon = \frac{C_\mu^{1/2} k u_*}{\kappa y} \quad (3.10.8)$$

(2.5.1), (3.10.7) and (3.10.8) comprise the 'wall functions'. In the thicker sublayer associated with the flow of a shear-thinning fluid, the Couette flow assumption may be less valid than in the sublayer associated with Newtonian fluid flow. Bearing this uncertainty in mind, in addition to that associated with the use of a Reynolds number, y^+ , in the flow of a shear-thinning fluid, 'wall functions' are used in this study as boundary conditions on solid walls. Shear-thinning behaviour is specifically accounted for through the definition of the local Reynolds number y^+ appearing in (2.5.1)

$$y^+ = y \left(\frac{\rho u_*^{2-n}}{K} \right)^{1/n} \quad (2.5.8)$$

and through the value of B used in (2.5.1).

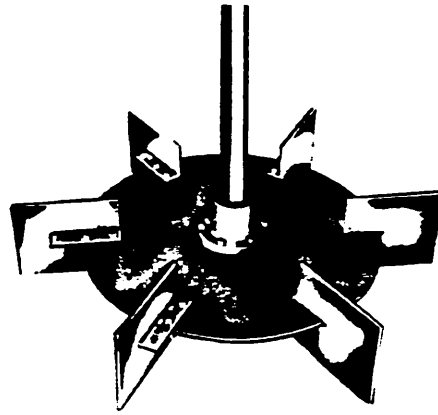


Figure 3.2 Rushton turbine

3.10.2 Mixing vessel impeller

The turbine impeller is one of the most widely used in industrial processes. Furthermore the most comprehensive mixing vessel flow data available for comparison with prediction is that of Yianneskis (1982, 1984) for a Newtonian fluid and of Hockey (1990) for Newtonian and non-Newtonian fluids, and these measurements have for the most part been made in flows driven by a six-blade Rushton turbine, illustrated in figure 3.2; accordingly this is the impeller type considered in this study.

The periodicity of the flow in the impeller region, imposed by the rotating blades, in principle requires a time dependent treatment of the flow. Alternatively, the unsteadiness can be absorbed in an approximate fashion into the characterisation of the flow in the immediate vicinity of the blades, and a time-dependent solution avoided altogether. In adopting this approach Issa and Gosman (1981) represented the impeller region as a porous cylinder, and prescribed uniform profiles for all velocity components and turbulence quantities on the cylinder 'surfaces' *ie.* the impeller region was excluded from the solution domain. Bolour-Froushan (1986) maintained this treatment but the experimental data of Yianneskis (1982) for the cylinder 'surfaces' was fitted by algebraic expressions and these, with some adjustments in order to satisfy continuity, were used to impose profiles as a function of axial and radial location on the vertical and horizontal 'surfaces', respectively.

The treatment employed here, however, is that employed by Politis (1989), in which the impeller is represented as an infinitely thin (for reasons of computational cost rather than inherent necessity), impermeable spinning disc attached to a hollow shell, corresponding to the volume swept by the rotating blades. Values

of circumferential velocity, turbulence energy and dissipation rate are imposed in the swept volume, and axial and radial velocity are solved for as elsewhere in the solution domain.

The swirl velocity is imposed as a proportion of impeller rotational speed *ie.* in terms of a slip factor f_{slip} :

$$w = f_{\text{slip}} \Omega R \quad (3.10.9)$$

where f_{slip} is defined as the ratio of measured circumferential velocity in the vicinity of the blade tip to the impeller tip velocity, Ω is the impeller frequency and R is the distance from the axis. Yianneskis' (1982) measurements provide the (time-averaged) mean circumferential velocity profiles in the vicinity of the impeller blade tip (2.1mm away), for the flow of water at an impeller speed of 300rpm ($Re_{\text{mv}} = 48,000$); Hockey (1990) provides measurements of the same quantity 3mm from the blade tip for the flow of a (shear-thinning) solution of CMC at an impeller speed of 600rpm ($Re_{\text{mv,st}} = 9,600$). Slip factors calculated from these data are given in table 3.2. The discrepancy between the data sets may be attributable either to the difference in distance from the blade tip at which they were obtained, and/or to the difference in impeller speeds. It cannot plausibly be attributed to differences in fluid rheology as this is the region of greatest turbulence intensity in the flow, and therefore that in which rheological effects would be least expected to manifest themselves.

Politis (1989) found it necessary to use somewhat higher slip factors than those derived from the measurements, and a symmetric distribution with respect to the impeller disc, to satisfactorily reproduce Yianneskis' measured volumetric throughput of the impeller and the ratio of flow rates above and below the disc. Numerical testing of a number of sets of slip factors in this study established that the same values of f_{slip} are required in order to obtain similar agreement for the flows measured by Hockey at an impeller speed of 600rpm. This is a positive finding insofar as it indicates that the prescription has some generality, important in establishing the present methodology as a design tool. The optimum values of f_{slip} established by Politis are used here in all cases for which predictions are later presented, they are listed in table 3.2.

In a similar manner the turbulence energy k is linked to the solid body rotational velocity within the swept volume, thus:

$$k_{\text{sw.vol.}} = C_k (\Omega R)^2 \quad (3.10.10)$$

a	b	c	d
-10		0.167	0.37
-8	0.287	0.299	0.50
-6		0.458	0.64
-4	0.439	0.617	0.74
-2		0.713	0.85
2		0.707	0.85
4	0.705	0.610	0.74
6		0.468	0.64
8	0.485	0.310	0.50
10		0.171	0.37

Table 3.2 Slip factors - experimental and adopted for present methodology
(a) Distance from impeller disc (mm) (b) Data of Yianneskis (1982), 300rpm
(c) Data of Hockey (1990), 600rpm (d) Adopted for present methodology

where the empirical coefficient C_k is determined by reference to experimental data. Both Yianneskis (1982) and Hockey (1990) provide r.m.s. data for all three velocity components; accordingly the C_k values listed in table 3.3 were obtained from k calculated as $1/2(u'^2 + v'^2 + w'^2)$. The values for the 600rpm case are based on Hockey's data for flow of the (shear-thinning) CMC solution. He does not provide data for all three components for the flow of the glycerine solution, but those r.m.s. values that are available are within 5% of those for the CMC case and the same values of C_k are accordingly employed in the prediction of both flows, to be presented in chapter 6.

Formulation of impeller boundary conditions for the rate of dissipation, ϵ , in the empirical manner adopted for the boundary conditions for w and k , is particularly difficult as ϵ is not directly measurable in any part of the flow. Yianneskis (1982) measured Reynolds stress $\overline{\rho v'w'}$ and mean velocities $\bar{v}$, $\bar{w}$, from which the mean strain $\bar{\dot{\gamma}_{r\theta}}$ in the $r - \theta$ plane can be estimated. Bolour-Froushan (1986) obtained estimates for ϵ from the relationship $\epsilon = C_\mu \rho k^2 / \mu_t$ with μ_t estimated from the ratio $(\overline{\rho v'w'}) / \bar{\dot{\gamma}_{r\theta}}$. In addition to the approximations involved in thus obtaining values for ϵ , however, there are significant uncertainties in the data themselves (see discussion of Yianneskis, who considers that ϵ values obtained in this manner are no better than an order of magnitude guide to the distribution). Politis (1989) therefore employed the earlier approach of Issa and Gosman (1981), based on di-

a	b	c
-10		0.048
-8	0.139	0.074
-6		0.098
-4	0.155	0.100
-2		0.103
2		0.095
4	0.150	0.093
6		0.087
8	0.142	0.066
10		0.042

Table 3.3 Empirical coefficients C_k in (3.10.10)

(a) Distance from impeller disc (mm), (b) 300rpm, (c) 600rpm

mensional arguments and taking the distance from the axis, R , as a characteristic length scale:

$$\epsilon_{\text{sw.vol.}} = C_\epsilon \frac{k^{3/2}}{R} \quad (3.10.11)$$

where C_ϵ is an empirical constant determined through numerical optimisation. This prescription is retained here.

The degree of empiricism embodied in this approach is freely acknowledged; the arguments for the bounding of the transport equation for ϵ being particularly tenuous. To address the problem conclusively requires that its time dependent nature be acknowledged. This is beyond the scope of this study.

3.10.3 Other boundaries

Duct/vessel axis

The duct/vessel axis is assumed to be a symmetry axis, and the following conditions are accordingly imposed:

- zero radial velocity
- zero shear stress
- zero normal fluxes of k and ϵ

Liquid surface

If no lid is used the surface of the liquid in the vessel is assumed to be flat. The

presence of baffles minimises surface troughing – see, for instance, Oldshue (1983) – and Yianneskis' (1982) experiments indicated little such surface distortion. It follows that the following quantities fall to zero at the surface:

- the axial (normal) velocity
- the tangential shear stress
- the axial fluxes of k and ϵ

Cyclic boundaries, mixing vessel

In the case of self-repeating *ie.* geometrically similar sectors of the vessel it is reasonable to assume that flow similarity between the sectors also exists. This implies cyclical repetition of flow behaviour *ie.* identical conditions at $x - r$ planes delimiting a sector. These are not known *a priori* but must be determined as part of the solution. The enforcement of the identical conditions on these boundaries depends on the method of solution and is accordingly described in section 4.7.3.

Inlet plane, duct

The duct cases are specified in terms of flow conditions obtaining at the inlet plane, and the values of all variables are accordingly treated as known here.

Outlet plane, duct

The flow at the outlet of the section of interest is treated as issuing into quiescent surroundings, and a zero axial (streamwise) gradient in all quantities is imposed.

3.11 Closure

In this chapter, the derivation of the time-averaged equations of motion and the Reynolds stress equation have been outlined, and the main mechanisms of turbulence and some of the principal approaches to its modelling briefly discussed. The superiority of the $k - \epsilon$ model to zero-, one- and other two-equation models has been noted, and it has been chosen in preference to algebraic and Reynolds stress models in view of the prohibitive extra cost of the latter in terms of currently available computing resources.

It has been shown that the fluctuating molecular viscosity – fluctuating strain rate correlation, resulting from decomposition and time-averaging of the viscous shear stress where the molecular viscosity is a field variable, is at most of equal magnitude to the mean molecular viscosity – mean strain rate correlation; it is thus disregarded.

The inappropriateness of evaluating molecular viscosity of a shear-thinning fluid from the mean strain rate in turbulent flow has been demonstrated; a method for its evaluation from the dissipation rate, ϵ , has been described.

The ϵ equation in the $k - \epsilon$ model has been rederived with molecular viscosity as a field variable. Four terms additional to those in the standard form of the equation result; two are disregarded as being relatively insignificant on the basis of an order of magnitude analysis and the remaining two are retained and modelled.

The empirical coefficients in the $k - \epsilon$ model are retained unchanged from the standard values and no additional coefficients are introduced.

‘Wall functions’ are employed in the prescription of solid boundary conditions, but with ‘standard’ coefficient values modified to account for shear-thinning fluid behaviour. Other boundary conditions are as established in previous work.

4 Solution procedure

4.1 Introduction

The equations describing the flows of interest have been assembled; their solution will be considered in this chapter. The first of the two tasks involved is the discretisation of the partial differential equations, in which they are replaced by algebraic equations with the values of the dependent variables at a finite number of spatial locations as the unknowns. Associated with this is the interpolation practice, or differencing scheme, to be used in obtaining values of the dependent variables between grid points, required during solution. The second task is the prescription of an algorithm for solving the (strongly) coupled sets of discretised equations, including the prescription of a subsidiary algorithm for the solution of each individual set of equations.

The discretisation concept, and the method used in this study, are introduced in section 4.2. Discretisation of the diffusion and source terms in the equations is outlined in section 4.3. Differencing schemes proposed to date in response to the problems associated with discretisation of the convection terms are reviewed in section 4.4; a description of a new scheme employed in this study follows in section 4.5. The relationship between the sets of spatial locations chosen for the values of each of the dependent variables – the grid layout – is discussed in section 4.6. The handling of boundary conditions is described in section 4.7. The solution algorithm for the coupled equations is described in section 4.8, and summarised in section 4.9, where convergence criteria for the iterative procedure are also presented. Solution algorithms for the individual equation sets are briefly discussed in section 4.10, with somewhat fuller consideration of the conjugate gradient method implemented in this study, and examination of its performance relative to that of several alternatives.

4.2 Finite volume discretisation

Discretisation of the distribution of a variable ϕ is the replacement of the continuous field by a set of discrete values of ϕ at a finite number of locations, or grid points, within the domain of interest. This involves the replacement of the partial differential equations by algebraic equations, one for each grid point. Patankar (1980) describes some of the possible approaches to discretisation; only the finite volume method used in this study will be described here.

The domain of interest is divided into non-overlapping control volumes such that one surrounds each grid point. The partial differential equation (3.9.1) for the transported quantity ϕ is integrated over the control volume, or cell:

$$\int_V \nabla(\rho u \phi) dV - \int_V \nabla(\Gamma \nabla \phi) dV = \int_V S(\phi) dV \quad (4.2.1)$$

which may be expressed as a set of surface integrals over the six cell faces using Gauss' theorem:

$$\int_{A_i} (\rho u \phi)_i dA - \int_{A_i} (\Gamma \nabla \phi)_i dA = \int_V S(\phi) dV \quad (4.2.2)$$

where $(\)_i$ is the component of $(\)$ normal to the face i of area A . (4.2.2) expresses conservation of ϕ for the cell surrounding any given grid point: the amount of ϕ convected (term 1) and diffused (term 2) into/out of the cell is equated to the net accumulation of ϕ in the cell (r.h.s. term). This satisfaction of the conservation of the conservation principle extends to any group of cells and thus to the calculation domain as a whole – this physical realism is followed irrespective of the coarseness of the grid. (4.2.2) also illustrates the transparency of the finite volume discretisation – the individual terms may be interpreted in terms of physical processes to fully the same extent as those in the differential equations.

4.3 Discretisation of the equations

Once the criteria for acceptability of the discretised equations have been established, as described in section 4.3.1, it transpires that discretisation of the diffusion and source terms in (4.2.2) conforming to these criteria is straightforward – this is outlined in sections 4.3.2 and 4.3.3, respectively. Discretisation of the convection terms in (4.2.2) is more problematic and this discussion is deferred to section 4.4.

4.3.1 Criteria for assessment of the discretised equations

Before proceeding to the derivation of discretised forms of (4.2.2) the criteria for their acceptability must be established.

Conservation

The partial differential equations (3.9.1) governing the flow were derived from conservation considerations, and it is evidently necessary that the equations continue

to represent this physical reality once discretised. Thus the flux across the face common to two control volumes must be represented by the same expression in the discretised equations for both.

Boundedness

In purely convective/diffusive flows, *ie.* in the absence of sources or sinks, the range of values in the solution domain is that bounded by the maximum and minimum boundary values, and this must also be a requirement of a numerical solution. If a_m are the algebraic coefficients of the discrete values ϕ_m , representing some combination of convective and diffusive fluxes, the algebraic equation for any node P must have the form

$$a_P \phi_P = \sum a_m \phi_m \quad (4.3.1)$$

It is then sufficient for the fulfillment of the boundedness criterion that

$$a_P = \sum a_m \quad (4.3.2)$$

and

$$a_m \geq 0, \quad \text{all } m \quad (4.3.3)$$

where (4.3.2) states that ϕ_P is some weighted average of the surrounding values ϕ_m , and (4.3.3) expresses the fact that if the value at any node changes, the values at neighbouring nodes must change in the same (positive or negative) direction. Coefficient positivity is purely a convention; a requirement that all be negative is exactly equivalent. Furthermore, it is less clear that (4.3.2) and (4.3.3) are always necessary than that they are sufficient; it will be apparent from the discussion in the following section that certain schemes remain bounded even with negative coefficients.

Accuracy

Accuracy may be assessed in terms of Taylor series analysis, in which the nodal values in the discretised equation are eliminated in favour of derivatives expressed at the location of the dependent variable; by using a unit cell analysis, the comparison of the exact analytical solution with the discretised equation estimate for ϕ ; or by performing full field calculations. The limitations and indeed potentially misleading nature of Taylor series analysis have been sufficiently well documented (Patankar, 1980; Lai, 1982) that mention here will suffice: the leading neglected

term is not always the largest, at least on the finite grids used in practice, while even a formal indication of second or third order accuracy does not necessarily mean that boundedness and transportiveness will be observed. Nevertheless it is used in preference to unit cell analysis in assessing differencing schemes as, unlike the latter, it gives the mathematical form of the first error term and hence an indication of the nature of the discretisation error.

In assessment of accuracy through full field calculations, either the calculation must be repeated on progressively finer grids until successive solutions are sensibly identical *ie.* until grid independence is achieved, or accurate experimental measurements must be used as the basis of comparison. In the latter case uncertainty as to the accuracy of the underlying partial differential equations should not be allowed to cloud the assessment of the proposed discretisation; accordingly laminar flows should be used as test cases. (This separation of modelling and numerical error to the fullest extent possible applies equally to assessment of modelling.)

Stability

The size of the equation sets necessitates iterative solutions; their sparseness makes such algorithms practicable, though the Scarborough criterion of diagonal dominance (Patankar, 1980)

$$\frac{|\sum a_m|}{|a_P|} \quad \begin{cases} \leq 1 & \text{all equations} \\ < 1 & \text{at least one equation} \end{cases} \quad (4.3.4)$$

used to assess the potential for convergence is a sufficient rather than always necessary condition – depending on the particular solution algorithm used. Insofar as (4.3.4) simply reinforces (4.3.2), it is the corollary of the boundedness issue, always associated with it.

Transportiveness

The greater the degree of dominance by convective mechanisms in the flow the greater the degree to which the values of dependent variables should be functions of upstream values. In the limit of absence of diffusive and source terms from the partial differential equations the value at a given location will be convected from upstream; the discretised equations should reflect this (Raithby, 1976a).

Linearity and pseudo-linearity

The ‘levelness’ principle requires that both ϕ and $\phi + c$ be valid solutions to the discretised equation with source term

$$a_P \phi_P = \sum a_m \phi_m + S \quad (4.3.5)$$

for a non-uniquely defined problem (boundary conditions of gradients in ϕ rather than ϕ itself). Lai (1982) has shown the necessary and sufficient condition to be (4.3.2) *ie.* that usually required for boundedness. Ziman (1990) points out the implications for non-linear discretisation schemes *ie.* those in which a_m are functions of ϕ : a_m cannot depend on ϕ at just one point, but rather on differences between values of ϕ at different points. For dimensional consistency a_m must then be functions of groups of the form

$$f(\phi) = \frac{\phi_1 - \phi_2}{\phi_3 - \phi_4} \quad (4.3.6)$$

4.3.2 The diffusion terms

A linear profile in ϕ between the grid point of interest, P , and its neighbours, E and W , is assumed. A stepwise profile assumption *ie.* constant ϕ throughout the control volume, leaves $\partial\phi/\partial x_i$ undefined at control volume faces. A quadratic profile assumption, on any other than an evenly spaced grid, will produce a different spatial gradient in ϕ , and hence flux, for the shared face of any pair of neighbouring cells (Patankar, 1980); such a scheme would not be conservative.

A ‘central difference’ approximation to the diffusion term in (4.2.2) is thus obtained:

$$\int_{A_e} (\Gamma \nabla \phi)_e dA = \Gamma_e \frac{\phi_E - \phi_P}{(\delta x)_e} dA \quad (4.3.7)$$

Implicit in (4.3.7) is the assumption that transverse variations in ϕ may be neglected. Consider the Taylor series expansion of the integrand (4.3.7), represented by ψ , about the midpoint of face e in the first transverse (y) direction, where the distance in the second transverse (z) direction is then taken as unity:

$$\psi(h) = \psi(0) + h \frac{d\psi}{dy} + \frac{1}{2} h^2 \frac{d^2\psi}{dy^2} + \text{HOT} \quad (4.3.8)$$

Neglecting the higher-order terms (HOT) the integration of the diffusion flux yields

$$\int_{y_s}^{y_n} \psi dy = (y_n - y_s) \psi(0) + \frac{1}{6} (y_n - y_s)^3 \frac{d^2\psi}{dy^2} \quad (4.3.9)$$

illustrating that even neglecting transverse variations in ϕ the discretisation error is third order – provided that the mid-point value is used in the flux approximation.

4.3.3 The source terms

When the source term S in (4.2.2) is a function of the dependent variable ϕ , expression of S in the linearised form

$$S = S_{\phi,P}^1 \phi_P + S_{\phi,P}^2 \quad (4.3.10)$$

permits implicit treatment of the first r.h.s. term and hence enhanced convergence in the iterative solution necessary for the coupled equation sets. Implicit in (4.3.10) is the assumption that the nodal value ϕ_P prevails over the cell volume as a whole. Enhancement of diagonal dominance of the coefficient matrix and hence of the stability of iterative solutions to the individual equation sets also results from this implicit treatment, *provided* that $S_{\phi,P}^1$ is negative. Indeed positive $S_{\phi,P}^1$ may drive a_P negative, in violation of the positivity of coefficients requirement (4.3.3). Hence the linearisation (4.3.10) of the source terms (3.9.1) to (3.9.5) is performed in accordance with a requirement that $S_{\phi,P}^1$ be negative, and the discretised equations expressed in the form

$$a_P \phi_P = \sum a_m \phi_m + S_{\phi,P}^2 \quad (4.3.11)$$

where

$$a_P = \sum a_m - S_{\phi,P}^1 \quad (4.3.12)$$

4.4 Review of differencing schemes for the convective terms

4.4.1 Central differencing (CD)

If the variation in the value of the dependent variable ϕ between nodes P and E is assumed linear, figure 4.1, the cell face value ϕ_e is given by

$$\phi_e = \phi_E \cdot f_{1,P} + \phi_P (1 - f_{1,P}) \quad (4.4.1)$$

where $f_{1,P}$ is a linear interpolation factor associated with a particular node P and co-ordinate direction x

$$f_{1,P} = \frac{(\delta x)_P}{(\delta x)_P + (\delta x)_E} \quad (4.4.2)$$

and $(\delta x)_P$ and $(\delta x)_E$ are the dimensions of the cells associated with nodes P and E in co-ordinate direction x , respectively.

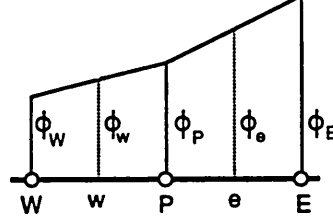


Figure 4.1 Schematic representation of CD in one dimension

Defining cell face values and interpolation factors for the other co-ordinate directions in a like manner to (4.4.1) and (4.4.2), the coefficients in the CD approximation to the convective terms in (4.2.2) are obtained as – see, for instance, Patankar (1980):

$$\begin{aligned}
 a_E^C &= -F_e \cdot f_{1,P} \\
 a_W^C &= F_w(1 - f_{1,W}) \\
 a_N^C &= -F_n \cdot f_{2,P} \\
 a_S^C &= F_s(1 - f_{2,S}) \\
 a_D^C &= -F_d \cdot f_{3,P} \\
 a_U^C &= -F_u(1 - f_{3,U}) \\
 a_P^C &= \sum_m a_m^C \quad m=E,W,N,S,D,U
 \end{aligned} \tag{4.4.3}$$

Boundedness is not assured by this scheme – if convective processes dominate, *ie.* $|a_m^C| > |a_m^D|$, the coefficient a_m will be negative for those neighbour nodes for which a_m^C is negative. Domination by convective processes, and hence an upper limit on CD scheme stability, is quantified, on a uniform Cartesian grid and in the absence of source terms, as a Péclet number Pe (equivalent to a grid Reynolds number for momentum equations) > 2 , where

$$Pe = \frac{\rho u \Delta x}{\Gamma} \tag{4.4.4}$$

Here Γ is the diffusion coefficient and Δx a characteristic cell dimension. The lack of boundedness is due to violation of the transportiveness principle, because of the employment of downstream nodes. In addition, the equation set resulting from CD becomes progressively less diagonally dominant, and hence less amenable to iterative solution, with increasing Pe (in the limit of $Pe = \infty$, $a_P = 0$).

Taylor series analysis indicates that the scheme is second-order accurate.

4.4.2 Upwind differencing (UD)

The principle alternative, in a three-point scheme, to linear interpolation between bracketing nodal values for the cell face value of ϕ , is to assume that it is equal to the value at the upstream node, figure 4.2. Thus

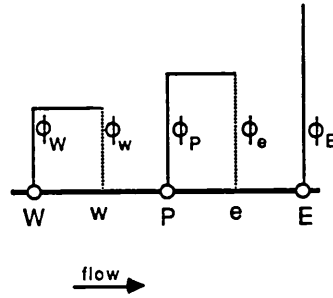


Figure 4.2 Schematic representation of UD in one dimension

$$\phi_e = \begin{cases} \phi_P & u_e \geq 0 \\ \phi_E & u_e < 0 \end{cases} \quad (4.4.5)$$

Defining values at the other cell faces in a like manner the coefficients in the UD approximation to the convective terms in (4.2.2) are obtained as

$$\begin{aligned} a_E^C &= \max(0, -F_e) \\ a_W^C &= \max(0, F_w) \\ a_N^C &= \max(0, -F_n) \\ a_S^C &= \max(0, F_s) \\ a_D^C &= \max(0, -F_d) \\ a_U^C &= \max(0, F_u) \\ a_P^C &= \sum_m a_m^C \quad m=E, W, N, S, D, U \end{aligned} \quad (4.4.6)$$

As a scheme derived from transportive considerations alone, boundedness is guaranteed, as confirmed by the always non-negative coefficients (4.4.6).

UD is formally (Taylor series analysis) first-order accurate, the leading neglected term being of the form $1/2\{u_i\Delta x_i(\partial^2\phi/\partial x_i^2)\}$. The diffusive nature of this

term has given rise to the expressions false or numerical diffusion, to describe the diffusion-like smearing, or reduction of sharp gradients in the solution, under the circumstances identified by Raithby (1976a): flow not closely aligned with grid lines and strong cross-flow gradients in ϕ . Leschziner (1980) has quantified the false diffusion coefficient as

$$\Gamma_f \approx 2^{-3/2} \sin(\frac{\pi}{4} + \theta) |\mathbf{V}| \sin 2\theta \quad (4.4.7)$$

for a (uniform) mesh width Δ , indicating that for the worst case of flow alignment to grid, θ , of 45° , the upwind approximation introduces a numerical diffusivity equivalent to $|Pe| = 2.8$ irrespective of the actual (physical) Péclet number.

4.4.3 Other three-point schemes

Spalding (1972) proposed that cell face values be evaluated according to central differencing when $Pe \leq 2$, and according to upwind differencing when $Pe > 2$. This Hybrid Scheme guarantees positive coefficients and thus a bounded solution, with accuracy in the diffusive flow limit, but does not remedy the numerical diffusion problem in the convective flow limit.

An alternative proposal also attributable to Spalding (1972) is based on the exact solution for ϕ_e for a sourceless equation between nodes P and E :

$$\phi_e = \frac{(\phi_E - \phi_P)e^{Pe \cdot f_{1,P}} - 1}{e^{Pe} - 1} + \phi_P \quad (4.4.8)$$

That this exponential scheme has not been widely implemented is due firstly to the expense of computing exponentials, particularly for situations (two or three dimensions and/or presence of source terms) where the inexactitude of (4.4.8) makes the value of such extra computational effort dubious, and secondly to the fact that it reduces to CD and UD in the convective and diffusive limits, respectively, as does hybrid differencing. Indeed hybrid differencing simply represents a piecewise approximation to exponential differencing.

4.4.4 Linear upwind differencing (LUD)

In interpolating/extrapolating for the value of ϕ at a given location, the net may be cast wider to include second-nearest nodes *ie.* the computational molecule may

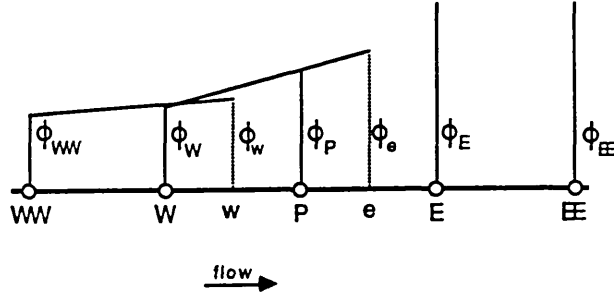


Figure 4.3 Schematic representation of LUD in one dimension

be expanded, in one dimension, from three to five points. The cell face values may then be obtained by

linear extrapolation from the two closest upstream neighbour nodes, figure 4.3, such that ϕ_e , for example, is given by

$$\phi_e = \begin{cases} \phi_P + (\phi_P - \phi_W)(1 - f_{1,W}) & u_e \geq 0 \\ \phi_E + (\phi_E - \phi_{EE})f_{1,E} & u_e < 0 \end{cases} \quad (4.4.9)$$

Defining values at the other cell faces in a like manner the coefficients in the LUD approximation to the convective terms in (4.2.2) are obtained as

$$\begin{aligned} a_E^C &= \max(0, -F_e)(1 + f_{1,E}) + \max(0, -F_w)f_{1,P} \\ a_W^C &= \max(0, F_w)(2 - f_{1,WW}) + \max(0, F_e)(1 - f_{1,W}) \\ a_N^C &= \max(0, -F_n)(1 + f_{2,N}) + \max(0, -F_s)f_{2,P} \\ a_S^C &= \max(0, F_s)(2 - f_{2,SS}) + \max(0, F_n)(1 - f_{2,S}) \\ a_D^C &= \max(0, -F_d)(1 + f_{3,D}) + \max(0, -F_u)f_{3,P} \\ a_U^C &= \max(0, F_u)(2 - f_{1,UU}) + \max(0, F_d)(1 - f_{3,U}) \\ a_{EE}^C &= -\max(0, -F_e)f_{1,E} \\ a_{WW}^C &= -\max(0, F_w)(1 - f_{1,WW}) \\ a_{NN}^C &= -\max(0, -F_n)f_{2,N} \\ a_{SS}^C &= -\max(0, F_s)(1 - f_{2,SS}) \\ a_{DD}^C &= -\max(0, -F_d)f_{3,D} \\ a_{UU}^C &= -\max(0, F_u)(1 - f_{3,UU}) \\ a_P^C &= \sum_m a_m \quad m=E,W,N,S,D,U,EE,WW,NN,SS,DD,UU \end{aligned} \quad (4.4.10)$$

Despite the adherence to the transportiveness criterion, unbounded solutions are possible due to the negative coefficients associated with the distant nodes EE , WW etc., which do not have a diffusive contribution.

The scheme is formally (Taylor series analysis) second order accurate, and where boundedness problems are avoided LUD produces a more accurate solution than UD on a given grid.

4.4.5 Quadratic upwind differencing (QUD)

Attributable to Leonard (1979), QUD determines cell face values from a quadratic function g of the two nearest upstream and the nearest downstream nodal values, figure 4.4, such that ϕ_e , for example, is given by

$$\phi_e = \begin{cases} g_{e1}^1 \phi_E - g_{e1}^2 \phi_W + (1 - g_{e1}^1 + g_{e1}^2) \phi_P & u_e \geq 0 \\ g_{e2}^1 \phi_P - g_{e2}^2 \phi_{EE} + (1 - g_{e2}^1 + g_{e2}^2) \phi_E & u_e < 0 \end{cases} \quad (4.4.11)$$

where g_{e1}^1 and g_{e1}^2 are the coefficients in the quadratic function g_{e1} of ϕ_W , ϕ_P and ϕ_E , and g_{e2}^1 and g_{e2}^2 are the coefficients in the quadratic function g_{e2} of ϕ_P , ϕ_E and ϕ_{EE} , calculable from the expressions

$$\begin{aligned} g_{e1}^1 &= \frac{(2 - f_{1,W})(f_{1,P})^2}{1 + f_{1,P} - f_{1,W}} \\ g_{e1}^2 &= \frac{(1 - f_{1,P})(1 - f_{1,W})^2}{1 + f_{1,P} - f_{1,W}} \\ g_{e2}^1 &= \frac{(1 + f_{1,W})(1 - f_{1,P})^2}{1 + f_{1,E} - f_{1,P}} \\ g_{e2}^2 &= \frac{(f_{1,E})^2 f_{1,P}}{1 + f_{1,E} - f_{1,P}} \end{aligned} \quad (4.4.12)$$

Values of ϕ and coefficients g may be defined by expressions analogous to (4.4.11) and (4.4.12) respectively, such that the coefficients in the QUD approximation to

the convective terms in (4.2.2) are obtained as

$$\begin{aligned}
a_E^C &= -\max(0, F_e)g_{e1}^1 - \min(0, F_w)g_{w2}^2 - \min(0, F_e)(1 - g_{e2}^1 + g_{e2}^2) \\
a_W^C &= \max(0, F_e)g_{e1}^2 + \min(0, F_w)g_{w2}^1 + \max(0, F_w)(1 - g_{w1}^1 + g_{w1}^2) \\
a_N^C &= -\max(0, F_n)g_{n1}^1 - \min(0, F_s)g_{s2}^2 - \min(0, F_n)(1 - g_{n2}^1 + g_{n2}^2) \\
a_S^C &= \max(0, F_n)g_{n1}^2 + \min(0, F_s)g_{s2}^1 + \max(0, F_s)(1 - g_{s1}^1 + g_{s1}^2) \\
a_D^C &= -\max(0, F_d)g_{d1}^1 - \min(0, F_u)g_{u2}^2 - \min(0, F_d)(1 - g_{d2}^1 + g_{d2}^2) \\
a_U^C &= \max(0, F_d)g_{d1}^2 + \min(0, F_u)g_{u2}^1 + \max(0, F_u)(1 - g_{u1}^1 + g_{u1}^2) \\
a_{EE}^C &= \min(0, F_e)g_{e2}^2 \\
a_{WW}^C &= -\max(0, F_w)g_{w1}^2 \\
a_{NN}^C &= \min(0, F_n)g_{n2}^2 \\
a_{SS}^C &= -\max(0, F_s)g_{s1}^2 \\
a_{DD}^C &= \min(0, F_d)g_{d2}^2 \\
a_{UU}^C &= -\max(0, F_u)g_{u1}^2 \\
a_P^C &= \sum_m a_m \quad m=E,W,N,S,D,U,EE,WW,NN,SS,DD,UU
\end{aligned} \tag{4.4.13}$$

QUD is conservative and formally third-order accurate – Leonard (1979) – thus promising solutions of a given accuracy on much coarser grids, with associated speed gains and storage savings. However, the scheme violates the transportiveness criterion, in including downstream nodes in the quadratic interpolations for ϕ (4.4.11). Furthermore, coefficients for the distant nodes EE, WW etc. are always negative, as for LUD, and the convective contributions to the coefficients of the nearest downstream node are negative. Thus in the case of a uniform grid with F_e, F_n and F_d all positive, the convective contributions

$$a_E^C = -\frac{3}{8}F_e; \quad a_N^C = -\frac{3}{8}F_n; \quad a_D^C = -\frac{3}{8}F_d \tag{4.4.14}$$

are obtained, and thus the coefficients a_E, a_N and a_D will be negative for $Pe > 8/3$. Leschziner's (1980) and Leschziner and Rodi's (1981) investigations of the merits of the scheme are the most comprehensive of a number in the literature; while found to simulate the effects of physical diffusivity on the spread of ϕ 'quite well' the scheme was also found to suffer from boundedness problems, attributable to the above-mentioned negative coefficients under certain circumstances. It has been noted in section 4.3.2 that the approximation used for the diffusion terms is second order accurate, and accordingly it is not necessarily of additional benefit

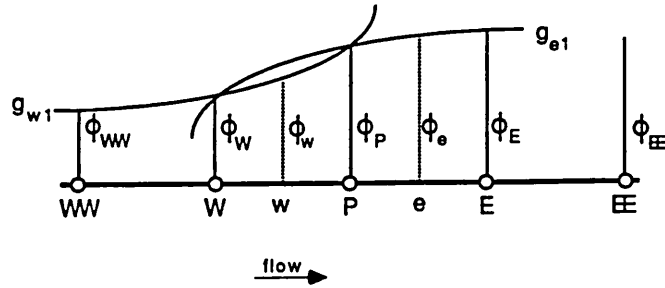


Figure 4.4 Schematic representation of QUD in one dimension

to employ an (albeit only formally) third order accurate approximation to the convective terms.

4.4.6 Flow-oriented differencing

Skew upwind differencing, attributable to Raithby (1976b) is representative of flow-oriented differencing schemes, which resemble upwind differencing insofar as they equate the cell face value to that at an upstream location. While in the case of upwind differencing, however, this location is the nearest node on the same co-ordinate, in the flow-oriented schemes it is the first point of intersection between the back projection of the tangent to the streamline passing through the cell face and a grid line, figure 4.5.

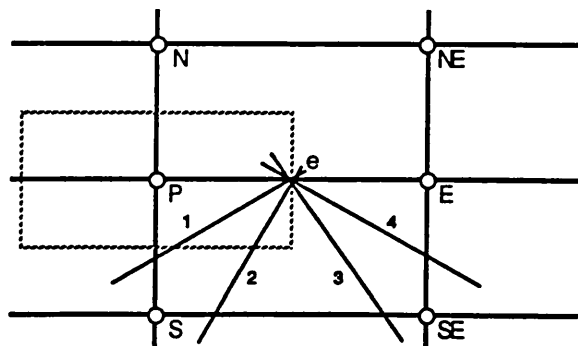


Figure 4.5 Schematic representation of SUD

While conservative and fully transportive, the main nodal coefficients a_W , a_E , a_N and a_S can become negative. Accordingly the scheme is neither unconditionally

bounded nor diagonally dominant, as borne out by Leschziner's (1980) investigations, which did, however, indicate considerably less under- and over-shoot than that associated with QUD. Lai (1982) showed SUD to be first-order accurate in Taylor series terms, but much less prone than UD to numerical diffusion. The improved accuracy (relative to UD) obtained in numerous two-dimensional implementations is however obtained at the expense of a 27-diagonal coefficient matrix (in three dimensions), as opposed to a 7-diagonal matrix for UD.

4.4.7 Total variation diminishing schemes

Given the convection-diffusion equation

$$\frac{\partial \phi}{\partial t} + \frac{\partial}{\partial x}(u\phi) - \frac{\partial}{\partial x}\left(\Gamma \frac{\partial \phi}{\partial x}\right) = 0 \quad (4.4.16)$$

for the non-dimensional function $\phi(x)$, the imposition of time-independent boundary conditions implies that the solution to (4.4.16) is bounded by the initial values *ie.* the total variation in ϕ must decrease with time *viz.*

$$\text{TV}(\phi^{n+1}) \leq \text{TV}(\phi^n) \quad (4.4.17)$$

A differencing scheme giving a solution obeying (4.4.17) is said to be total variation diminishing (TVD). Harten (1984) has given the basic theory for explicit TVD schemes, and extended it to implicit ones, summarised as follows.

A one-parameter family of schemes in conservation form, on a uniform grid of spacing Δx and time step Δt for convenience, is considered, *viz.*

$$L \cdot \phi^{n+1} = R \cdot \phi^n \quad (4.4.18)$$

where L and R are the following finite-difference operators:^{*}

$$(L \cdot \phi)_P = \phi_P + \eta \lambda (f_e - f_w) - \eta \lambda (\gamma_e(\Delta \phi)_e - \gamma_w(\Delta \phi)_w) \quad (4.4.19)$$

and

$$(R \cdot \phi)_P = \phi_P - (1 - \eta) \lambda (f_e - f_w) + \lambda (1 - \eta) (\gamma_e(\Delta \phi)_e - \gamma_w(\Delta \phi)_w) \quad (4.4.20)$$

where f_e and $\gamma_e(\Delta \phi)_e$ are the numerical approximations of the convection and diffusion fluxes, respectively, at face e of the computational molecule of figure 4.3, *ie.*

$$f_e = (u\phi)_e \quad (4.4.21)$$

^{*} λ is defined as $\Delta t / \Delta x$

and

$$\gamma_e = \Gamma_e / \Delta x \quad (4.4.22)$$

The parameter η ranges in value from 0, corresponding to the explicit forward-Euler scheme, to 1, corresponding to the implicit backward-Euler scheme. The scheme is TVD if

$$\text{TV}(R \cdot \phi) \leq \text{TV}(\phi) \quad (4.4.23)$$

and

$$\text{TV}(L \cdot \phi) \geq \text{TV}(\phi) \quad (4.4.24)$$

since

$$\text{TV}(\phi^{n+1}) \leq \text{TV}(L\phi^{n+1}) = \text{TV}(R\phi^n) \leq \text{TV}(\phi^n) \quad (4.4.25)$$

The forms of L and R satisfying these conditions are

$$(L \cdot \phi_P) = \phi_P - \eta[\lambda\gamma_e + C_e^+](\Delta\phi)_e + \eta[\lambda\gamma_w + C_w^-](\Delta\phi)_w \quad (4.4.26)$$

where

$$C_e^+ = \frac{1}{2} \left(q_e - \lambda \frac{(\Delta(u\phi))_e}{(\Delta\phi)_e} \right) \quad (4.4.27)$$

$$C_e^- = \frac{1}{2} \left(q_e + \lambda \frac{(\Delta(u\phi))_e}{(\Delta\phi)_e} \right) \quad (4.4.28)$$

and the function q must satisfy the condition

$$\lambda \frac{(\Delta(u\phi))_e}{(\Delta\phi)_e} \leq 2\lambda\gamma_e + q_e \leq \frac{1}{(1-\eta)} \quad (4.4.29)$$

This may be alternatively expressed as

$$\frac{\Delta t}{\Delta x} \frac{(\Delta(u\phi))_e}{(\Delta\phi)_e} \leq \frac{2\Delta t \Gamma_e}{(\Delta x)^2} + q_e \leq \frac{1}{(1-\eta)} \quad (4.4.30)$$

The left-hand inequality here is

$$\frac{(\Delta(u\phi))_e}{(\Delta\phi)_e} \leq \frac{2\Gamma_e}{\Delta x} + Q_e \quad (4.4.31)$$

where Q_e is defined as

$$Q_e = \frac{q_e}{\lambda} \quad (4.4.32)$$

and is the numerical diffusion coefficient in the expression for the numerical approximation to the convection term

$$f_e = \frac{1}{2}(u\phi)_E + \frac{1}{2}(u\phi)_P - \frac{1}{2}q_e \frac{(\Delta\phi)_e}{\lambda} \quad (4.4.33)$$

The constraint (4.4.31) is equivalent to the requirement of positive coefficients; if

$$Q_e = \frac{(\Delta(u\phi))_e}{(\Delta\phi)_e} \quad (4.4.34)$$

(4.4.33) reduces to upwind differencing. (4.4.34) may be interpreted as a flux limiter, introducing numerical diffusion to maintain boundedness. Harten (1984) has extended the above first-order scheme to one of second-order accuracy in both space and time by applying it to a modified flux $\tilde{f}$, where $\tilde{f}$ reduces the effects of numerical diffusion everywhere except where boundedness is violated. $\tilde{f}$ is then given by

$$\tilde{f}_e = \frac{1}{2}(u\phi)_E + \frac{1}{2}(u\phi)_P - + \frac{(g_E + g_P)}{2\lambda} - \frac{q\left(\lambda \frac{\Delta(u\phi)_e}{(\Delta\phi)_e} + \frac{(\Delta g)_e}{(\Delta\phi)_e}\right)(\Delta\phi)_e}{2\lambda} \quad (4.4.35)$$

and g is defined as

$$g_P = s \cdot \max\{0, \min(\sigma_e |(\Delta\phi)_e|, s \cdot \sigma_w |(\Delta\phi)_w|)\} \quad (4.4.36)$$

where

$$s = \text{sgn}((\Delta\phi)_e) \quad (4.4.37)$$

It is apparent from (4.4.36) that g , and hence the flux correction, is non-zero only when $(\delta\phi)_e$ and $(\delta\phi)_w$ are of opposite sign *ie.* only at extrema.

This modified scheme is a 5-point scheme – $\tilde{f}_e$ depends on g_P and g_E and hence

$$\tilde{f}_e = \tilde{f}(\phi_W, \phi_P, \phi_E, \phi_{EE}) \quad (4.4.38)$$

Harten proves, however, that $\tilde{f}_e = 1/2[f(v_P) + f(v_E)] = f(v)$, and thus that

$$\tilde{f}(u, v, v, w) = f(v), \quad \text{all } u, v, w \quad (4.4.39)$$

– a consistency relation similar to that of the first-order 3-point scheme. This property results in a tri-diagonal coefficient matrix when the scheme is implemented implicitly; such an implementation is reported by Yee, Warming and Harten (1985) for the solution of Euler equations.

Harten (1984) concludes that 2 seems to be the maximum order of accuracy for TVD schemes, and while the gain in accuracy in one dimension is significant, it has not been theoretically proven in two or more dimensions; nor has the guaranteed boundedness of the scheme in the same circumstances. The lack of conclusive

theoretical or empirical proof of robustness and cost-effective accuracy gains for multi-dimensional analysis excludes TVD schemes from further consideration here.

4.4.8 Conclusions

It will be apparent from the foregoing that while all of the schemes mentioned are conservative, and while transportiveness is adhered to by the majority, none successfully reconcile the unconditional requirement for boundedness with the goal of avoidance of numerical diffusion in convection-dominated flow. Both extended computational molecule and flow-oriented schemes offer formal (and for a number of flow cases demonstrated) improvements in accuracy over upwinding in convection-dominated flow. All have also been noted to exhibit unboundedness in the form of oscillatory solutions, however, and even when such behaviour does present difficulties in solution it usually negates any gain in formal accuracy. The goal of a reliable (bounded), cost-effective and accurate scheme for analyses of three-dimensional flow provided the motivation for Ziman's (1990) differencing scheme work, presented in the following section.

4.5 Self-filtered central differencing

The self-filtered central differencing (SFCD) scheme of Ziman (1990) is based on the ideas expounded by Runchal (1987) in developing his CONDIF scheme. SFCD is a 5-point scheme in one dimension, using the same extended computational molecule as used by LUD, and calculates ϕ_e as

$$\phi_e = \begin{cases} \phi_P + f_{1,P}(\phi_P - \phi_W)r_e & u_e \geq 0 \\ \phi_E - f_{1,P}(\phi_{EE} - \phi_E)r_e & u_e < 0 \end{cases} \quad (4.5.1)$$

where

$$r_e = \begin{cases} \max\left\{0, \min\left(\frac{\phi_E - \phi_P}{\phi_P - \phi_W}, r_{\max}\right)\right\} & u_e \geq 0 \\ \max\left\{0, \min\left(\frac{\phi_E - \phi_P}{\phi_{EE} - \phi_E}, r_{\max}\right)\right\} & u_e < 0 \end{cases} \quad (4.5.2)$$

and similarly for ϕ_w, r_w etc. In the circumstances where (4.5.2) gives

$$r_e = \frac{\phi_E - \phi_P}{\phi_P - \phi_W} \quad \text{or} \quad r_e = \frac{\phi_E - \phi_P}{\phi_{EE} - \phi_E}$$

it can be seen that (4.5.1) is equivalent to central differencing. However (4.5.2) prevents corruption of ϕ_e by physically unrealistic maxima or minima in the computational molecule. Figure 4.6 illustrates that negative values of

$$\frac{\phi_E - \phi_P}{\phi_P - \phi_W} \quad \text{or} \quad \frac{\phi_E - \phi_P}{\phi_{EE} - \phi_E}$$

represent such extrema and that under these circumstances (4.5.2) ensures that (4.5.1) reverts to upwind differencing.

The convection terms discretised using SFCD are here separated into those terms which would be obtained using UD, and non-linear correction terms. The rationale behind this decomposition will be apparent when solution algorithms are discussed in section 4.8.1.

In three dimensions the differenced convective terms are then given by

$$\begin{aligned} & a_P^c \phi_P - a_E^c \phi_E - a_W^c \phi_W - a_N^c \phi_N - a_S^c \phi_S - a_D^c \phi_D - a_U^c \phi_U + \\ & + f_{1,P}(\phi_P - \phi_W)[\max(0, F_e)]r_e + f_{1,P}(\phi_{EE} - \phi_E)[\max(0, -F_e)]r_e \\ & - f_{1,P-1}(\phi_W - \phi_{WW})[\max(0, F_w)]r_w - f_{1,P-1}(\phi_E - \phi_P)[\max(0, -F_w)]r_w \\ & + f_{2,P}(\phi_P - \phi_S)[\max(0, F_n)]r_n + f_{2,P}(\phi_{NN} - \phi_N)[\max(0, -F_n)]r_n \\ & - f_{2,P-1}(\phi_S - \phi_{SS})[\max(0, F_s)]r_s - f_{2,P-1}(\phi_N - \phi_P)[\max(0, -F_s)]r_s \\ & + f_{3,P}(\phi_P - \phi_U)[\max(0, F_d)]r_d + f_{3,P}(\phi_{DD} - \phi_D)[\max(0, -F_d)]r_d \\ & - f_{3,P-1}(\phi_U - \phi_{UU})[\max(0, F_u)]r_u - f_{3,P-1}(\phi_D - \phi_P)[\max(0, -F_u)]r_u \end{aligned}$$

The coefficients a_m^c are those obtained by upwind differencing, given by (4.4.6); they are independent of ϕ , and thus unconditionally positive. The nonlinear terms associated with the outermost cells (EE , WW , NN , SS , DD and UU) are always non-positive, though the remaining SFCD contributions are positive. The presence of negative terms does not have boundedness implications (boundedness being ensured by filtering out of maxima and minima as aforesaid) but may reduce the central coefficient a_P sufficiently to impair the stability of an iterative solution. The introduction of the upper bound $r_{\max}$ on r_e on (4.5.2) limits the value of the negative contributions to a_m in order to preclude this problem.

If r_e has a value of unity SFCD is equivalent to LUD. Thus if $r_{\max}$ is set to unity SFCD may be interpreted as a non-linear blend between UD and LUD, with the r_e 's as blending factors ranging in value between zero and unity.

Ziman (1990) has performed a Taylor series analysis for the assessment of the accuracy of SFCD for the various values of r_e , and demonstrated that the

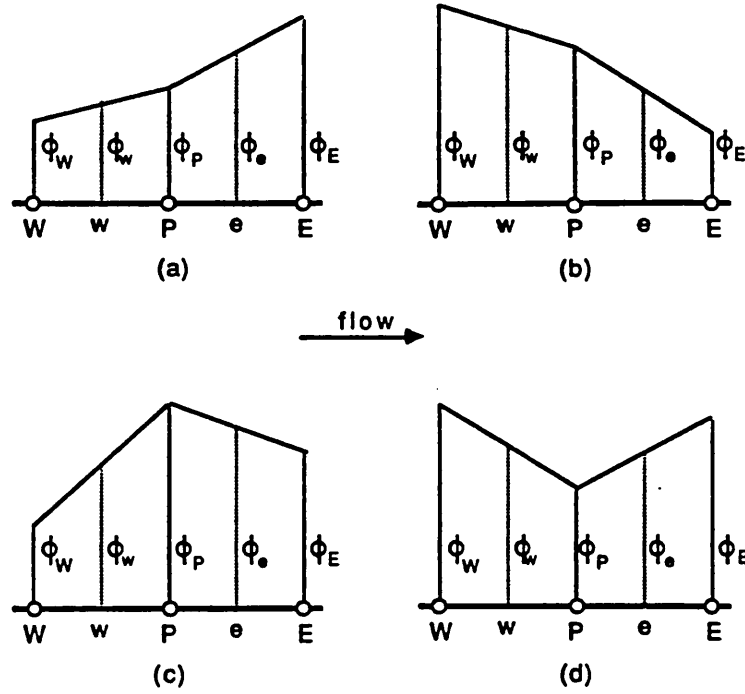


Figure 4.6 SFCD filtering mechanism: r_e is non-negative if the profile is monotonic, (a) and (b); negative in cases of local maxima or minima, (c) and (d)

scheme is formally second-order accurate for the cases

$r_e = (\phi_E - \phi_P)/(\phi_P - \phi_W)$ or $r_e = (\phi_E - \phi_P)/(\phi_{EE} - \phi_E)$ (central differencing) and $r_e = r_{\max}$.

Furthermore, Ziman argues that SFCD fulfills the transportiveness requirement. This is self-evident in the case $r_e = 0$, in which only upstream node values are used. In the case $r_e = (\phi_E - \phi_P)/(\phi_P - \phi_W)$ or $r_e = (\phi_E - \phi_P)/(\phi_{EE} - \phi_E)$, there is some spatial variation due to terms other than that being discretised, and the incorporation of a downstream node, i.e. the use of central differencing, ensures that these effects are taken into account (the failure to do so is the source of numerical diffusion in the case of upwind differencing and the cause of unboundedness in the case of linear upwind differencing). In the case $r_e = r_{\max}$ values at downstream points which are markedly different are excluded from the interpolation i.e. they cannot be transmitted upstream in violation of the transportiveness criterion.

4.6 Grid layout and variable arrangement

For both the pipe and mixing vessel cases the solution domains are divided into a finite number of control volumes by an orthogonal rectilinear grid. The spatial arrangement of the storage locations employed is different in each case, however. For the pipe cases the co-located approach perfected by Perić (1985) has been adopted, and this is described in section 4.6.1. The earlier staggered grid arrangement, the various versions of which have been reviewed by Perić (1985), has been retained for the mixing vessel studies as its replacement by the co-located grid arrangement is outside the scope of this study; it is described in section 4.6.2. The relative merits of the schemes are summarised in section 4.6.3.

4.6.1 Pipe flow procedure

The domain of solution is comprised of a cylindrical sector of geometric symmetry of unit radian thickness. Due to the assumption of circumferential invariance this is discretised into a finite number of four-sided control volumes the faces of which are sections of the x and r co-ordinate surfaces, and the volumes of which accordingly are $r\Delta r\Delta x$. The values of all variables are stored at grid nodes (symbol $\bullet$) centred in the control volumes. The outermost control volumes are of zero thickness *ie.* the grid arrangement is such that the outermost grid nodes lie on the domain boundary, as do the faces of the second outermost control volume – figure 4.7.

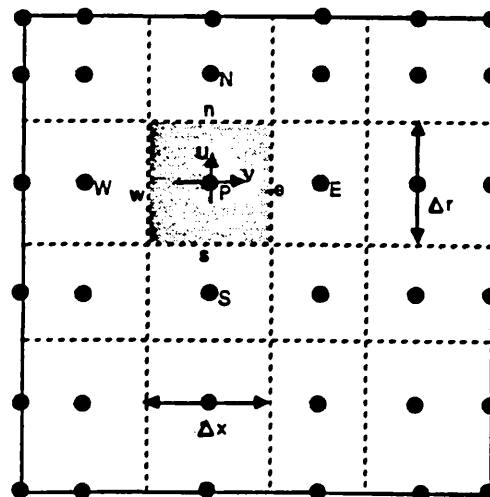


Figure 4.7 Solution domain, grid layout and variable arrangement, pipe cases

4.6.2 Mixing vessel procedure

The domain of solution is comprised of a cylindrical sector of geometric symmetry enclosing a single baffle. This is discretised into a finite number of six-sided control volumes the faces of which are sections of the x, r and θ co-ordinate surfaces. Figure 4.8 shows the grid locations at which the dependent variables are calculated; it will be noted that scalar quantities, including pressure, are calculated at grid nodes (symbol $\bullet$) centred in the control volumes while the locations at which velocities are calculated (symbol $\rightarrow$) are defined such that the component normal to each control volume boundary lies on the intersection of that boundary with the grid line passing through the scalar node locations which straddle it. Furthermore, the grid is so arranged that the outermost control volume boundaries coincide with the outer surfaces of the calculation domain and so also therefore do the normal velocity component locations.

As a consequence of the staggered arrangement of the velocity locations the control volumes associated with the velocity nodes are displaced relative to the main control volumes surrounding the scalar nodes, as illustrated in figure 4.8.

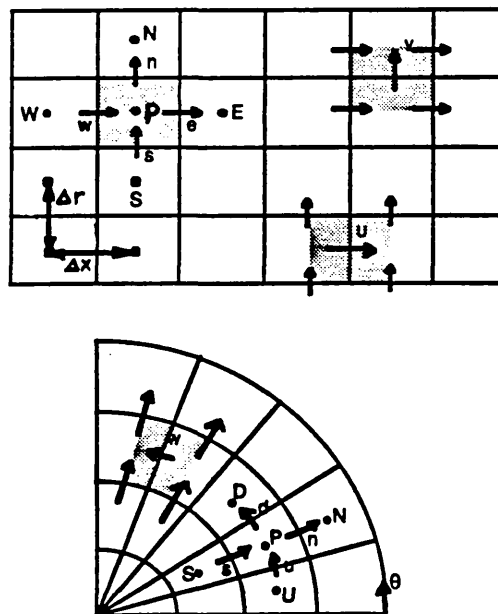


Figure 4.8 Solution domain, grid layout and variable arrangement, mixing vessel cases

4.6.3 Relative merits of staggered and co-located arrangements

Perić *et al* (1988) have conducted a detailed comparison, using staggered and co-located grids, of the performance of the finite volume method in the prediction of a range of two-dimensional laminar flows. They showed that typical differences between the results of the two methods were of the order of 0.01% of appropriate reference values, with differences of up to 0.1% limited to small regions, and, by comparison with reference numerical solutions, that the differences are significantly smaller than the solution errors. Furthermore, the total computing times were about the same for both methods.

The primary advantage to be expected from the co-located grid arrangement is the relative simplicity (and hence economy and flexibility) it affords on non-orthogonal grids – this is of little consequence here. Of greater potential interest is the fact that for a co-located grid the coefficients in all of the discretised transport equations are identical, and this should in general reduce computational effort substantially when higher-order differencing schemes are employed.

The treatment of boundary conditions is in most cases more straightforward with the co-located arrangement – the half cells appearing near some boundaries with the use of staggered grids require special treatment. However the disadvantage of the latter arrangement when higher-order differencing schemes such as QUDS or LUDS are employed, that a lower-order treatment of the near-boundary control volumes has to be accepted, does not apply to the use of SFCD on a staggered grid, as Ziman (1990) has demonstrated.

An advantage of the staggered arrangement is that since velocities normal to the boundaries are usually known, or taken as such, zero gradient boundary conditions can be specified for the pressure correction equation (to be presented in section 4.8.3), avoiding explicit reference to boundary pressures. While this is also true for the pressure correction equation with the co-located arrangement, values of the pressure at the boundary nodes are required to evaluate the pressure gradient in the momentum equations; the linear extrapolation from interior values of the pressure used is thus an additional slight uncertainty.

Overall, however, the differences in accuracy and computing effort to be expected between the approaches are sufficiently small as to have no significance for the purposes of this study.

4.7 Boundary conditions

4.7.1 Solid boundaries

The convective flux normal to solid boundaries is zero, and the wall shear stress τ_w is given by

$$\tau_w = \mu \frac{u_{i,P}}{y_P} \quad (4.7.1)$$

for the case where P is in the laminar sublayer *ie.* $y_P^+ \leq y_{lt}^+$, where $u_{i,P}$ is the velocity component parallel to the wall at node P , distance y_P from the wall. For the case where P is in the fully turbulent region *ie.* $y_P^+ > y_{lt}^+$, τ_w may be obtained by writing (3.10.7) as

$$\begin{aligned} \tau_w &= \rho C_\mu^{1/2} k^{1/2} \frac{u_*}{C_\mu^{1/4}} \\ &= \rho C_\mu^{1/4} k^{1/2} \frac{\kappa}{\ln(E y_P^+)} u_{i,P} \end{aligned} \quad (4.7.2)$$

This boundary condition for the momentum equations is thus implemented by setting the appropriate coefficient a_m in the equation for the next-to-solid boundary cell to zero, and specifying the source terms as (*cf.* section 4.3.3):

$$S_{u_i}^1 = 0 \quad (4.7.3)$$

with

$$S_{u_i}^2 = -\Delta_i p + \mu \frac{u_i}{y_P} \quad y_P^+ \leq y_{lt}^+ \quad (4.7.4)$$

$$S_{u_i}^2 = -\Delta_i p + \frac{\rho C_\mu^{1/4} k_P^{1/2} \kappa}{\ln(E y_P^+)} u_{i,P} \quad y_P^+ > y_{lt}^+ \quad (4.7.5)$$

The sink term in the transport equation for k for the next-to-wall cell is obtained by integration of (3.10.8) over the cell; this term is treated implicitly (*cf.* section 4.3.3) and thus

$$S_k^1 = \frac{\rho C_\mu^{3/4} k_P^{1/2} u_P^+}{y_P} \quad (4.7.6)$$

In the calculation of the generation of turbulence energy term (3.9.7) in the next-to-wall cell the contribution of the wall shear stress τ_w , given by (4.7.2), replaces the relevant, *ie.* wall face, turbulent stress component τ_{ij} as approximated by the effective viscosity model. Hence the source term in the transport equation for k in this cell (treated explicitly) becomes

$$S_k^2 = S_k^2 + \frac{\rho C_\mu^{1/4} k_P^{1/2} \kappa}{\ln(E y_P^+)} \frac{u_{res,P}^2}{y_P} \quad (4.7.7)$$

where u_{res} is the resultant velocity parallel to the wall at the next-to-wall node.

The transport equation for ϵ is abandoned for the next-to-wall cell – the value is prescribed from the wall function (3.10.8), in which the friction velocity u_* is given by (3.10.7). The solution procedure is forced to return this value by ensuring source term domination of the next-to-wall cell equation, thus:

$$S_\epsilon^1 = -L \quad (4.7.8)$$

and

$$S_\epsilon^2 = L \frac{C_\mu^{3/4} k^{3/2}}{\kappa y_P} \quad (4.7.9)$$

where L is a large number, *eg.* 10^{30} .

4.7.2 Mixing vessel impeller

The grid layout in the impeller region is illustrated in figure 4.9; the practice is to choose the scalar control volumes such that their surfaces are coincident with the impeller disc and nodes with the blade edges. Within the volume swept out by the blades (shaded area in figure 4.9) the circumferential velocity, w , turbulence energy, k , and dissipation rate, ϵ , are prescribed, and this is performed in a like manner to that for the dissipation rate at next-to-wall nodes, (4.7.8) and (4.7.9):

$$S_{\phi_{sw.vol.}}^1 = -L \quad (4.7.10)$$

and

$$S_{\phi_{sw.vol.}}^2 = L \phi_{sw.vol.} \quad (4.7.11)$$

where L is a large number, *eg.* 10^{30} , and $\phi_{sw.vol.}$ is the prescribed value in the swept volume.

The axial and radial momentum equations are solved in unconstrained form in the blade swept region, as are all equations in the volume inboard of the blades. The setting of normal velocities u to zero on the impeller disc is performed using the same mechanism as for the swept volume variable prescription, (4.7.10) and (4.7.11) *ie.* the S_2 component of the axial momentum source term is set to a large negative value. Since the impeller disc is treated as any other solid boundary, wall functions are used to bound the remaining transport equations, for the control volumes on both sides of the disc from the axis to the disc edge, and the no slip

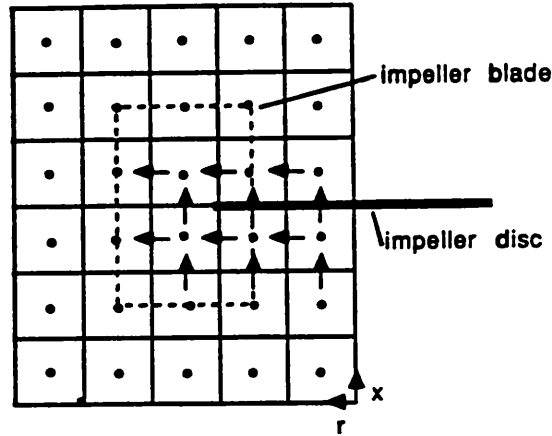


Figure 4.9 Grid layout in the impeller region

condition implies that the value of the circumferential velocity on the disc surface at radius r is $\omega.r$, where ω is the impeller rotational speed.

4.7.3 Other boundaries

Duct/vessel axis

The zero convection and diffusion fluxes assumed to obtain at the axis – section 3.10.3 – are enforced by setting the appropriate coefficients a_s in the transport equations to zero. The zero gradient condition is also assumed to hold for the pressure distribution from the axis to the next-to-axis node and radial gradients of pressure across this interval are accordingly set to zero.

Cyclic boundaries, mixing vessel

Values of the variables and fluxes on the upstream and downstream boundaries of the domain are not known in advance – they must be determined as part of the solution. Since the fluxes on the upstream face of the first plane of cells must by definition be equal to those on the downstream face of the last plane, the coefficient links across the inlet plane, IP , are evaluated from expressions for the fluxes crossing the outlet plane, OP , thus:

$$a_u|_{IP} = a_d|_{OP} + c_d|_{OP} \quad (4.7.12)$$

where c_d denotes the convective flux through the downstream face of the cell in

question, and

$$c_d|_{OP} = c_u|_{IP} \quad (4.7.13)$$

Inlet boundary, pipe cases

Since the inlet mass fluxes are known, they need not be corrected. Flux correction is accordingly suppressed by setting to zero the coefficients a_w in the transport equations (4.3.11) for the next-to-inlet cells.

Outlet boundary, pipe cases

The zero gradient boundary condition for all variables is imposed by setting to zero the coefficients on the outlet face of the next-to-outlet cells.

4.8 Solution procedure for the coupled equation sets

The procedure for determination of the terms in the discretised equations (4.3.11) having been determined, and practices for handling boundary conditions having been established, the method of solution of the coupled equation sets may now be addressed. The first issue arising is the handling of the SFCD correction terms in the transport equations; this is discussed in section 4.8.1. The mechanism for ensuring stability of the overall iterative procedure is briefly described in section 4.8.2, and the handling of the pressure-velocities coupling is outlined in section 4.8.3.

4.8.1 Handling of the SFCD correction terms

A number of solution algorithms for the treatment of the non-linearity and extended computational molecule associated with SFCD have been examined by Ziman (1990). Apart from the possibility of using a time-marching approach, some of the other alternatives are linearisation and implicit solution of the SFCD corrections to UD, or explicit treatment of the corrections as source terms to be updated after each iteration of the algorithm employed in the solution of the individual equation sets (section 4.10). The last-named, explicit approach has been adopted in this study since it avoids the extra storage requirement and solver complexity associated with the extended computational molecule, and the necessity to recalculate coefficients at each iteration of an implicit treatment.

The correction terms are handled as follows:

- The (transport) equation set is assembled with convective contributions to the coefficients evaluated using upwind differencing, and the SFCD corrections are evaluated from values of the transported variable at the previous iteration level and added to $S_{\phi,P}^2$.
- After each iteration of the equation set solution algorithm (*cf.* section 4.10) the SFCD corrections are recalculated from the new values of the dependent variable.

Explicit handling of the convection terms means that the question of preservation of diagonal dominance of the matrix (section 4.5) does not arise. $r_{\max}$ was maintained at a value of unity for all cases in this study, however, as there is some evidence (Ziman, 1990) that higher values of $r_{\max}$ limit permit such large correction at certain points in the flow field that convergence of the equation set solution algorithm is slowed substantially, with a rise in computing cost disproportionate to the gain in solution accuracy. The use of the $r_{\max}$ limit in this study is also with a view to prevention of another possible type of instability. An extremum formed at any given point on iteration N is eliminated by reversion to UD on iteration $N + 1$. However the lack of an extremum on completion of iteration $N + 1$ will result in the filter being inactive on iteration $N + 2$, making it possible for the extremum to reform. To prevent such an oscillation the r terms could be prevented from increasing from one iteration to the next, making the solution more UD-like, and, much more seriously, somewhat path dependent. Such oscillations were not observed in this study.

4.8.2 Under-relaxation

To obtain stability of the overall iterative scheme it is necessary to retard the changes in the dependent variable from iteration to iteration. Consider (4.3.11) recast in the form

$$\phi_P^N = \phi_P^{N-1} + \left(\frac{\sum a_m \phi_m + S_{\phi,P}^2}{a_P} - \phi_P^{N-1} \right) \quad (4.8.1)$$

where N and $N - 1$ denote the current and previous iteration levels, respectively, and the term in parentheses represents the change in ϕ_P effected during this iteration. This change is reduced by the introduction of an ‘under-relaxation’ factor α_ϕ in the range 0 to 1,

$$\phi_P^N = \phi_P^{N-1} + \alpha_\phi \left(\frac{\sum a_m \phi_m + S_{\phi,P}^2}{a_P} - \phi_P^{N-1} \right) \quad (4.8.2)$$

such that the final equation takes the form

$$\frac{a_P^\phi}{\alpha_\phi} \phi_P^N = \sum a_m \phi_m + S_{\phi,P}^2 + \frac{1 - \alpha_\phi}{\alpha_\phi} a_P \phi_P^{N-1} \quad (4.8.3)$$

Implicit in the above procedure is that it fulfills the requirement of final solution independence from the solution path followed *ie.* the final solution will not be a function of the value of α_ϕ .

4.8.3 Handling of the pressure-velocities coupling

The pressure-velocities coupling is handled via the PISO algorithm of Issa (1985), in which the solution process is split into a series of steps whereby operations on pressure are decoupled from those on velocity at each step, with the split sets of equations each applying to a single variable and thus being amenable to simple solution. Only a statement of the algorithm is made here, its relative merits having been thoroughly documented in the literature.

In the following, * and ** denote intermediate values between iteration levels N and $N + 1$, obtained during the splitting process. The predictor-corrector sequence proceeds as follows:

Predictor step

The momentum equations are solved using the pressure field from the previous iteration level, p^N to obtain the velocity field u_i^*

$$\frac{A_P^{u_i}}{\alpha_u} u_i^* = \sum_m A_m^u u_{i,m}^* - \Delta_i p^N + S_{u_i,p}^{2'} + \frac{1 - \alpha_u}{\alpha_u} A_P^{u_i} u_{i,p}^N \quad (4.8.4)$$

where

$$S_{u_i,p}^{2'} = S_{u_i,p}^2 + \Delta_i p^N \quad (4.8.5)$$

This satisfies the momentum equation for the given pressure field but not, in general, the continuity equation.

It is necessary to ensure that the axial velocities at the outlet plane in the pipe flow cases satisfy continuity, *ie.* that the sum of the outlet mass fluxes F^O equals the sum of the inlet mass fluxes F^I . Accordingly the axial velocity components are corrected after the predictor stage, by multiplying them by the ratio F^I/F^O .

First corrector step

Corrections u'_i and p' are sought such that the fields

$$u_i^{**} = u_i^* + u'_i$$

and

$$p^* = p^N + p' \quad (4.8.6)$$

satisfy the momentum equation and the continuity equation:

$$\Delta_i u_i^{**} = 0 \quad (4.8.7)$$

(4.8.4) is written in updated form as

$$\frac{A_P^{u_i}}{\alpha_u} u_i^{**} = \sum_m A_m^u u_{i,m}^* - \Delta_i p^* + S_{u_i,p}^{2'} + \frac{1 - \alpha_u}{\alpha_u} A_P^{u_i} u_{i,P}^N \quad (4.8.8)$$

Subtraction of (4.8.4) from (4.8.8) yields an equation in u'_i :

$$\frac{A_P^{u_i}}{\alpha_u} u'_i = \Delta_i (p^* - p^N) \quad (4.8.9)$$

When the divergence of (4.8.9) is combined with the continuity relation (4.8.7) the first pressure correction equation is obtained:

$$\Delta_i \left(\frac{\alpha_u}{A_P^{u_i}} \Delta_i p' \right) = \Delta_i u_i^* \quad (4.8.10)$$

(4.8.10) is solved for p' , p^* is obtained from (4.8.6), (4.8.9) yields u'_i and the updated velocity field is then available from (4.8.6).

Second corrector step

Further corrections u''_i and p'' are then sought, giving updated values

$$u_i^{N+1} = u_i^{**} + u''_i$$

and

$$p^{N+1} = p^* + p'' \quad (4.8.11)$$

which satisfy the continuity equation:

$$\Delta_i u_i^{N+1} = 0 \quad (4.8.12)$$

(4.8.8) is written in updated form as

$$\frac{A_P^{u_i}}{\alpha_u} u_i^{N+1} = \sum_m A_m^u u_{i,m}^{**} - \Delta_i p^{N+1} + S_{u_i,p}^{2'} + \frac{1 - \alpha_u}{\alpha_u} A_P^{u_i} u_{i,P}^N \quad (4.8.13)$$

Subtraction of (4.8.8) from (4.8.13) yields an equation in u_i'' :

$$\frac{A_P^{u_i}}{\alpha_u} u_i'' = \sum_m A_m^u u_i' - \Delta_i p'' \quad (4.8.14)$$

When the divergence of (4.8.14) is combined with the continuity relation (4.8.12) the second pressure correction equation is obtained:

$$\Delta_i \left(\frac{\alpha_u}{A_P^{u_i}} \Delta_i p'' \right) = \Delta_i \left(\frac{\sum_m A_m^u u_i'}{A_P^{u_i} / \alpha_u} \sum_m A_m^u u_i' \right) \quad (4.8.15)$$

(4.8.15) is solved for p'' , p^{N+1} is obtained from (4.8.11), u_i'' is then obtained from (4.8.14) and the velocity field at the new iteration level u_i^{N+1} from (4.8.11).

The mass fluxes F_i , appearing in the convective terms of the transport equations, are then updated from u_i^{N+1} .

The transport equations for k and ϵ are strongly coupled through their source terms, and a similar splitting procedure is employed in their solution. They are initially effectively decoupled by solving them in a predictor step as

$$\left(A_P + \frac{C_\mu \rho^2}{\mu_{t,P}^N} k_P^N \right) \frac{k_P^*}{\alpha_k} = \sum_m A_m k_m^* + \mu_{t,P}^N g + \frac{1 - \alpha_k}{\alpha_k} A_P^N k_P^N \quad (4.8.16)$$

$$\left(A_P + \frac{C_2 \rho}{k_P^*} \epsilon_P^N \right) \frac{\epsilon_P^*}{\alpha_\epsilon} = \sum_m A_m \epsilon_m^* + C_1 C_\mu g \rho k_P^* + \frac{1 - \alpha_\epsilon}{\alpha_\epsilon} A_P^N \epsilon_P^N \quad (4.8.17)$$

The viscosity μ_t^* is then obtained from

$$\mu_t^* = C_\mu \rho \frac{k_P^{*2}}{\epsilon_P^*} \quad (4.8.18)$$

Equations for the corrected *ie.* new iteration level, values of k and ϵ are written:

$$\left(A_P + \frac{C_\mu \rho^2}{\mu_{t,P}^*} k_P^* \right) \frac{k_P^{N+1}}{\alpha_k} = \sum_m A_m k_m^* + \mu_{t,P}^* g + \frac{1 - \alpha_k}{\alpha_k} A_P^* k_P^N \quad (4.8.19)$$

where

$$A_P^* = A_P^N + C_\mu \rho^2 \left(\frac{k_P^*}{\mu_{t,P}^*} - \frac{k_P^N}{\mu_{t,P}^N} \right) \quad (4.8.20)$$

and

$$\left(A_P + \frac{C_2 \rho}{k_P^{N+1}} \epsilon_P^*\right) \frac{\epsilon_P^{N+1}}{\alpha_\epsilon} = \sum_m A_m \epsilon_m^* + C_1 C_\mu g \rho k_P^{N+1} + \frac{1 - \alpha_\epsilon}{\alpha_\epsilon} A_P^* \epsilon_P^* \quad (4.8.21)$$

where

$$A_P^* = A_P^N + C_2 \rho \left(\frac{\epsilon_P^*}{k_P^{N+1}} - \frac{\epsilon_P^N}{k_P^*} \right) \quad (4.8.22)$$

By subtracting (4.8.16) from (4.8.19), and (4.8.17) from (4.8.21), the corrected values k^{N+1} and ϵ^{N+1} are obtained from the following explicit relations:

$$k_P^{N+1} = (1 - \alpha_k) k_P^N + \frac{\alpha_k}{A_P^*} \left\{ \frac{A_P^N}{\alpha_k} [k_P^* - (1 - \alpha_k) k_P^N] + (\mu_{t,P}^* - \mu_{t,P}^N) g \right\} \quad (4.8.23)$$

and

$$\epsilon_P^{N+1} = (1 - \alpha_\epsilon) \epsilon_P^N + \frac{\alpha_\epsilon}{A_P^*} \left\{ \frac{A_P^N}{\alpha_\epsilon} [\epsilon_P^* - (1 - \alpha_\epsilon) \epsilon_P^N] + (k_P^{N+1} - k_P^*) C_1 C_\mu g \rho \right\} \quad (4.8.24)$$

The term A_P^* , (4.8.20), in the corrector equation for k , (4.8.23), is replaced for next-to-solid boundary cells by

$$A_P^* = A_P^N + \frac{\rho C_\mu^{3/4}}{y_P} (\sqrt{k^*} u^{+*} - \sqrt{k} u^+) \quad (4.8.25)$$

consistent with the prescriptions (4.6.6) and (4.6.7) for the predictor step.

The molecular viscosity is updated if the fluid is shear-thinning, based on the ϵ^{N+1} field. The iteration is completed by updating μ_t , based on k^{N+1} and ϵ^{N+1} .

4.9 Summary of algorithm

The complete solution algorithm may be summarised as

- (i) Initialise all field values by an initial guess
- (ii) Solve the momentum equations (4.8.4) to obtain u_i^* , using the prevailing pressure as p^N
- (iii) Solve the pressure correction equation (4.8.10) to obtain p'
- (iv) Correct the velocities and pressures using (4.8.6) to obtain the u_i^{**} and p^* fields
- (v) Solve the second pressure correction equation (4.8.15) to obtain p''
- (vi) Correct the velocities and pressures using (4.8.11), to obtain the u_i^{N+1} and p^{N+1} fields

114 4: Solution procedure

- (vii) Calculate the cell face mass fluxes F_i^{N+1} from the u_i^{N+1} and p^{N+1} fields
- (viii) Solve the transport equation for the scalar product $r.w$, and obtain the swirl velocity w
- (ix) If the flow is turbulent, solve the predictor equations (4.8.16) for k^* and (4.8.17) for ϵ^*
- (x) Obtain μ_t^* from (4.8.18), and the corrected values k^{N+1} and ϵ^{N+1} from (4.8.23) and (4.8.24), respectively
- (xi) Calculate μ^{N+1} if the fluid is shear-thinning, based on the ϵ^{N+1} field. Calculate μ_t^{N+1} , based on the k^{N+1} and ϵ^{N+1} fields.
- (xii) Return to step (ii)

The sequence of steps (ii) to (xi) is repeated until the convergence criterion, to be defined below, is satisfied.

Convergence criterion for the iterative procedure

The residual at node P is defined as

$$R_P^N = \left| \sum_m A_m^N \phi_m^{N-1} + S_P^{2,N-1} - A_P^N \phi_P^{N-1} \right| \quad (4.9.1)$$

and the sum of the residuals over the solution domain is given by

$$SR_\phi = \sum R_P^N \quad (4.9.2)$$

where N represents the iteration level. This sum is calculated at each iteration, for each dependent variable, before the equation is solved. The sums SR_ϕ are then normalised by the appropriate ‘inlet’ fluxes SN_ϕ , given in table 4.1

$$r_\phi = \frac{SR_\phi}{SN_\phi} \quad (4.9.3)$$

It is then required that

$$\max(r_\phi) \leq \xi_{\text{norm}} \quad (4.9.4)$$

where ξ_{norm} is the maximum value of normalised residual sums consistent with sensibly invariant solution vectors (fields). The values of the dependent variables are also monitored at a particular grid point, in a region considered sensitive, to ensure that changes in them from iteration to iteration are negligible when convergence is declared.

	Equation	Normalisation quantity SN_ϕ
Pipe flow	Momentum	Momentum at inlet, $\rho \sum_{i=1,n} (u_i^{in})^2 A_i^{in}$
	Pressure correction	Volume flowrate at inlet, $\sum_{i=1,n} u_i^{in} A_i^{in}$
	Turbulence kinetic energy	Inlet flux of mean kinetic energy, $\bar{k} \rho \sum_{i=1,n} u_i^{in} A_i^{in}$, where $\bar{k} = (\bar{u}^{in})^2$
	Energy dissipation	Nominal inlet flux of dissipation rate, $\bar{\epsilon} \rho \sum_{i=1,n} u_i^{in} A_i^{in}$, where $\bar{\epsilon} = \bar{k}^{3/2} / l$, and $1/10$ of the pipe diameter is taken as the characteristic length scale l $n = \text{no. of cells in inlet plane}$
Mixing vessel flow	Momentum	Momentum at impeller blade tip, $\rho \sum_{i=1,n} (r_{tip} \omega)^2 A_i^{tip}$
	Pressure correction	Volume flowrate at impeller blade tip, $\sum_{i=1,n} r_{tip} \omega A_i^{tip}$
	Turbulence kinetic energy	Impeller blade tip flux of mean kinetic energy, $\bar{k} \rho \sum_{i=1,n} r_{tip} \omega A_i^{tip}$, where $\bar{k} = (r_{tip} \omega)^2$
	Energy dissipation	Nominal impeller blade tip flux of dissipation rate, $\bar{\epsilon} \rho \sum_{i=1,n} r_{tip} \omega A_i^{tip}$, where $\bar{\epsilon} = (r_{tip} \omega)^3 / l$, and the blade tip radius, r_{tip} , is taken as the characteristic length scale l $n = \text{no. of cells on impeller blade tip}$

Table 4.1 Quantities used to normalise residual sums

4.10 Solution algorithms for the individual equation sets

The number of algorithms available for the solution of the system of equations (4.3.11) is very large. While direct solution offers exact solution (to the degree of accuracy afforded by a digital computer) it is impractical for matrices of the size associated with grids of interest, certainly in three dimensions. Matrix inversion involves complete fill-in, necessitating storage of all elements, which is impractical; inversion is also computationally intensive. Furthermore, exact solution to an individual equation set is an excessive requirement in the context of an overall iterative procedure.

Iterative methods exploit matrix sparseness, thus minimising storage requirements. They also prove very much faster in achieving solutions to the level of

accuracy established through experience as being optimum in minimising overall computing effort. (The optimum level of accuracy proves to be a reduction in equation set imbalance to within 5 – 10 % of the initial value for the transport equations, and to within 1 – 5% for the pressure correction equations, for the type of problems of interest in this study.) Amongst the most widely-used iterative methods may be listed the ‘Alternating Direct Implicit (ADI) method of Peaceman and Rachford (1955) and the ‘Strongly Implicit Procedure (SIP) of Stone (1968). The method used here for the transport equations is a line-by-line counterpart of the Gauss-Seidel technique (which propagates boundary conditions across the domain at each iteration, rather than only one node per iteration as with the basic Gauss-Seidel technique). The grid lines are scanned along the axial, radial and circumferential directions successively, and along each line scanned, the equations are solved by the **Tri-Diagonal Matrix Algorithm (TDMA)** – see, for example, Householder (1964). Acceptable accuracy is achieved within a very few (often 1) iteration(s) for the problems of interest here.

The pressure correction equations, however, require a large number of iterations before convergence to a satisfactory level is achieved. This is emphasised by table 4.2 in which CPU time requirements for solution of the axial momentum and of the first pressure correction equation in the first ‘outer’ iteration, for the example of the (three-dimensional) mixing vessel flow, on three grids, relative to the requirement for the solution of the axial momentum equation on the coarsest of the grids, are listed. The ratio of the CPU time requirements for the solution of the former to that for the solution of the latter equation set is seen to be 32 on a 2,000-point grid, and this increases linearly with equation set size, to 127 and 386 on 16,000- and 87,000-point grids, respectively.

This ratio is a quantity of primary interest in selecting solution algorithms for the different equation sets. It is also instructive, however, to note the rate of increase of solution effort required with increasing grid size for a particular equation set; the CPU time requirement for solution of the pressure correction set increases as the increase in grid size to the power of 1.9 and 1.8 with an increase from a 2,000-point grid to 16,000- and 87,000-point grids, respectively. This rate of increase is a chief incentive for the development of higher-order differencing techniques, in order to obtain solutions of acceptable accuracy on the coarsest grids possible.

The **Conjugate Gradient (CG)** algorithm of Hestenes and Steifel (1952) has been adopted for the solution of the (symmetric) pressure correction equations in

Grid	Equation	CPU requirement
2,240	Axial momentum	1
	Pressure correction	31.7
15,903	Axial momentum	10.0
	Pressure correction	1,259
87,048	Axial momentum	58.9
	Pressure correction	22,708

Table 4.2 CPU time requirements, for the solution to a tolerance of initial/final residual ratio of 5%, of axial momentum and pressure correction equation sets, using the TDMA algorithm. Relative to requirement for axial momentum set on 2,240 point grid (=1)

this study.

The CG method is direct in the sense that if calculation is exact, the exact solution will be obtained in N iterations, though as Reid (1971) has pointed out it is not as such competitive with Gaussian elimination. With the finite precision arithmetic of a digital computer the finite termination property no longer holds, and the solution obtainable to machine precision is obtainable only after, at best, a very large number of steps. Nevertheless, as Reid points out, as an iterative method it gives a sufficiently accurate approximation in many less than N iterations if the matrices are reasonably well-conditioned (eigenvalues clustered around a small number of distinct values). A further advantage is that no *a priori* parameter estimates are required. There is opinion, *eg.* that of Jackson and Robinson (1985) that CG and related methods may be the best algorithms currently available for general problems, particularly those arising from finite difference discretisation in three dimensions, provided that they are used in conjunction with procedures to improve the conditioning of the coefficient matrices if ill-conditioned (eigenvalues distributed over a wide range), as are the pressure correction equation sets. The preconditioning used here to transform the system of equations into a form for which a conjugate gradient method 'converges' faster – one in which the eigenvalues are clustered – is Incomplete Cholesky (IC) factorisation. The details of the CG method and of IC factorisation are given in Appendix H.

Table 4.3 quantifies the relative performances of the CG and TDMA methods in the solution of the first pressure correction equation in the first outer iteration, on the same grids used in the momentum/pressure correction solution comparison.

Grid	Algorithm	Tolerance	CPU requirement
2,240	CG	5%	1
		1%	1.17
	TDMA	5%	3.95
		1%	10.42
15,903	CG	5%	14.19
		1%	17.44
	TDMA	5%	156.9
		1%	354.6
87,048	CG	5%	131.2
		1%	160.4
	TDMA	5%	2,830
		1%	6,150

Table 4.3 CPU time requirements, solution of pressure correction equation sets to initial/final residual ratios of 1% and 5%, using the CG and TDMA algorithms. Relative to CG algorithm requirement on 2,240-point grid to 5% tolerance (=1)

It is apparent that the CG algorithm reduces the computing effort by a factor of 4 on the coarsest grid, by a factor of 11 on the intermediate grid and by a factor of 22 on the finest, solving to the final/initial residual ratio of 5%. The relative advantage of the CG method increases still further as the convergence tolerance requirement is tightened to the 1% of initial residual level, since only a marginal extra computing effort is required (factors of 1.17, 1.23 and 1.22 on the three grids), whereas with the TDMA method tightening the convergence criterion from the 5% to 1% levels more than doubles the required CPU time (factors of 2.63, 2.26 and 2.17 on the 2,000-, 16,000- and 87,000-point grids, respectively). Iteration histories using the two algorithms on the 2,000- and 16,000-point grids are presented in figure 4.10; while convergence to a residual ratio of $\sim 20\%$ is achieved in approximately the same number of iterations with each method, a rapid fall-off in the rate of residual reduction per decade of iterations in the TDMA solution as residual ratios are reduced below this level contrasts sharply with the consistent rate of convergence of the CG method.

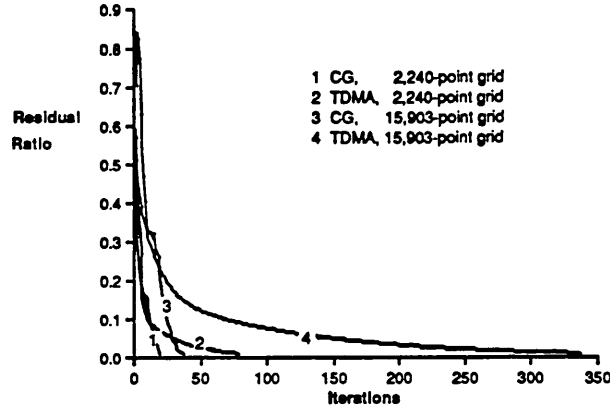


Figure 4.10 Iteration history, solution of pressure correction equation sets to initial/final residual ratios of 1%, using the CG and TDMA algorithms

4.11 Closure

In this chapter, the numerical methodology for the solution of the coupled partial differential equation set describing the flows of interest has been presented.

The equations are discretised using the finite volume method. A novel form of central differencing is employed in the discretisation of the convection terms of the transport equations which ensures boundedness while offering second-order accuracy. An explicit implementation *ie.* deferred flux correction is employed, with the degree of deferral limited by updating the correction after each iteration of the TDMA solution method employed for the sets of transport equations.

The PISO algorithm is employed in the solution of the coupled equations.

It has been shown that the ratio of the computing effort in the solution of a representative transport equation set and a pressure correction set rises linearly from 32 on a 2,000-point grid to 386 on an 87,000-point grid. The conjugate gradient algorithm is employed in the solution of the pressure correction equation sets in view of this discrepancy; the reduction in computing effort occasioned by its use, by comparison with the use of the TDMA algorithm, has been quantified as a factor of > 20 on an 87,000 point grid. It has also been shown that the increase in computing effort associated with obtaining a solution to an final/initial ratio of 1% as opposed to a ratio of 5% is a factor of only ~ 1.2 using the conjugate algorithm, compared to a factor of > 2 using the TDMA algorithm.

5 Flow predictions with SFCD

5.1 Introduction

Predictions of flows of a Newtonian fluid (water) are presented in this chapter. The prediction of laminar flow considered in section 5.2 provides a vehicle for assessment of the SFCD scheme presented in section 4.5 in the absence of the uncertainties associated with turbulence modelling, the case of a pipe with a step contraction having been chosen for the availability of recent and comprehensive experimental data against which comparison is made. Predictions of the flow in the mixing vessel described in chapter 1 are considered in section 5.3, both for their intrinsic significance, having been made on a much finer grid than used in previous work and using SFCD, and as a reference in the analysis of flow of a shear-thinning fluid to follow in chapter 6. The performance of SFCD relative to that of UD is again assessed for this flow, in section 5.4, through detailed comparison of the predictions obtained with both schemes on several grids. The accuracy of the predictions is simultaneously assessed by comparison with experimental data. Section 5.5 summarises the findings.

Figures for this chapter are appended to the thesis.

5.2 Laminar Newtonian fluid flow, pipe with sudden contraction

The case of laminar flow of water in a pipe with a 3.5:1 step contraction, at $Re = 196$, is considered here; predictions on 4 computational grids using UD and SFCD in turn are compared and costed. The solution domain extends $1.3D$ upstream and downstream of the contraction, with a fully-developed axial velocity profile prescribed at inlet : Durst and Loy (1985), with whose LDA measurements the predictions are compared, observed the flow profile still to be that of a fully developed flow at $1.0D$ upstream of the contraction. All other boundary conditions were specified as in sections 4.7.1 and 4.7.4.

The 23×24 , 35×33 , 47×44 and 78×60 cell grids used are illustrated in figure 5.2.1. The flow field predicted on the finest of these meshes using SFCD is illustrated in figure 5.2.2.

No convergence problems were experienced in obtaining solutions with SFCD. The CPU times taken to reach convergence for the various cases, relative to that

Grid	UD	SFCD
23×24 (=552)	1	1.1
35×33 (=1155)	4.8	7.8
47×44 (=2068)	34.7	37.9
78×60 (=4680)	59.7	95.9

Table 5.1 Comparison of CPU time requirements using SFCD and UD, case of laminar flow through a step contraction. Relative to requirement for 23×24 grid with UD

taken on the coarsest grid using UD, are listed in table 5.1. The same solution parameters (under-relaxation factors, individual equation set convergence criteria and the overall convergence criterion) were employed in all cases.

Velocity profiles at three locations, 0.039D upstream, and 0.052D and 0.209D downstream, are presented as figures 5.2.3, 5.2.4 and 5.2.5, respectively. There appears to be a systematic error in the experimental data, as the comparison is made on a normalised basis and the fulfillment of the continuity criterion is inherent in the computational methodology (this error has also been noted by Perić (1985) in comparing results obtained on orthogonal and non-orthogonal grids with this data). The important comparison here, however, is between the UD and SFCD predictions, and solution accuracy is judged with respect to the SFCD result on the finest grid; the measurements serve as a reference for the distributions.

At 0.039D upstream the SFCD predictions are seen to be indistinguishable at $r < 0.5R$ and $r > 0.7R$, figure 5.2.3a, while discrepancies between the result on the 23×24 grid and the remainder using UD are identifiable across the full radius, figure 5.2.3b. At 0.052D downstream it is again apparent that a result considerably closer to that on the finest grid is obtained on the coarse grids with SFCD (figure 5.2.4a) than with UD (figure 5.2.4b). In particular it may be noted from figure 5.2.4c that the velocity peak resulting from incomplete momentum redistribution is already resolved on the 23×24 grid using SFCD, whereas using UD the first indication of its existence is on the 78×60 grid, and its magnitude is very much underpredicted. Figure 5.2.5 repeats the pattern of predictions with the various grids being in much closer agreement using SFCD than UD; the 23×24 grid SFCD prediction is in close agreement with the 78×60 grid UD result.

In both the planes for which comparisons are presented and elsewhere, the 35×33 grid prediction is of comparable or better (in the vicinity of the contraction)

accuracy than the 78×60 grid UD prediction; at locations removed from the contraction this is also true of the 23×24 grid SFCD result, with attendant CPU time savings of the order of a factor of 10 to 50. While it must be borne in mind that all quantification of relative performance is case-dependant, the conclusion that SFCD is cost-effective is reinforced by the reduction in storage requirements of a factor of 4 to 8.

5.3 Analysis of predictions, Newtonian fluid flow, mixing vessel

Predictions of mixing vessel flow are considered here. The details of the vessel configuration and of the computation are given in section 5.3.1. Analysis of the flow predictions proceeds from consideration of the mean flow patterns in successive vertical and horizontal planes in sections 5.3.2 and 5.3.3 respectively, to examination of turbulence energy and dissipation rate distribution in section 5.3.4, of the turbulence time and length scales, as quantities of significance for macro-scale mixing, in section 5.3.5, and of the Kolmogorov time scale distribution, as the principal quantity governing micro-scale mixing, in section 5.3.6.

5.3.1 Case details

The vessel configuration is that for which detailed flow measurements (Yianneskis, 1982, 1984) are available, and consists of a flat-bottomed cylinder with four equally-spaced wall-mounted baffles extending from bottom to liquid surface. The blade Rushton turbine impeller extends from $r = 0.166R$ to $0.333R$ (outer edge), where R is the vessel radius; the impeller disc is located at $x = 0.333H$, and the blades extend from $x = 0.299H$ to $0.367H$, where H is the height of the fluid free surface above the bottom. The details of the geometry of the vessel employed by Yianneskis are illustrated by figure 5.3.1; for the predictions the impeller was approximated in the manner described in sections 3.10.2 and 4.7.2. Fixed features were represented exactly – this was one of the considerations in devising the grids employed, the others being the the necessity for concentration in regions of large changes in gradients and the (contradictory) requirement of ratios of successive inter-nodal distances as close to unity as possible to avoid amplification of truncation errors.

The predictions presented in this section were obtained on a $62 \times 39 \times 36 = 87,048$ point grid, as depicted in figure 5.3.2. As will be shown later, these results are close to being grid-independent.

In obtaining predictions on a grid of 15,903 points (which will be considered in comparison with these predictions in section 5.4) it was found that the use of SFCD for all transport equations *ie.* including the k and ϵ equations, resulted in unboundedness *ie.* negative values of k and ϵ , at a small number of grid points in the early solution iterations. This problem rapidly corrected itself, and did not reappear; the overall rate of convergence was not affected. Owing to the fact that the time constraints of this study did not permit more than one solution on the 87,000 point grid to be obtained, however, it was decided to employ SFCD for the momentum equations only. This decision was partly conditioned by the fact that differences between solutions obtained on the 15,903 point using SFCD for the momentum equations only and those obtained using SFCD on all transport equations were found to be negligible – this result is not unexpected as the k and ϵ equations are source-term-dominated and as such the form of differencing employed for the convection and diffusion terms would not be anticipated to greatly affect the outcome. Thus the conclusion is that while SFCD has been used here for the momentum equations only in order to avoid potential unboundedness problems and associated difficulties of stability, the predictions to be considered would be negligibly different had it been employed on all equations.

It did not prove possible to obtain solution convergence, within the time available, to the tolerance criterion (4.9.4), where ξ_{norm} was specified as 10^{-3} (this being the value employed for coarser grid runs, to be considered later, and found to ensure sensible iteration-to-iteration field value invariance). For the solutions presented here r_ϕ , defined by (4.9.3), was reduced to a value of 4×10^{-3} for the axial momentum equation set, $< 1 \times 10^{-3}$ for the other equation sets. This corresponds to a per-decade-of-residual change, averaged over the final five decades performed, of 0.1% in the most sensitive velocity component value at the most sensitive of four monitoring point locations, and of 0.4% in the values of pressure and turbulence kinetic energy at the same location.

While time constraints did not permit a solution on the 87,000 point grid using UD to be obtained, several hundred iterations of such a solution were performed, and very similar rates of convergence (and CPU time required per iteration) to the values for the case using SFCD were observed. Thus it is considered that the employment of SFCD was not responsible for the difficulty encountered in

obtaining convergence to the level achievable on coarser grids; rather the likeliest cause is considered to be the cyclic boundary conditions.

5.3.2 Flow patterns in vertical ($x - r$) planes

The principal flow patterns have been well established in the literature – experimentally by Yianneskis (1987) and computationally by Politis (1989): a radial impeller jet and two toroidal vortices, one each above and below the jet. The jet has a slight upward tilt due to the location of the impeller nearer the vessel bottom than the liquid surface; the lower vortex is the stronger for the same reason. This presentation serves, through the detail and accuracy obtained from grid refinement and higher-order differencing, to document the flow pattern more fully and quantitatively.

Velocity vectors in successive planes are presented in figure 5.3.3, axial and radial velocity profiles in figures 5.3.4 and 5.3.5, respectively, and the complementary isobars in figure 5.3.6. It should be noted that throughout this and the following chapter the circumferential location θ is measured with respect to the plane midway between successive baffles; thus the baffle in the quadrant taken as the domain of interest is located in the plane $\theta = 45^\circ$.

The impeller jet

As expected, the impeller jet is inclined slightly upwards, upon leaving the blade edge, in all planes. The degree of inclination is greatest in the plane midway between the baffles – this is illustrated by figure 5.3.3a, in which only every third vector in the radial direction in the jet is plotted for greater clarity. It is also noted that the point of impingement on the vessel wall shifts downward as the baffle is approached, from $x \approx 0.352H$ at $\theta = 1.5^\circ$ to $x \approx 0.337H$ at $\theta = 44^\circ$ – in this context note also the shift from an asymmetric (relative to the plane of the impeller disc) to a symmetric distribution of positive static pressure on the wall from plane $\theta = 1.5^\circ$ to plane $\theta = 44^\circ$ – figures 5.3.6a and 5.3.6f, respectively. The radial velocity profiles indicate little circumferential variation in jet strength, with the exception of somewhat higher velocities outboard of the baffle edge from the baffle plane to $\sim 0^\circ - 25^\circ$ downstream of the baffle, and an associated sensible circumferential invariance in jet width.

The below-impeller region

The toroidal vortex, which is the predominant flow feature in this part of the vessel,

has an elliptical cross-section in the inter-baffle region, centred at $x \approx 0.182H$ and $r \approx 0.800R$ at $\theta = 1.5^\circ$, changing to a circular cross-section with an associated upward and inward shift at $\theta = 25.5^\circ$, centred now at $x \approx 0.233H$ and $r \approx 0.721R$, followed by a downward and further inward shift as the baffle itself is approached – centred at $x \approx 0.177H$ and $r \approx 0.653R$ at $\theta = 44^\circ$. Downstream of the baffle outward return and recovery of elliptical cross-section is more rapid than upstream loss of these characteristics, with centre locations of $x \approx 0.167H$ and $r \approx 0.800R$ at $\theta = 58^\circ$ and $x \approx 0.162H$ and $r \approx 0.800R$ at $\theta = 70.5^\circ$.

The wall jet, the shape of which is best appreciated from the axial velocity profiles, figure 5.3.4, is virtually constant in width, at $0.2R$, from $\theta = 58^\circ$ to $\theta = 13.5^\circ$, but broadens and flattens significantly upstream of the baffle, reflecting the very much enlarged region of positive and therefore driving static pressure in the region encompassing the impeller jet/baffle/wall intersection – figure 5.3.6 – which augmentation is in turn due to the impingement of the swirling flow on the baffle face. This linkage between the swirling flow and the wall jet serves to emphasise that while the analysis is of necessity conducted on a plane-by-plane basis, the flow is truly three-dimensional. That the velocity components are not independent quantities but three parts, one whole must always be borne in mind, particularly in consideration of comparison with experiment in section 5.4. Increased wall jet strength in the ‘pre-baffle’ region also manifests itself in markedly higher static pressure at the vessel bottom – figure 5.3.6 – and consequently in a stronger ‘floor’ jet, figure 5.3.5d, the augmented wall and floor jets being associated with the upward and inward shift of the vortex noted earlier.

The discontinuity in the gradient near the wall illustrated by the axial velocity profiles, figure 5.3.4, reflects the approximation of a continuous distribution by a finite number of piecewise linear intervals; the peaks are at the next-to-wall nodes and the gradients between these locations and the wall itself are those imposed by the use of (4.7.2) for the prescription of wall shear stress.

Circumferential variation in the magnitude of the positive on-axis pressure resulting from floor jet impingement is unremarkable – worthy of comment, however, is the conically vortical structure evident in the near-axis region in planes $\theta = 70.5^\circ$ to $\theta = 1.5^\circ$ and to which reference will again be made in considering the flow from the standpoint of the $r - \theta$ planes.

The above-impeller region

The upper toroidal vortex has an elliptical cross-section at all circumferential locations, the major axis of which has a slight outward tilt from $\theta = 70.5^\circ$ to $\theta = 13.5^\circ$, and centred at $x \approx 0.578H$ and $r \approx 0.810R$ at $\theta = 1.5^\circ$. A pronounced inward tilt is observable immediately upstream and downstream of the baffle (major axis at $\sim 35^\circ$ to the vessel axis) – the strengthening of the vortex here being associated with an inward and downward shift: $x \approx 0.483H$ and $r \approx 0.789R$ at $\theta = 25.5^\circ$ and $x \approx 0.456H$ and $r \approx 0.707R$ at $\theta = 44^\circ$. As with all other quantities characterising the flow, downstream recovery is slower than upstream loss of inter-baffle flow pattern – the vortex is centred at $x \approx 0.564H$ and $r \approx 0.810R$ at $\theta = 58^\circ$, but has the same location on reaching $\theta = 70.5^\circ$ as at $\theta = 1.5^\circ$.

The axial velocity profiles, figure 5.3.4, demonstrate that the upper wall jet also has a width of $0.2R$, or equal to that of the baffle, to a height $x \approx 0.7H$, between the planes $\theta = 58^\circ$ and 25.5° , the slight decrease of width with height reflecting the not-quite-vertical orientation of the vortex axis. The pronounced broadening of the jet immediately upstream of the baffle again results from deflection of swirl and the associated rise in pressure at the baffle/wall/jet intersection. Notable also is the greatly diminished jet strength in the upper third of the vessel downstream of the baffle, with virtually no axial flow near the surface and at $r > 0.8R$ at $\theta = 58^\circ$ – figure 5.3.4f. Of potentially greater practical significance is the downflow across most of the vessel radius just below the liquid surface, midway between the baffles, identifiable in figures 5.3.3h and 5.3.3i, which is markedly different from the parallel-to-surface flow from $\theta = 13.5^\circ$ to 58° . The vortical structure suggested by figures 5.3.3h and 5.3.3i will be confirmed through examination of $r - \theta$ plane velocity vectors; of interest is the indication of surface troughing away from the baffles (one of the functions of which is to inhibit the phenomenon) which is associated with air entrainment, to be avoided in many processes. The suggestion of a tendency to troughing (albeit slight) is despite the imposition of a zero-axial-velocity boundary condition at the free surface *ie.* the assumption of a level surface.

5.3.3 Flow patterns in horizontal ($r - \theta$) planes

Velocity vectors, in planes identified in terms of proportion of overall liquid free surface height H , are presented in figure 5.3.7, and swirl velocity profiles in figure 5.3.8. Several representative plots of pressure distribution are included as figure

5.3.9. The direction of impeller rotation is counter-clockwise.

The below-impeller region

At $x = 0.054H$ the flow is nearly everywhere directed inward, with the exception of the vortex centred at $r \approx 0.33R$ and $\theta \approx 70^\circ$, the presence of which was alluded to earlier in consideration of figure 5.3.3. This counter-rotation is accompanied by evidence of a developing co-rotation in its wake, which has come to dominate the former structure on reaching the level $x = 0.105H$, centred at $r \approx 0.42R$ and $\theta \approx 80^\circ$ – figure 5.3.7. The latter structure is still evident at $x = 0.146H$, shifted slightly further downstream. Noteworthy here is the strength of the swirl flow at $r \approx 0.8R$ in the $\theta \approx 60^\circ$ to $\theta \approx 70^\circ$ segment, this being just below the vortex centre as noted in consideration of the $x - r$ planes; the toroidal nature of the vortex is thus emphasised. The planes of negligible radial flow at the next level of flow depiction, $x = 0.187H$, are midway between the baffles and immediately upstream of the baffle, corresponding to the vortex centre, which, it will be recalled, was earlier identified as being at approximately this height at $\theta \approx 1.5^\circ$ and at $\theta \approx 44^\circ$.

The approach to a purely radial flow downstream of the baffle under the influence of the impeller jet is evident at $x = 0.248H$ and $0.289H$ (the plane of the impeller disc is at $x = 0.333H$) – this is emphasised by the swirl velocity profiles, figure 5.3.8, in which the maintainance of a greater proportion of the impeller swirl with increasing radial distance upstream of the baffle is also noteworthy. This radial flow is sufficiently strong to suppress recirculation on the upstream of the baffle at $x = 0.289H$; while the decrease in radial velocities with progress down the face permits recirculation ($x = 0.187H$) it is indicative not of separation but of conversion of primary flow direction to the axial (recall the broadening of the wall jet indicated by the axial profiles in figure 5.3.4).

On the downstream face of the baffle a helical vortex has already formed at $x = 0.289H$, and may be identified, if much weakened, down to $x = 0.105H$, (the counter-rotation at this level is more clearly seen from the velocity profile, figure 5.3.8). A slight downstream shift in the locus of the vortex centre as it progresses downward is attributed to wall jet impingement on the wall/baffle/jet intersection. Again the maintainance of flow attachment is due solely to the strength of the axial flow, as is indeed the case on the vessel wall both immediately upstream and downstream of the baffle.

The above-impeller region

A consistent feature of the predicted flow above the impeller is the considerably

greater strength of swirl upstream of the baffle than down, at $r > 0.3R$ and $x < 0.7H$ – most evident from the swirl velocity profiles, figure 5.3.8. The strength of the vortex on the downstream face of the baffle which is largely responsible for this difference is best gauged from the pressure contours at $x = 0.442H$ – figure 5.3.9c. It will be noted that the negative pressure associated with this vortex is higher than that associated with the upper toroidal vortex. From $\theta \approx 49^\circ$ and $r \approx 0.88R$ at $x = 0.442H$ the vortex centre is shifted inward and downstream to $\theta \approx 54^\circ$ and $r \approx 0.83R$ at $x = 0.551H$, the last plane in which a true vortex structure is identifiable. A small helical vortex on the upstream face of the baffle retains a vertical alignment from $x = 0.442H$ to $x = 0.714H$.

A strong co-rotational helical vortex associated with the downward flow is clearly identifiable at $x = 0.932H$, centred at $\theta \approx 83^\circ$ and $r \approx 0.76R$. Its centreline traces an inward and downstream locus through $\theta \approx 10^\circ$ and $r \approx 0.50R$ at $x = 0.714H$ to $\theta \approx 24^\circ$ and $r \approx 0.37R$ at $x = 0.551H$, below which it vanishes.

A second, counter-rotating, vortex may also be seen in the $x = 0.932H$ plane; this is absorbed into the wake of the counter-rotating vortex once the $x = 0.850H$ plane is reached.

Strong counter-rotation is illustrated by the swirl velocity profiles in the upper third of the vessel in the near-axis region; it is noted however that the boundary conditions adopted do not take account of the impeller shaft, which would have a suppressive effect on any such development.

5.3.4 Turbulence energy and dissipation rate distributions

In reactive mixing processes, the relationship between the reaction rate and the mixing rate is crucial in determining whether homogeneity of reactants is maintained, for process efficiency, or whether segregation, with its attendant low product yield, occurs – see, for instance, Oldshue (1983). Processes with rapid kinetics require the very much higher mixing rates associated with turbulent, rather than molecular, diffusion. The requirement of high given levels of shear, associated with turbulence, in many multi-phase processes *eg.* the enhancement of droplet breakup/inhibition of coalescence, the maintenance of equilibrium in liquid/liquid dispersions etc. is a further indication of the significance of turbulence levels in their own right as a qualitative indicator of mixer performance.

The dissipation rate is required in the estimation of the characteristic scales of the macro and micro scales of turbulence, to be considered presently; it is also

of interest in estimating impeller power requirements.

Both turbulence energy and dissipation rate are here presented in normalised form, $\tilde{k}$ and $\tilde{\epsilon}$. The normalising quantities are $1/2(\omega r_{\text{imp}})^2$ and $1/2\omega(\omega r_{\text{imp}})^2$, respectively, corresponding to values of 0.03 (m/s)^2 and $0.15 \text{ m}^2/\text{s}^3$. It will be remembered (section 3.10.2) that turbulence energy levels and dissipation rates are imposed in the blade swept volume; these correspond to values of $\tilde{k}$ and $\tilde{\epsilon}$ on the blade tip, in the plane of the disc, of 11.85 and 115.4, respectively. Presentation of distributions is primarily in $x - r$ planes, figures 5.3.10 for $\tilde{k}$ and 5.3.11 for $\tilde{\epsilon}$, with distributions in a small number of $r - \theta$ planes as figure 5.3.12 for $\tilde{k}$ and 5.3.13 for $\tilde{\epsilon}$. Note should be taken of the piecewise linear (contours A-C, then D-G) interval scale chosen to illustrate the $\tilde{k}$ distribution, and the pseudo-logarithmic scale chosen to illustrate the $\tilde{\epsilon}$ distribution.

That the highest levels of turbulence kinetic energy should be associated with the source of energy input to the vessel is unsurprising; levels in the impeller jet as a whole are an order of magnitude higher than in the remainder of the vessel. The local Reynolds number of turbulence

$$Re_t = \nu k^{0.5} \frac{k^{1.5}}{\epsilon} = \frac{\nu k^2}{\epsilon} \quad (5.3.1)$$

is of the order of 3×10^3 in the jet, and of the order of 1×10^3 elsewhere in the vessel. (Since Re_t may alternatively be expressed as

$$Re_t = \frac{1}{C_\mu} \frac{\mu_t}{\mu} \quad (5.3.2)$$

it is seen to be a direct measure of the relative importance of turbulent and molecular diffusion.) Radial gradients in $\tilde{k}$ in the jet are little changed from one circumferential location to the next, with the exception of the vicinity of the baffle, where gradients are substantially higher from a radius of $\sim 0.6R$ outward. This is attributed not to higher dissipation rates arising from baffle proximity but to very much lower local generation (that local dissipation rates are actually lower on the downstream face of the baffle may be seen from the $r - \theta$ plane $\tilde{\epsilon}$ distributions, figure 5.3.13).

Much the steepest gradients in $\tilde{k}$ are those across the jet periphery – the very high production associated with these thin shear layers is dissipated locally due to the weakness of cross-stream transport.

The highest levels of $\tilde{k}$ elsewhere in the vessel are associated with the vortices. Strain rates are relatively high and the associated generation is sufficient to maintain turbulence levels away from the suppressive influence of the vessel wall and

baffle. That local production and dissipation rather than convection of impeller jet turbulence energy by the wall jet govern these levels is borne out by the very different distributions at 42° and 44° – the correspondence of the lowest-energy contour with the face of the baffle in the latter plane is complete. The broadened and strengthened wall jet convects little energy – the sink-dominated nature of the k transport equation in these and the 47.5° and 49° planes is clear.

Locally-high levels of turbulence are in all planes predicted in the downflow region immediately above the impeller and on the peripheries of the upflow midway between the vessel bottom and the impeller; these again are due to locally-high strain rate/moderate dissipation rate ratios.

The $r - \theta$ plots of figure 5.3.12 serve to clarify that in areas removed from the impeller jet the peak values of $\tilde{k}$ are associated with the regions of highest strain rate removed from solid boundaries *viz.* the toroidal vortices and particularly their peripheries, while levels on the downstream face of the baffle are even lower than in the regions of ‘lazy flow’ near the surface.

The correspondence of the $\tilde{\epsilon}$ distribution to that of $\tilde{k}$ reflects the strong coupling of their transport equations and the degree of source domination thereof. Thus a logarithmic rate of decay from peak values at the blade tip is observed in the impeller jet; a reduction in gradients in the impingement zone immediately upstream and downstream of the baffle mirrors rather than directly corresponds to the $\tilde{k}$ distribution in this zone but local maxima elsewhere in the vessel are co-located with those of $\tilde{k}$.

The $r - \theta$ plots, figure 5.3.13, serve to re-emphasise the correspondence between $\tilde{k}$ and $\tilde{\epsilon}$ – it is interesting to note that predicted levels of the latter are even higher between the toroidal vortex and the wall than on the wall itself.

5.3.5 Turbulence length and time scale distributions

The significance of the larger scales of turbulence in various processes is discussed by Oldshue (1983); apart from the breakup and coalescence phenomena alluded to in the previous section, mechanisms which are governed wholly or in part by macro-scale parameters include fermentation with biological solids, particle size and degradation in emulsions, particularly where the particles are friable and do not coalesce, and many polymerisation processes.

Before proceeding further in consideration of this and the other turbulence parameters, it is perhaps worth emphasising that they offer only qualitative guid-

ance to the efficacy of mixing and reaction processes in a sense completely independent of uncertainties as to the accuracy of the primary quantities used in their calculation. The random nature of turbulence implies that fields are more truly characterised by spectra than by individual values, and the ultimate goal must therefore not be establishment of these values with certainty but their resubstitution by probability distributions. (It is interesting to note in this context attempts to solve transport equations for length scales at a number of scales of turbulence in the course of turbulent flow prediction; Launder (1984a) summarises these efforts.)

Making a virtue of present necessity, it is noted that understanding, and thus modelling, of secondary processes (breakup & coalescence, mixing & reaction rates etc.) is as yet in terms of characteristic quantities. Recalling then that $k^{3/2}/\epsilon$ has the dimensions of a length scale, the particular form

$$L = C_\mu^{3/4} \frac{k^{3/2}}{\epsilon} \quad (5.3.3)$$

is adopted here since it reduces to the Prandtl mixing length κy in the logarithmic region of a boundary layer (it is shown in appendix G that

$$\epsilon = \frac{C_\mu^{1/2} k u_*}{\kappa y} \quad (G.11)$$

where

$$u_* = k^{1/2} C_\mu^{1/4} \quad (G.7)$$

in the logarithmic region).

Hinze (1975) notes that it is not the largest eddies which contain the maximum turbulence kinetic energy but those in a somewhat higher wavenumber range; he further states that it is reasonable to assume that the Eulerian longitudinal integral length scale Λ_f , which is determined mainly by the size of the larger energy-containing eddies (being a measure of the longest connection, or correlation distance between the velocities at two points in the flow field), is of the same order as the size of these eddies. Hinze (1975) demonstrates that the ratio Λ_f/L is in the range $\sim 1-3$, but with a probable value in the range 1.94-2.19, for isotropic turbulence.* Thus the distributions presented here are of a length scale approx-

* Hinze does not consider Λ_f/L *per se* but rather Λ_f/Λ_L , where Λ_L is the Lagrangian integral time scale. The latter he writes, however, in terms of the former (pp. 397-398) viz. $\Lambda_L = (2/C)(u'^3/\epsilon)$, where $C = (1.36/\alpha)(\Lambda_f/\Lambda_L)$ i.e. $\Lambda_f = (0.68/\alpha)(u'^3/\epsilon)$, which may be related to $L (= C_\mu^{3/4} u'^3/\epsilon)$. The value of the Heisenberg exchange coefficient α must be calculated from experiment and values in the range 0.2-0.6 are quoted by various workers (as summarised by Hinze), with a most plausible value (in terms of theoretical expectation) of 0.4-0.45 for isotropic turbulence.

imately half that characteristic of the energy-containing eddies, an insignificant factor in terms of the orders-of-magnitude range of the spectrum of length scales.

As the ratio $\tau = k/\epsilon$ has the dimensions of time it is the quantity presented here as characteristic of energy-containing-eddy lifetimes *ie.* the time required for the energy of these eddies to pass to the high-wavenumber (small) eddies. The Eulerian temporal correlation is defined in a manner analagous to the spatial correlation, *viz.*

$$T = \int_0^\infty R(t') dt \quad (5.3.4)$$

with the analagous interpretation of the longest non-negligible temporal correlation of the fluctuation $u'(t)$, *viz.*

$$R(t') = \frac{\overline{u'(t)u'(t+t')}}{\overline{u'^2}} \quad (5.3.5)$$

– see, for example, Hinze (1975). While it is difficult to establish a relationship between τ and T to the same level of precision as that between L and Λ_L , Watkins (1977) demonstrates that τ and T are of the same order of magnitude.

The length scales are presented on a normalised basis, $\tilde{L}$, with the impeller radius r_{imp} ($= 0.049\text{m}$) as the normalising quantity *ie.* $\tilde{L} = L/r_{\text{imp}}$. The distribution contours are presented in $x - r$ planes as figure 5.3.14 and in $r - \theta$ planes as 5.3.15; the smaller contour intervals at the lower end of the scale in the $x - r$ plane figures should be noted. $\tilde{L}$ is seen to range in value from $\sim 0.025 - 0.2$, with close correspondence between minimum values and the thin shear layers on the upper and lower faces of the impeller jet and on the wall, bottom and baffle faces, as expected.

Length scale growth from the high-turbulence impeller tip zone to the radius of the baffle edge is consistent with the growth in width of the jet in inter-baffle planes (a factor of ~ 2) but at $\theta = 44^\circ$ the baffle is seen to inhibit this growth to the extent that little variation in the scale is evident over the full radial extent of the jet in this plane.

The somewhat greater sizes in the region above the impeller by comparison with those in the region below are attributable partly to the greater overall dimensions of the former and partly to the absence of a shear layer on the surface comparable to that on the vessel bottom; again, while the scales are (apparently paradoxically in a region of relatively high Re_t) largest above and inboard of the impeller tip, the physical plausibility of this is based on the absence of substantial mean velocity gradients to inhibit eddy growth.

The parallelism of the minimum value contours and the solid boundaries – most easily seen in the $r - \theta$ plane plots, figure 5.3.15 – simply reflects the proportional-to-distance-from-wall condition implicit in the wall functions. In considering the distributions in horizontal planes it is interesting to note the extent to which they reflect the flow patterns. Little circumferential variation in $\tilde{L}$ is apparent in planes of outward radial flow, at $x = 0.248H$ and $0.442H$ (flow patterns in figure 5.3.7), consistent with the imposition by near-wall shear layers of a maximum eddy size irrespective of the dimensions of those convected in, but substantial inward convection of the smaller scales is evident in planes of inward radial flow, at $x = 0.105H$ and $0.660H$; smaller eddies will of course be convected further. It is of course to be understood that such hypotheses are not incorporated in the turbulence model *per se* but are cited here to indicate the plausibility of the predictions obtained from its use.

Figures 5.3.16 and 5.3.17 present the time scales in $x - r$ and $r - \theta$ planes, respectively, on a normalised basis, $\tilde{\tau}$, with the inverse of the impeller blade frequency ($= 0.2sec$) as the normalising quantity. The smaller contour intervals at the lower end of the scale in the $x - r$ plane figures should be noted. $\tilde{\tau}$ is seen to range in value from $\sim 0.25 - 3.4$, with a minimum value of 0.1 on the blade tip, and this is comparable to the inverse of the blade frequency, since for a six-blade impeller $\tilde{\tau}_{blade} = 0.16\bar{6}$. The lifetime of energy-containing eddies may reasonably be expected to be of similar duration to that of blade-to-blade passage; while the impeller model does not explicitly calculate the effects of periodicity they are incorporated in the 90° -averaged turbulence kinetic energy values imposed along the blade edge.

The increase in the value of $\tilde{\tau}$ with increasing radial distance along the impeller jet reflects the increase in the value of $\tilde{L}$; the former increase, however, is of a factor of ~ 4.7 from blade tip to baffle tip while the latter is of a factor of ~ 1.8 over the same interval. The difference in distribution of the length and time scales in the impeller jet is worthy of remark: the former quantity is a stronger function of k , and hence of turbulence energy generation, the primary location of which is in shear layers, hence the concave contour pattern of its distribution as opposed to the convex contour pattern of that of the time scales. This is physically plausible: while length and time scales would be expected to move broadly in step (since larger eddies have longer lifetimes) locally high shear rates will limit eddy size while locally high dissipation rates (as in the jet core) will limit eddy lifetimes.

The steep gradients in $\tilde{\tau}$ on solid boundaries reflect those in $\tilde{L}$, as do the

locally-high values in the lower toroidal vortex and the upflow region near the bottom. The $r - \theta$ plane distributions are also qualitatively similar to those of $\tilde{L}$, with substantially greater circumferential gradients in the $40^\circ - 60^\circ$ zone at the $x = 0.105H$ and $0.660H$ levels than at the $x = 0.248H$ and $0.442H$ levels. More generally, the distributions in the horizontal planes emphasise that there is little circumferential variance outside the baffle zone, and indeed within it for some distance above and below the impeller jet *ie.* the latter has a considerable influence on characteristic scales of turbulence beyond the limits of its own extent. In areas removed from the jet the reduction in cross-sectional area occasioned by the baffle is mirrored by a reduction in $\tilde{\tau} - x = 0.105H$ and $0.660H$, figures 5.3.17a and 5.3.17d – plausibly in the sense that in the absence of other factors such a reduction in area would be expected to be accompanied by some reduction in macro-scale turbulence parameters.

5.3.6 Kolmogorov length and time scale distributions

The characteristic length scale of the Kolmogorov eddies, η , has been defined earlier in terms of quantities available from the computations:

$$\eta = \left(\frac{\mu^3}{\rho^3 \epsilon} \right)^{1/4} \quad (3.7.18)$$

The characteristic time scale, τ_k , is defined in terms of the same quantities as

$$\tau_k = \left(\frac{\mu}{\rho \epsilon} \right)^{1/2} \quad (5.3.6)$$

Both quantities are presented here in dimensional terms, as macro-scale parameters are inappropriate for the normalisation of micro-scale quantities, and there is no reason to expect these micro-scale quantities to be independent of bulk Reynolds number (in the fully turbulent regime) if so normalised, contrary to the case for the macro scales of turbulence.

The length scale distributions are presented in $x - r$ planes as figure 5.3.18, and they are seen to range in value from $\sim 2 - 9 \times 10^{-5}m$. The impeller tip value of η , in the plane of the disc, is $1.5 \times 10^{-5}m$, by comparison with a value of $1.2 \times 10^{-2}m$ for L at the same location, while the value of η obtaining over the greater part of the volume above the impeller, $\sim 9 \times 10^{-5}m$, compares with a value of L of $\sim 1 \times 10^{-2}m$ in the same region.

With μ invariant the distribution of η follows that of ϵ and thus of the macro-scale fields in general. Growth in eddy size with progress from blade tip to wall in the impeller jet is by a factor of ~ 2.4 , before rapid collapse at the wall itself. In contrast to the macro length scale of turbulence, values of η obtaining over the bulk of the below- and above-impeller regions are broadly similar *ie.* η does not display the dependence on vessel geometry exhibited by L . That the distribution is in this sense physically plausible is less a judgement regarding the predictions, as η is a derived rather than directly calculated quantity, but rather an at-least-partial vindication of the relationship (3.7.18).

Again, while the values of L characteristic of the above-impeller region change by a factor of $\sim 1.5 - 2.5$ between the 1.5° and 47.5° planes (figures 5.3.14a and 5.3.14c) little change in the magnitudes of η in the reduced area of the plane of the baffle is evident from the relevant figures, 5.3.18a and 5.3.18c. Nor are the lesser variations in η (by comparison with those in L) just enumerated explicable in terms of a smaller overall range of η values, as this is fully as great as that of the L values in all planes.

The range of τ_k is seen from the relevant figures, 5.3.19 and 5.3.20 for the $x - r$ and $r - \theta$ plane distributions, respectively, to be $\sim 4 \times 10^{-4} - 1.1 \times 10^{-2} \text{ sec}$, substantially greater than that of the other characteristic scales, at either the macro or micro levels. The distributions, however, mirror those of η , being again a function of the same variable, ϵ . The impeller blade tip value, in the plane of the disc, of $2.2 \times 10^{-4} \text{ sec}$, compares with a value of τ of $2 \times 10^{-2} \text{ sec}$; the impeller-blade-tip to baffle-blade-tip increase of a factor of ~ 5.8 is comparable with the factor of ~ 4.7 for τ . Some difference in the values of τ_k prevailing over the lower and upper regions of the vessel is evident, but the factor of < 1.5 is still very much less than the equivalent ratio for τ of > 3 *ie.* τ_k is seen to be also essentially independent of vessel bulk dimensions.

The $r - \theta$ plane distributions show that while circumferential gradients are greater at $x = 0.105H$ and $0.660H$ than at intermediate locations, as for L and τ , of more significance is the predicted degree of dissipative eddy lifetime growth in the baffle wake, both on the downstream face of the baffle itself immediately inboard of the baffle tip and in the region of reverse flow on the wall side of both the downward and upward baffle vortices. This growth in τ_k is of the order of 2 by comparison with neighbouring values, and contrasts with the pattern at the macro level – figure 5.3.17 – suggesting that while the baffles, used to achieve certain mean flow patterns, do not thereby inhibit macro-scale mixing in their

immediate vicinity (but rather promote it), they do suppress the rate at which micro-scale mixing may proceed.

5.4 Mixing vessel predictions: differencing scheme & experimental comparisons

5.4.1 Computational details

The predictions for the flow of water in the mixing vessel presented in the previous section are compared here with those obtained using UD and SFCD in turn, on grids of $31 \times 27 \times 19 = 15,903$ points and $44 \times 34 \times 26 = 38,896$ points – these grids are illustrated in figure 5.3.2. A simultaneous comparison of the 87,000 point SFCD predictions is made with the detailed LDA measurements of Yianneskis (1982, 1984).

From the viewpoint of mixing vessel flow prediction as a design tool the objectives here are determination of the degree of grid independence achieved, and by comparison with experimental data, assessment of the overall prediction accuracy and of the degree of error due to the turbulence modelling and boundary conditions in the hoped-for circumstance of relatively unimportant numerical error.

From the more general standpoint of methodologies for CFD the issue is the costeffectiveness of SFCD, again to be assessed in the terms of section 5.2 *ie.* the degree to which it facilitates grid independence on coarser grids than necessary using UD, and the relative computing effort required.

The relative CPU time requirements for solutions satisfying the tolerance criterion (4.9.4), where $\xi_{\text{norm}} = 1 \times 10^{-3}$, on three grids and using UD and SFCD in turn, are given in table 5.2. As meaningful comparison cannot be made with the CPU time requirement data for the 87,000 point SFCD case, since as indicated in section 5.3.1, it did not prove possible to obtain solution convergence to this tolerance for this case, the data is not included here. The CPU time requirements for calculations performed on a 2,240 point grid, the results of which have been omitted here for clarity, have thus been included to provide a basis of comparison for the finer grid runs.

The data provides some indication that the relative increase in CPU time requirements associated with the employment of SFCD decreases with grid refinement, and this result is not unexpected, as the degree of flux correction necessary should decrease as inter-nodal spacing is reduced. (Qualitative support for this

Grid	UD	SFCD
2,240	1	3.74
15,903	65.2	135
38,896	710	992

Table 5.2 Comparison of CPU time requirements using SFCD and UD, mixing vessel cases. Relative to requirement for 2,240 point grid with UD

statement is in the form of the result that the value of the ratio r in (4.5.1) is on average much lower, in the 0° plane, on the 87,000 point than on the 16,000 point grid).

The comparisons are presented for each of the velocity components and the turbulence energy level in turn, in sections 5.4.2 to 5.4.5, respectively.

5.4.2 Mean axial velocity comparisons

The predicted and measured mean axial velocities are presented as figures 5.4.1 to 5.4.8, plotted along radii and progressing from vessel axis to wall.

The below-impeller region

0° plane, figure 5.4.1

The improved resolution of gradients with grid refinement is apparent at all levels; the degree of numerical smearing associated with the 16,000 point grid prediction using UD is highlighted by the comparison with the 87,000 point grid prediction using SFCD. These observations apply to most of the comparisons of mean velocity predictions and are to be expected.

Encouraging, however, is the close identity of the 39,000 and 87,000 point predictions using SFCD, permitting the assertion that further grid refinement would have little effect on the prediction of this quantity at these locations. Furthermore the 16,000 point SFCD prediction identifies considerably more closely with the 87,000 point prediction than does the 16,000 point UD prediction, as does the 39,000 point SFCD prediction than the 39,000 point UD prediction. Indeed the 16,000 point SFCD prediction is in most respects closer than the 39,000 point UD prediction – note in particular the prediction of wall jet strength at $x = 0.170H$ and above.

In comparing the ‘grid-independent’ solution with the experimental data it

is apparent that qualitative agreement is good, with resolution of the positive gradient $\partial u/\partial r$ in the near-axis zone, and negative thereafter. The chief differences may be identified as a substantial overprediction of the near-axis upward flow at $x = 0.068H$, and underprediction of wall jet strength at the same level and of the upflow below and near the inner edge of the impeller blade, at $x = 0.282H$. It is noted that the measured wall jet velocity at $x = 0.068H$ is anomalously larger than those at the same height in the 22.5° and 67.5° planes, indeed larger than the (baffle-amplified) velocities in the 33.75° and 56.25° planes, and is thus open to question.

22.5° plane, figure 5.4.2

The coincidence between the 39,000 and 87,000 point SFCD predictions in the upflow zone does not hold across the wall jet region, and the change in values with grid refinement and/or higher-order differencing is not unidirectional, suggesting that discrepancies between coarser and finer grid predictions are not attributable solely to the larger truncation errors associated with the former but also to substantial changes in predictions of the other components with grid refinement. This hypothesis will receive further mention in the context of the mean swirl velocity comparisons.

The overall agreement with experiment is very good, with (smaller than previous) disparities in the wall jet near the bottom and immediately below the impeller.

33.75° plane, figure 5.4.3

While differences between the 39,000 and 87,000 point SFCD predictions are again clearly identifiable, their magnitude is considerably less than differences between these and the other predictions shown. The degree to which numerical diffusion reduces gradients is very evident from the 16,000 point UD prediction at $x = 0.068H$ and $x = 0.170H$. The superiority of the 16,000 point SFCD predictions to the 39,000 point UD predictions (where, as throughout these comparisons, it is emphasised that superiority is assessed by reference to the finest grid predictions and not by reference to the experimental measurements) is also noted.

Yianneskis' later (1984) measurements offer greater detail, in just the 33.75° and 56.25° planes. Comparison confirms the extremely good agreement at the intermediate levels in the previous planes, but also the underprediction of the jet strength at the $x = 0.068H$ level. The broadening of the jet at $x = 0.281H$ is also not predicted.

56.25° plane, figure 5.4.4

Once more many of the discrepancies between the 39,000 and 87,000 point SFCD predictions contradict the trend of the discrepancies between these and the coarser grid predictions, and explanation must await consideration of profile comparisons of the other mean velocity components. Attention is, however, drawn to the superior gradient resolution on the 16,000 point grid with SFCD to that on the 39,000 point grid with UD in this plane also.

While the upflow in this plane is underpredicted over most of its extent, overprediction is evident approaching the impeller disc ($x = 0.281H$). The strength of the wall jet is overpredicted at its origin ($x = 0.281H$), but satisfactorily resolved further down the vessel.

67.5° plane, figure 5.4.5

Differences between the 39,000 and 87,000 point SFCD predictions are quantitative rather than qualitative, confined to the upflow region and in the main of much less consequence than differences between these and coarser grid predictions. The reversal of trends in differences between predictions when the fine grid results are considered is again in evidence; this is also counterbalanced by the superiority of the 16,000 point SFCD prediction to the 39,000 point prediction.

*The above-impeller region**0° plane, figure 5.4.6*

The prediction is grid-independent for the $x = 0.544H$ plane, with differences between the 39,000 and 87,000 point SFCD predictions at the higher levels again smaller than those between these results and the rest. No uniform trend to final values is evident with grid refinement/higher-order differencing, however, indicating even greater sensitivity in this region of the predictions of (smaller) axial velocities to changes in the values of other components with changes in grid/differencing scheme.

The agreement with experiment is again satisfactory to $x = 0.680H$, and is poor only in the overprediction of near-axis downflow at $x = 0.861H$ and of the (very weak) wall jet at $x = 0.884H$.

22.5° plane, figure 5.4.7

The coincidence of the 39,000 and 87,000 point SFCD predictions at all levels is quite remarkable; these are also distinctly different from the 39,000 point UD

predictions. This again is strong evidence of the potential for higher-order differencing schemes to produce grid-independent solutions on considerably coarser grids than first-order schemes.

At the lower levels agreement with experiment is satisfactory, particularly given the sparseness of the data; higher up the underprediction of the wall jet is the least satisfactory of all the axial velocity predictions.

67.5° plane, figure 5.4.8

In this plane also it may be asserted that grid independence has been achieved, and the differences between the coincident 39,000 and 87,000 point SFCD predictions and the 39,000 point UD prediction are marked.

Agreement with experiment is extremely good across the full vessel radius at the lower levels. There is substantial overprediction of downflow strength, and underprediction of wall jet strength and width, at $x = 0.884H$ – this cannot, however, be viewed in isolation from the predictions for radial and swirl velocity at these locations – figures 5.4.18 and 5.4.28. Both quantities are underestimated in the downflow region in particular, indicating that the error in prediction noted here is as much one of velocity direction as magnitude.

5.4.3 Mean radial velocity comparisons

The predicted and measured mean radial velocities are plotted in the vertical direction and progressing upward, from the vessel bottom to the impeller region – figures 5.4.9 to 5.4.14, and from the impeller region to the free surface – figures 5.4.15 to 5.4.18. (The axial distance indicated on the co-ordinate is in all cases measured from the vessel bottom; and it will be recalled that the impeller disc is located at $x = 0.333H$.) Note that the plotting range reflects that over which measurements were available at each radial location and is therefore not the same in all cases.

The below-impeller region

0° plane, figure 5.4.9

A greater degree of grid sensitivity for the radial than for the axial velocities is evident at most radial locations in this plane. While the predictions of the 39,000 and 87,000 point SFCD cases exhibit differences which are non-negligible by comparison with those coarser grid predictions, the former do however indicate

qualitative self-similarity and dissimilarity with the latter – particularly from $r = 0.340R$ outward. The 39,000 point SFCD prediction is consistently superior to the UD prediction on the same grid, and where differences between the 16,000 point SFCD and 39,000 point UD predictions are discernible, the former are also generally superior – $r = 0.051R$ and $r = 0.510R$ outward. The greater grid sensitivity of the predictions to $r = 0.646R$ is consistent with the sensitivity of the axial velocity predictions in the upflow region compared to the wall jet region, figure 5.4.1.

Comparison with experiment shows that gradients are particularly well predicted, as is the point of crossover from inward- to outward-directed flow. This latter indicates that the axial location of the vortex centre is at least approximately correctly located. The peak velocity at $r = 0.748R$ is underpredicted by $\sim 8\%$; the prediction of jet asymmetry i.e. the location of the peak above the plane of the impeller disc, is qualitatively correct but does not match the extent of the measured asymmetry.

22.5° plane, figure 5.4.10

The predictions in this plane exhibit considerably less grid sensitivity; differences between the 39,000 and 87,000 point predictions are confined to the floor jet and are not large by comparison with other inter-prediction differences.

Agreement with experiment is poor only at the $r = 0.102R$ location, where small magnitudes are involved.

33.75° plane, figure 5.4.11

Grid sensitivity manifests itself to a greater extent in terms of gradients than magnitudes at $r = 0.510R$ and $0.646R$ – but changes are such that it may again be said that further grid refinement would have little effect on the 87,000 point SFCD predictions. The superiority of the 16,000 point SFCD to 39,000 point UD predictions is marked at the forementioned locations.

General agreement with experiment is again so good as to highlight the one failing: the underprediction of the jet peak (by 15%) at the impeller tip, attributable to the impeller boundary condition treatment, and typical of the level of discrepancy in other planes. The measured asymmetry of the jet is not quite reproduced, although the peak is correctly located.

45° plane, figure 5.4.12

Discrepancies between the 39,000 and 87,000 point SFCD predictions are smaller than between these and the coarser grid predictions, significant in magnitude only for the near-axis floor jet. The superiority of the 16,000 point SFCD to the 39,000 point UD prediction is noted here also.

The predictions agree satisfactorily with experiment, with the exception of a floor jet overprediction of the order of 5 – 10% (greater for the weak near-axis flow) and an indication that the predicted vortex centre (located, it will be recalled, at $r \approx 0.65R$ and $x \approx 0.18R \approx 0.052m$ at $\theta = 44^\circ$) may be slightly too low – see profile at $r = 0.646R$.

56.25° plane, figure 5.4.13

Differences between the 39,000 and 87,000 point SFCD predictions are negligible in all but the floor jet region; as in previous planes the differences are inconsistent in trend with those between the other predictions and the 87,000 point SFCD results. This points to the influence of grid-sensitive swirl velocity predictions, and should be borne in mind when these are examined. Yet again the 16,000 point SFCD predictions are superior to the 39,000 point UD predictions.

The only unsatisfactory aspects of the comparison with experiment are the underprediction of the impeller jet peak velocities, by 23% at $r=0.340R$ and 15% at $r = 0.510R$ and the repeated failure of the predictions to reflect the full extent of jet asymmetry.

67.5° plane, figure 5.4.14

The grid sensitivity of the floor jet predictions near the axis is repeated in this plane – $r = 0.102R$ – this is linked to the sensitivity of the swirl velocity predictions in this region – see the profile at $x = 0.068H$ in this plane, figure 5.4.24. The coupling between the radial and swirl components, in the absence of substantial axial velocities, is strong – a substantial increase in inward radial velocity prediction will cause ‘spin up’ i.e. an increase of swirl velocity due to angular momentum conservation. The grid sensitivity of the predictions at the $r = 0.340R$ location is exaggerated by the small magnitudes involved; the gradients of the 39,000 and 87,000 point SFCD predictions are consistent. At locations further from the axis grid independence is sensibly achieved on the 39,000 point grid with SFCD.

The agreement with experiment is sufficiently good that comment may again be limited to the deficiencies of floor jet prediction (at worst, underpredicted by

$\sim 40\%$ at $r = 0.510R$), and a slightly ($\sim 0.03H$) too low prediction of zero velocity location at $r = 0.782R$, which corresponds approximately to the predicted location of vortex centre at this radius.

The above-impeller region

0° plane, figure 5.4.15

Radial velocities above the impeller are an order of magnitude smaller than those below in the downflow region ($r < 0.388R$), and in this light the discrepancies between the 39,000 and 87,000 point predictions, confined in any case to the upper third of the vessel, are unimportant (and again considerably less than differences between these and the other predictions). The velocity predictions at the $r = 0.728R$ and $r = 0.864R$ locations are grid-independent.

Agreement with experiment is qualitatively good at all locations. The extent of near-zero velocity (and thus vortex height at this radius) is underestimated at $r = 0.728R$; the strength of the inward-directed flow in the upper third of the vessel is universally underpredicted.

22.5° and 45° planes, figures 5.4.16 and 5.4.17

Grid independence has been achieved; it is, however, noted that in the case of the 22.5° plane the predictions are in general grid-insensitive in any case.

Agreement with experiment is excellent in the lower half of this region and satisfactory above in all but the weak near-axis flow.

67.5° plane, figure 5.4.18

Differences between the 39,000 and 87,000 point SFCD predictions are significant only at a radial location ($r = 0.388R$) in which the flow is almost perfectly axial; apart from the factor of small velocity magnitudes the cause of these discrepancies is again suggested to be sensitivity to the values of the other components, themselves grid-sensitive, as much as truncation error, given the lack of a uniform trend to final profile prediction.

Serious disagreement with experiment is evident at $r = 0.252R$, qualitative agreement, and at radii of larger velocity magnitude ($r = 0.728R$ and $r = 0.864R$) quantitative agreement is satisfactory elsewhere. Some question must attach to the measurements at $r = 0.252R$, in view of the fact that the positive gradient $\partial v / \partial x$ is opposite to that at all other radial locations in this plane and at this radius in all other planes. It is not particularly obvious why the downflow should

be strongly directed toward the axis here. Furthermore the axial velocity is well predicted, figure 5.4.8. It remains possible that the poor prediction of momentum exchange between $x - r$ planes, in the form of the swirl velocity, figure 5.4.28, is responsible for the present discrepancy, though the discrepancy in the swirl velocity comparison is no greater in this plane than elsewhere.

5.4.4 Mean swirl velocity comparisons

The below-impeller region

0° plane, figure 5.4.19

Grid sensitivity is more pronounced, at most of the locations in this and other planes, for the swirl velocity component than either of the other two. It is noteworthy, however, that the greatest sensitivity is exhibited near the axis, where considerable sensitivity is also evident in the radial velocity predictions, and there is a close relationship between the two components in terms of the necessity for angular momentum conservation in response to flow strength directed toward the axis.

There is a qualitative difference between the monotonic increase in swirl with radius obtained with UD at $r > 0.5$ and the plateau/local minimum resulting from the employment of SFCD (most pronounced on the 39,000 point grid but evident also on the 16,000 point and 87,000 point grids at $x = 0.170H$). The considerable variation in magnitudes apparent at most locations is partly attributable to the above and partly to shifts in the location of flow features (in particular, the location of a pronounced minimum value of swirl between $r \approx 0.04m$ and $r \approx 0.06m$ at $x \leq 0.238H$).

Grid independence is further from being achieved for this than for the other velocity components – though it is noted that the 39,000 and 87,000 point SFCD predictions are in closer agreement than any of the others.

In very broad qualitative terms the predictions agree with experiment, insofar as the measurements indicate that from being (weakly) co-rotational (with the impeller) close to the vessel axis the flow is almost purely radial at intermediate locations, and reverses nearer the vessel bottom, before becoming increasingly strongly co-rotational from $r \sim 0.07R - 0.1R$ to the wall. The near-axis value is consistently and considerably overpredicted, however, to a height of $x = 0.238H$, while the counter-rotation is under-predicted in strength and extent from the bot-

tom upwards (*cf.* the comparison at $x = 0.170H$). There is some experimental support for the aforementioned prediction of a local minimum in positive swirl, at $x = 0.238H$, albeit very much closer to the wall and with a more pronounced surrounding maximum and minimum. In other words, swirl velocity gradient underprediction is such that measured flow behaviour is only tentatively suggested rather than defined.

The peak in predicted velocity at $r = 0.05m$ at $x = 0.281H$ reflects the imposed swirl velocities in the impeller swept volume (height of lower edge of impeller blade = $0.299H$); while the experimental data indicates the flow to be purely radial at this point it is insufficient to indicate whether a peak exists further inboard or not. The inability of the impeller boundary condition to anticipate the formation of trailing vortices, which have been reported to exist behind the impeller blades by van't Riet and Smith (1973) among others, is likely to be a principal factor, as the lower of these would be expected to be positioned at or close to this location.

22.5° plane, figure 5.4.20

Quantitative differences between predictions at $r > 0.3R$ in this plane are non-negligible; however the qualitative mutual agreement evident at $x = 0.281H$ is maintained between the SFCD predictions to the vessel bottom, the UD predictions not maintaining and deepening the minimum in swirl velocity at $r \approx 0.12m$, which represents a change to almost purely radial flow in anticipation of the baffle (baffle edge at $r = 0.117m$).

The disappearance of near-axis co-rotation at all locations indicated by the measurements is not reflected in the predictions, which differ little from those for the 0° plane in this zone. The aforementioned prediction of a local minimum at $r \approx 0.12m$, again repeating the pattern at the previous plane, is also contradicted by experiment. The greatest quantitative differences between prediction and experiment are at $x = 0.281H$, where a measured velocity of $0.018m/s$ contrasts with a prediction of $0.134m/s$, though in this case the discrepancy is attributable to circumferential variation in predicted values where the measurements indicate little circumferential change.

33.75° plane, figure 5.4.21

The same observations regarding anomolous predictions near the axis with SFCD on the 39,000 point grid, qualitative mutual agreement of predictions immedi-

ately below the impeller, and a notable difference in between the UD and SFCD predictions further down the vessel, apply in this plane.

Swirl velocity magnitude is generally overpredicted in this plane as before, with the most serious overprediction below and outboard of the impeller. An encouraging feature of the comparison with experiment, however, is the degree to which the characterisation of the flow as purely radial near the bottom ($x = 0.068H$) is confirmed by the measurements.

45° plane, figure 5.4.22

The lesser radial distance over which the profiles are plotted in this, the plane of the baffle, should be noted.

Apart from the 39,000 point SFCD near-axis result the predicted flow patterns are in complete qualitative agreement. Quantitatively, the mutual agreement between the SFCD predictions of gradient $\partial w / \partial r$ is very close at $r > 0.05m$. While definitive conclusions regarding differencing scheme performance cannot be drawn in the absence of a grid-independent reference of absolute values, the gradients are sufficiently invariant to suggest the superiority of the 16,000 point SFCD solution to the 39,000 point UD one. This is true to an extent of the predictions in all planes outboard of the impeller, it is clearest here, for $x > 0.170H$.

With the repeated exception of substantial overprediction near the axis, the extent of the increase in swirl velocity over that in the previous plane at $x = 0.068H$, and the gradient $\partial w / \partial r$, are moderately well reproduced by the predictions. Elsewhere the comparison shows qualitative as well as quantitative disagreement, however. The overprediction originating in the just-below-impeller zone, for $r < 0.1m$, extends down to $x = 0.170H$, and the flow rate past the inner edge of the baffle is substantially underpredicted at $x = 0.170H$ and $x = 0.238H$.

56.25° and 67.5° planes, figures 5.4.23 and 5.4.24

The observations already made regarding the comparison of the various predictions apply equally here.

While the swirl is overpredicted below the impeller as before, the prediction of counter-rotation for $0.07m < r < 0.12m$ at $x = 0.238H$ and $x = 0.281H$ in the 56.25° plane, and for $0.07m < r < 0.10m$ at $x = 0.281H$ in the 67.5° plane, is borne out by the measurements, as, qualitatively, are the gradient and strength of the forward swirl downstream of the baffle in both planes. Experiment suggests the (very weak) continuation of the counter-rotation down to $x = 0.068H$ in the

56.25° plane, and with much greater strength in the 67.5° plane; the predictions merely suggest a weakening of co-rotating flow.

The above-impeller region

The differences between the 16,000 point and the 39,000 point/87,000 point grid predictions are marked, qualitatively and quantitatively, and this necessitates some caution in assessing the extent to which the predictions continue to embody grid dependency effects; nevertheless the correspondence between both 39,000 and the 87,000 point SFCD predictions is such as to strongly suggest that grid independence has indeed been achieved, albeit as a result more of grid refinement than differencing scheme employed.

These remarks apply equally to predictions in all planes, and the plane-by-plane discussion will concern itself with comparison with experiment only.

0° plane, figure 5.4.25

A feature of the predictions in the below-impeller region, which is repeated here, is the underestimation of axial gradients, $\partial w / \partial x$, for $r < 0.5m$ and extending from the impeller to the vessel bottom and free surface. Thus the overprediction of swirl immediately above the impeller on the 16,000 point grid becomes an accurate prediction at $x = 0.544H$, and an underprediction at higher levels. Likewise the apparently (given the sparsity of the experimental data) equally inaccurate prediction of small negative values of swirl at $x = 0.401H$ on the finer grids only changes by a factor of ~ 2 at the higher levels; the measurements indicate a strengthening of positive swirl by an order of magnitude. The inaccuracy at $x = 0.401H$, as at $x = 0.281H$ (below the impeller) may be attributable to the impeller model employed. The failure to predict $\partial w / \partial x$ must, however, be ascribed to the turbulence model.

Nearer to the vessel wall ($r > 0.10m$) an overprediction of the order of 2 at the $x = 0.401H$ level is replaced by reasonable agreement with what measurements are available at the higher levels. At these radial locations the measurements display less an axial gradient in magnitude than in radial gradient, $\partial w / \partial r$; this is not reproduced by the predictions which again exhibit little variation with height.

22.5° plane, figure 5.4.26

The experimental indication of counter-rotation at $r = 37mm$ and $x = 0.401H$ suggests that the prediction of weak counter-rotation at this level in this and the

previous plane is of an actually-existing phenomenon, incorrectly located. The measurements indicate a much greater sensitivity in general than the predictions to circumferential location; thus a negative gradient $\partial w/\partial r$ for $r > 0.10m$ at $x = 0.680H$ in the previous plane is positive in this plane while the predicted positive gradient changes little. Similarly a positive gradient $\partial w/\partial r$ for $r > 0.10m$ at $x = 0.884H$ in the previous plane is negative in this plane while the predicted positive gradient reduces only slightly.

45° plane, figure 5.4.27

The predictions are again characterised by qualitative axial and circumferential invariance, even in this, the plane of the baffle (note the reduction in the radial range over which the data is presented). The (very limited) data appear to confirm the prediction of purely radial flow directly above the impeller blade, but also suggest a more uniformly distributed increased velocity in the reduced cross-sectional area – $x = 0.401H$. At $x = 0.544H$ this prediction of positive $\partial w/\partial r$ is in agreement with experiment, but the repeated failure to predict the substantial axial gradients measured results in serious qualitative and quantitative disagreement in the upper third of the vessel.

67.5° plane, figure 5.4.28

The discrepancy between prediction and experiment at $x = 0.401H$ and $r < 0.05m$ is greatest in this plane. The circumferential gradients in w are demonstrably non-negligible (note in particular the difference in measured $\partial w/\partial r$ between this and the 22.5° plane), and the imposition of circumferentially-invariant impeller boundary conditions, apart from anything else, prevents resolution of these gradients.

5.4.5 Turbulence kinetic energy comparisons

The below-impeller region

As measurements of all three components of r.m.s. velocity are available in this region, the comparison made here is between turbulence kinetic energy calculated as $1/2(u'^2 + v'^2 + w'^2)$ and the predicted quantity k . The presentation is made in the vertical direction and progressing upward, from the vessel bottom to the impeller region – figures 5.4.9 to 5.4.14, and from the impeller region to the free

surface – figures 5.4.15 to 5.4.18. (The axial distance indicated on the co-ordinate is in all cases measured from the vessel bottom; and again it is instructive to view the distributions relative to the impeller disc location of $x = 0.098\text{m} = 0.333H$.)

0° plane, figure 5.4.29

The increase in predicted turbulence levels with both grid refinement and higher-order differencing averages a factor of ~ 4 and results entirely from the improved mean velocity gradient resolution, since SFCD was not employed for the k and ϵ transport equations, as explained in section 5.3.1.

The most important and encouraging aspect of the comparison of the predictions is the agreement between the 39,000 and 87,000 point SFCD predictions at all but the $r = 0.252R$ location, and the consistency of the trends with grid refinement and higher-order differencing, which lends further weight to the assertion that grid independence is close to being achieved, particularly at $r = 0.728R$ and $r = 0.864R$. Where the 39,000 point SFCD predictions are not coincident with the 87,000 point SFCD predictions – $r = 0.116$ and 0.252 – they are nonetheless clearly superior to the 39,000 point UD predictions. At all radial locations for $x > 0.2 - 0.3$ the 16,000 point SFCD predictions are also superior to the 39,000 point UD predictions.

Similar remarks applies to nearly all of the remaining predictions; further comment on the prediction comparisons is limited to the few departures from this pattern.

Reasonable agreement with experiment is obtained immediately below the impeller and jet (the lower edge of the impeller blade is located at $x = 0.088\text{m} = 0.3H$) and on the inner periphery of the toroidal vortex – $r = 0.388R$ and $x > 0.05\text{m}$. Elsewhere turbulence kinetic energy and its axial gradients are universally underpredicted. The turbulence energy underestimate is severest near the vessel bottom: 71% at $r = 0.116R$, 69% at $r = 0.728R$. An element of the discrepancy may be attributed to amplification of the r.m.s. measurements by vortex processing (Hockey, 1990); a greater part must be ascribed to the deficiencies of the $k - \epsilon$ model in strongly curved flow. Bolour-Froushan (1986) has reviewed the literature on the effects of streamline curvature on turbulence intensity, and more specifically, the failure of the $k - \epsilon$ model to characterise the distributions of turbulence parameters with sufficient accuracy in the presence of such curvature. Briefly, the inaccuracy is attributable to the inadequacy of the effective viscosity

hypothesis

$$\overline{u'v'} = \mu_t \frac{\partial u}{\partial y} \quad (5.4.1)$$

– this cannot be generalised to

$$\overline{u'_i u'_j} = \mu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (3.6.1)$$

since the effect of a second strain rate, *eg.* $\partial v / \partial x$, is not to raise the Reynolds stress by a factor

$$f = 1 + \frac{\partial v / \partial x}{\partial u / \partial y} \quad (5.4.2)$$

permitting one to write

$$\overline{u'v'} = \mu_t \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \quad (5.4.3)$$

but rather to raise it by an order of magnitude – Bradshaw (1973) – such that the effect is more accurately represented by an expression of the form

$$\overline{u'v'} = \mu_t \left(\frac{\partial u}{\partial y} + a \frac{\partial v}{\partial x} \right) \quad (5.4.4)$$

where a is of order 10. The use of such a linearised expression is an unpromising approach where curvature effects are large – Bradshaw (1973) – and furthermore would not represent the transport of curvature-amplified Reynolds stresses. This represents a strong argument for the adoption of Reynolds stress models as soon as computer resources are such as to make this feasible in large-scale three-dimensional flow studies. The findings of Gibson and Rodi (1981), using the Launder, Reece and Rodi (1975) Reynolds stress closure, of improved predictions for flows over curved surfaces, may be cited as representative practical evidence of the potential value of such modelling for the flows of interest here.

The other major cause of the underprediction of k is believed to result from the treatment of the impeller region on an ensemble-averaged basis. The r.m.s. data against which comparison is made here are amplified by blade periodicity effects – the problem of ‘pseudo-turbulence’. This amplification is incorporated in the impeller boundary conditions for k , insofar as these are tuned to reproduce the measured values (*cf.* section 3.10.2). The impeller treatment cannot, however, reproduce the flow structures in the blade swept volume and its vicinity, most specifically the phenomenon of trailing vortices behind each blade, first reported by Van’t Riet and Smith (1973) and confirmed by subsequent investigations, as

summarised by Politis (1989). The presence of the vortices means that problem of 'pseudo-turbulence' extends beyond the immediate vicinity of the swept volume, and the element of the discrepancy between prediction and experiment thereby resulting is thus attributable to the nature of the experimental data. The trailing vortices will themselves give rise to vortex shedding, however, with which genuine production of turbulence will be associated. That the model does not 'see' the shear layers which would be associated with vortex shedding thus means that this element of the underprediction is attributable to the impeller boundary condition treatment.

22.5° plane, figure 5.4.30

While grid independence is not quite achieved in this plane the differences between the finer grid predictions are sufficiently small for the differences between calculation and experiment to be attributed primarily to the model and boundary conditions.

Experiment indicates a drop in turbulence energy levels from values at the previous plane of a factor of $\sim 4 - 5$ near the axis, bottom and wall, and of a factor of ~ 2 in the regions of the impeller and vortex; the predictions exhibit small circumferential gradients and the turbulence energy is accordingly almost universally overpredicted here. The distribution is however almost universally well predicted, with the exception of poor gradient resolution near the axis.

45° plane, figure 5.4.31

As in the other planes, what variations are still evident at the most accurate discretisation reached are near the axis and wall, and insufficiently large for numerical error to be a significant factor in predictive inaccuracy.

The measurements show a return to approximately the turbulence energy levels of the 0° plane, but with a markedly different distribution. The near-axis region excepted, axial gradients are small, particularly as the baffle is approached ($r = 0.728R$). Thus the circumferentially-insensitive predictions understate the turbulence level at all locations. They do, however, satisfactorily characterise distribution in all but the near-axis region.

67.5° plane, figure 5.4.32

Similar levels of turbulence are indicated by experiment at this as in the previous plane. Axial gradients are somewhat larger and, within the limits of data sparsity, lower values are suggested in the vicinity of the vortex than at the bottom and

impeller/jet periphery, in contrast to the pattern in the previous plane. While the predictions overall continue to show little variation with circumferential location, the pronounced increase in axial gradient, compared with the 45° plane, at $r = 0.388R$ and $0.728R$ for $x < 0.01m$, is accompanied by a weakly negative axial gradient for $x > 0.02m$. This is in contrast to the negligible axial gradient at $r = 0.728R$ in the 45° plane, and represents a qualitative reproduction of experimentally-observed behaviour.

The above-impeller region

As measurements of all only two components of r.m.s. velocity are available, the comparison made here is between the average of these and the quantity $\sqrt{2/3k}$ obtained from the predictions. The not-always-valid assumption of isotropy is implicit in the above; this should be borne in mind in considering the comparison with experiment. It should also be noted that in all planes at $r = 0.116R, 0.252R$ and $0.388R$ the reference value of the ordinate is non-zero.

Bearing in mind that the quantity of interest here is the square root of that compared below the impeller, the average increase between the coarsest grid UD and the finest grid SFCD results of a factor of $\sim 1.5 - 2$ is as significant as the in the lower third of the vessel. At the nearest-to-axis location ($r = 0.116R$) and near the wall and free surface ($r = 0.864R$ and $x > 0.280m$) the predictions exhibit continued sensitivity to grid refinement/discretisation; elsewhere it is concluded that further refinement would not change the results. The 16,000 point SFCD predictions are seen to be closer or as close to the grid-independent as the 39,000 point UD results. These comments apply equally to all planes.

Turbulence levels are reasonably predicted in the region immediately above the impeller and the impeller jet (the upper edge of the impeller blade is located at $x = 0.108m = 0.367H$) and in the wall jet/vortex region ($x < 0.2m \approx 0.7H$ and $r = 0.728R$ and $0.864R$). Levels are underpredicted in the downflow region and near the free surface, by an average of $\sim 30 - 40\%$ at the grid-independent $r = 0.252R$ location (which translates to an underprediction of $\sim 50 - 65\%$ of the square of this quantity, to be borne in mind when comparing the relative accuracy of prediction below and above the impeller). The degree of discrepancy varies as below the impeller because of the failure of the predictions to reproduce the measured circumferential variability. Thus an accurate prediction at $r = 0.728R$ and $x = 0.16m$ in the 0° and 22.5° planes is replaced by a deficit of 50% in the 45° plane, where the predicted value remains sensibly constant throughout.

5.5 Summary of findings

5.5.1 Mixing vessel flow: analysis of predictions

Predictions of the flow of a Newtonian fluid in a mixing vessel, on a considerably finer – 87,000-point – grid than employed in previous work and using SFCD, have been analysed in detail, and the chief features identified as:

- The impeller jet has an upward inclination, reduced in the plane of the baffle.
- The lower toroidal vortex changes from an elliptical to circular cross section in travelling inward and downward past the baffle; the upper vortex has a pronounced inward tilt where squeezed by the baffles and is also shifted downward.
- Secondary vortices are predicted within the radius of the impeller near the vessel bottom, in the baffle wake extending from the impeller jet upward and downward, and in association with the downward flow extending from near the fluid surface to half the vessel height.
- The distribution of k and ϵ is characterised by rapid decay from the impeller blade tip region, with locally high values associated with the vortices and the downflow region immediately above the impeller.
- Turbulence length and time scales increase from minimum values in the blade tip region to maxima on solid boundaries – the increase in the vicinity of the baffle is marked. Minimum values of the former quantity in the jet are associated with the periphery, and of the latter with the jet core.
- Distributions of Kolmogorov length and time scales are qualitatively similar to those of the turbulence scales, but do not exhibit the dependence on vessel geometry of the latter. Blade tip values of Kolmogorov length scale are three orders of magnitude smaller than those of turbulence length scale, those of Kolmogorov time scale two orders of magnitude smaller than the turbulence time scale.

5.5.2 Mixing vessel flow: comparison with experiment

Comparison of the fine grid results with measurements has shown that:

- Overall agreement is very good, throughout the vessel, for the axial and radial mean velocity components, less satisfactory for the swirl component, with consistent underprediction below the impeller and overprediction above it.
- Deficiencies in the prediction of impeller jet strength have been attributed to the impeller boundary condition treatment.

- Turbulence energy is underpredicted, though by a factor of < 2 in most of the vessel. Underprediction is more severe near the vessel bottom. Circumferential variations in k are underpredicted.

The underprediction of turbulence kinetic energy has been attributed in part to the inadequacy of the eddy viscosity hypothesis, and thus of the $k - \epsilon$ model, in strong flow curvature. The generation of turbulence energy associated with vortex shedding in the wake of the baffle blades is not accounted for by the present methodology due to the treatment of the impeller region adopted. It has also been pointed out that the measured r.m.s. values incorporate ‘pseudo turbulence’ effects due to vortex processing and flow periodicity in the vicinity of the impeller; while these are accounted for on the blade tip itself through the boundary conditions they will amplify the prediction/measurement discrepancy elsewhere.

5.5.3 SFCD performance

For the case study of laminar flow in a pipe with a step contraction it has been shown that the use of SFCD enables results of comparable accuracy to be obtained as on a grid of four times as many grid points if Upwind Differencing (UD) is used, with a consequent saving in memory requirement of the same magnitude; the reduction in processor time needed has been quantified as a factor of 10 to 50.

For the case study of a mixing vessel it has been found that the increase in CPU time requirement associated with the use of SFCD decreases with grid refinement, while comparison of mean velocity and turbulence energy predictions on three grids and using UD and SFCD has shown that:

- Predictions obtained on each of the coarser grids with SFCD are for the most part much closer to the finest grid solution than those obtained with UD.
- Finest grid results are for most variables in the greater part of the vessel close to grid independence.
- The swirl velocity shows the greatest grid/discretisation sensitivity.
- Turbulence energy predictions are increased by a factor of four from a 16,000-point UD to an 87,000-point SFCD prediction, as a result of better mean velocity gradient resolution.

It has been found that with the use of SFCD for scalar transport equations boundedness is not guaranteed at intermediate solution levels for these quantities, but also that, for the mixing vessel case of interest here, little difference is occasioned to the final solution whether or not SFCD is employed for these equations.

6 Predictions of flows of shear-thinning fluids

6.1 The flow cases considered

Predictions of several flows of shear-thinning fluids are presented here. Emphasis is placed on assessment of the predictions, and thereby of the modelling of turbulent flow of shear-thinning fluids presented in chapter 3, by comparison with newly-available and comprehensive experimental data.

Pipe flow is considered in section 6.2. Comparisons with experiment for fully developed turbulent pipe flows of Newtonian fluids are presented in section 6.2.1, and of shear-thinning fluids in section 6.2.2. Comparison with data for turbulent flow of a Newtonian fluid in a pipe with an axially-mounted baffle are presented in section 6.2.3, and of shear-thinning fluids in the same configuration in section 6.2.4.

Predictions for the flow of a shear-thinning fluid in a mixing vessel, of the same configuration as that in which the flow of a Newtonian fluid was considered in the previous chapter, are presented in section 6.3, and comparisons with data are made in section 6.4.

Finally, findings are summarised and conclusions drawn in section 6.5.

6.2 Turbulent pipe flow predictions

6.2.1 Fully developed turbulent pipe flow of Newtonian fluids

The $k - \epsilon$ model of turbulence is tuned to two-dimensional boundary-layer and free jet flows, in the sense that the values of the empirical coefficients in the model itself are chosen such that the model reproduces experimental data for such flows of Newtonian fluids (section 3.8.5), and those in the wall functions chosen by reference to experimental data for such flows of Newtonian or shear-thinning fluids as appropriate (section 3.10.1). There is, however, a perhaps surprising (in view of its widespread use) paucity of reportage in the literature of the predictive capacity of the ‘standard’ model with wall functions employed here, for pipe flow. It is necessary that this be established for Newtonian fluid flow before assessment of non-Newtonian fluid flow predictions, as the former may reasonably be expected to provide an upper bound on the accuracy obtainable with the latter. This in turn provides a basis of reference when predictions for more complex two- and three-dimensional flows are considered.

Predictions of the fully developed turbulent pipe flow of Newtonian fluids are presented here. The solutions in all cases were generated using successive cycling through the solution domain *ie.* values of field variables at the outlet of each domain were supplied as inlet values for the next. The flow was deemed fully developed when a solution domain was reached for which the convergence criterion specified in section 4.9 was satisfied by fields equated to the distributions at inlet *ie.* of zero axial gradient.

Figures 6.2.1a and 6.2.1b illustrate predictions of mean axial velocity, at a Reynolds number of 194,000, on semi-logarithmic ‘law-of-the-wall’ and on linear co-ordinates, respectively. It is seen that location of the next-to-wall node has little effect, provided that it lies outside the sublayer *ie.* provided that the value of y^+ at this node, given by (2.5.5), is greater than 11.62. The consequence of the node being located at $y^+ < 11.62$ is a downward-shifted profile on ‘law-of-the-wall’ co-ordinates, since prescription of laminar shear stress according to (4.7.1) will locate the next-to-wall node correctly on the $u^+ = y^+$ profile, but prescription of ϵ according to (4.7.9) causes the velocity gradient between the next- and second next-to-wall nodes to be $1/\kappa$ (through the dependence of ϵ on κ and the dependence of μ_t on ϵ). Thus the location of the next-to-wall node, in terms of y^+ , is seen to be significant if the ‘wall function’ approach is employed, particularly in terms of predicted pressure drop, and is all the more significant in the context of flows of fluids for which substantially higher values of y_{it}^+ are apparently appropriate, since greater care has to be exercised in the location of next-to-wall nodes. The predicted velocities for the ‘correct’ distribution have been found to be in agreement with experiment to the degree reported in the literature – by, for instance, Stephenson (1976) – with the qualification that the predicted distribution is somewhat steeper than that measured.

The pressure drop is consistently underpredicted by 6.8% – 8% over a range of Reynolds numbers from 20,000 to 194,000, relative to that given by (2.5.12).

Figure 6.2.2 shows representative predictions of normalised turbulence kinetic energy ($k^+ = k/u_*^2$), with the data of Laufer (1954) and Lawn (1971) for comparison. With a value of C_μ of 0.09, the wall functions prescribe a value of k^+ of 3.3 at the next-to-wall node (see appendix G). While the predictions are indistinguishable in the pipe core for various next-to-wall node locations (provided that these are outside the sublayer) this prescription results in a non-monotonic distribution in the near-wall region if the next-to-wall node is located at a y^+ of less than ≈ 200 , with a peak value at a location much further from the wall than

that indicated by experiment.

The predictions lie well within the range of experimental data in the pipe core. It is clear, however, that experiment indicates a value of k^+ in the near-wall region which is considerably higher than 3.3, albeit with considerable scatter. Launder and Spalding (1974), in recommending the value of 0.09 for C_μ which has been retained by the majority of users of the $k - \epsilon$ model, did not state which boundary layer flows were examined in determining this value; it must be concluded that pipe flows were not amongst those considered.

A lower value of C_μ results in an upward shift in the $k^+ - y^+$ profile, thereby improving predictions in the near-wall region at the expense of those in the pipe core. Furthermore, changes in the values of the empirical coefficients in an effort to improve predictive accuracy for a particular flow may degrade predictions for other flows, given that the coefficients have been optimised with a view to $k - \epsilon$ model generality. Explicit recognition of the failure of the $k - \epsilon$ model with standard empirical coefficient values and wall functions to accurately predict turbulence levels in the near-wall region of fully developed turbulent pipe flow has not been found in the literature; it is, however, implicit in the work on low Reynolds number models referred to in section 3.10.1.

6.2.2 Fully developed turbulent pipe flow of shear-thinning fluids

Predictions for the fully developed turbulent pipe flow of several shear-thinning solutions are considered here – the computational details are as described in the previous section for Newtonian fluid flow.

Figures 6.2.3 illustrates mean axial velocity predictions, on semi-logarithmic and on linear co-ordinates, for the flow of the 0.3% aqueous solution of Carbopol measured by Bogue (1963) and already referred to in section 2.5.1 – this being the solution concentration in the flow of which a logarithmic region of the velocity distribution could be identified with most confidence. The values of the wall function parameters used are as given in table 2.1; the index n of this fluid, 0.70, is indicative of non-negligible shear-thinning behaviour.

The predictions are seen to reproduce the measured values to the same level of accuracy as for Newtonian fluid flow. Centreline velocity is underpredicted by 3.2%. Pressure drop is also predicted to the same level of accuracy: the underprediction of the measured value is 9%. Bogue did not make r.m.s. measurements, having used a Pitot tube.

Solution	n	B	κ	y_{lt}^+	Re_μ	f (exp.)	f (pred.)
0.1%	0.905	12.10	0.271	23.79	45,000	2.20×10^{-3}	2.21×10^{-3}
0.2%	0.73	7.76	0.180	31.99	32,000	2.07×10^{-3}	1.50×10^{-3}
		5.77	0.174	24.01			2.00×10^{-3}

Table 6.1 Fluid and flow parameters for fully developed turbulent pipe flow of aqueous CMC solutions, from data of de Pinho (1990)

De Pinho (1990) has, in parallel to the present work and using laser doppler anemometry, measured mean and r.m.s. values of velocity in turbulent pipe flow of shear-thinning, aqueous solutions of CMC of varying concentration. From the semi-logarithmic representation of de Pinho's data in figures 6.2.4a and 6.2.7a for the two most dilute solutions he measured, it is clear that the profiles are not only shifted upward relative to the Newtonian but substantially steeper; the trend towards a laminar distribution is more pronounced still for the flows of the more concentrated solutions employed by de Pinho (not shown). These latter are not considered here in view of the difficulty in identifying a logarithmic region in the profiles and of the likelihood that the flows are transitional. The curve $u^+ = 8.49(\log y^+) + 12.10$ is the least squares fit to the data for the 0.1% solution, over a y^+ range of 55 – 370 – figure 6.2.4a. Likewise the curve $u^+ = 12.32(\log y^+) + 7.76$ is the least squares fit to the data for the 0.2% solution, over a y^+ range of 120 – 280, while the curve $u^+ = 13.22(\log y^+) + 5.77$ is the least squares fit to the data for the 0.2% solution over a y^+ range of 90 – 230 – figure 6.2.7a.

The wall function parameters thus obtained are listed in table 6.1.

The agreement of the predicted axial mean velocity with the experimental data, for the flow of the 0.1% CMC solution, as shown on semi-logarithmic and linear co-ordinates in figures 6.2.4, respectively, is reasonable. Centreline velocity is underpredicted by 5%. It will, however, be noted that the predicted distribution is flatter than that measured, in contrast to the predictions for Newtonian fluids and for the Carbopol solution. The error in the pressure drop prediction is less than 1% of the measured value. The greater accuracy of this prediction by comparison with that for Newtonian fluid flow is somewhat fortuitous – the prediction is a function of the value of y_{lt}^+ . This will be obvious below from the predictions for the flow of the 0.2% solution.

The comparison of predicted turbulence kinetic energy with the data of de

Pinho (1990) is presented in figure 6.2.5. De Pinho's data for the fully developed pipe flow of a Newtonian fluid (water) show somewhat higher turbulence energy levels than the data of Laufer (1954) and Lawn (1971) – figure 6.2.6. The discrepancy may be attributable to the small size of pipe used (25 mm diameter) – de Pinho (1990), which necessitates location of measurement points at very small absolute distances from the wall in order to satisfactorily characterise near-wall flow patterns. The measurement control volume *ie.* volume of intersection of the beams in the Laser Doppler Anemometry measurement technique used was 400×10^{-6} m across, to be compared with a nearest-to-wall measurement location of 300×10^{-6} m from the wall. The other principal potential source of error (de Pinho, 1990) relates to the values of pressure by which the k values are normalised – these were obtained using a transducer operating in the lowest 5% of its operating range (having been selected with a view to measurement of the much greater pressure drops obtaining in the baffled flow to be considered presently). While this introduces an element of uncertainty as to the magnitude of the turbulence energy data for the flow of the CMC solution, obtained in the same pipe, the difference in the distribution in the flows of the water and CMC solutions is clear, and this is reflected in the prediction/experiment comparison for the latter case: the underprediction of the measured value at the axis is 15%, while at $y^+ = 37$ it is 65%.

De Pinho's measurements show that maximum radial and tangential velocity fluctuations are approximately five times less than those of the axial velocity fluctuations and considerably less than those associated with a Newtonian fluid. This is in accord with the measurements of Patterson *et al* (1977) and Allan *et al* (1984) amongst others, who confirm that very dilute polymer solutions can cause damping of the radial and cross-flow normal stresses and increase the axial normal stress very close to the wall – the significant point for present purposes is that the fluids used by these investigators were not shear-thinning. Much discussion has appeared in the literature concerning the mechanisms involved, the balance of which is in agreement with the conclusion of Lumley (1977) that molecular expansion has a preferential effect on normal Reynolds stresses other than those associated with the main flow direction, and this confirms that prediction of the phenomenon of augmented near-wall turbulence in the flow of drag-reducing fluid flow is outside the scope of this work.

Figures 6.2.7 illustrates predictions of mean axial velocity for the flow of the 0.2% CMC solution, using both sets of wall function parameters listed in table

6.1. Using parameters resulting from the least squares fit of smallest standard deviation produces a flatter axial velocity prediction than the experimental (with centreline velocity underprediction of 10%) and a pressure drop underprediction of 27%. Using those obtained from the least squares fit of second smallest standard deviation reduces the centreline velocity underprediction to 8% and the pressure drop underprediction to $< 4\%$. Predictions were also obtained with wall function parameters obtained from least squares fits over other ranges of y^+ , all less accurate than those shown.

The above illustrates the difficulty of characterising this flow in law-of-the-wall terms – the velocity distribution is more characteristic of transitional than fully turbulent flow despite a Re_{μ_w} of 32,000 obtaining.

The predictions of turbulence kinetic energy for each of the sets of wall function parameters in table 6.1 are compared with the data of de Pinho in figure 6.2.8. Again the predictions made with the second set of wall function parameters are the least inaccurate (underprediction of k of 32% at centreline as opposed to underprediction of 49% with the first set; predictions with other parameter sets are more inaccurate). The underprediction at $y^+ = 50$ is 58%. The comments regarding the inability of the $k - \epsilon$ model to predict the gradient of the turbulence energy in the flow of the 0.1% solution apply equally here. In order to illustrate the degree of modification to C_μ which would be required to even qualitatively reproduce the turbulence energy distribution in the boundary layer flow of this fluid, however, prediction of the turbulence energy distribution with a value of C_μ of 0.04 is included in figure 6.2.8; the error in the on-axis prediction is $< 3\%$, with an underprediction of 36% at $y^+ = 50$. This essentially confirms the unlikelihood of success in employing the ‘wall function’ approach for the flows of these fluids in general, given that the modification of C_μ to this degree is likely to degrade solutions in regions removed from boundaries where the flow is truly inertially dominated, but it also indicates that even a low-Reynolds-number approach offers an uncertain chance of success, given the degree of modification to the damping function, f_μ , defined by (3.10.3), which would be required. (Whether any correlation of this degree of modification with fluid properties could be established is of course another issue, a reiteration of the problem stated in chapter 2 of establishing empirical boundary condition parameters for general use with a given class of non-Newtonian fluids on the basis of a few specific cases which may be dynamically dissimilar.)

6.2.3 Turbulent Newtonian fluid flow in pipe with baffle

The case of turbulent flow of water in a pipe with an axially-mounted baffle, at a Reynolds number based on disc diameter of 138,000, (corresponding to an annular jet bulk velocity of 7.68m/s) is considered here. This will provide a basis for assessment of predictions of flows of shear-thinning fluids in the same configuration, to be examined in the next section.

The configuration is as illustrated in figure 6.2.9 – the sharp-edged baffle reduces the flow cross-sectional area by 50%, and is mounted on a rod itself located on the pipe axis by four radial ribs.

The orthogonal grid used in this study precludes the exact representation of the 45° chamfer on the upstream face of the baffle. The results presented here were obtained with the problem specified in terms of an impermeable, rigid surface of zero thickness, which approximates the sharp edge of the experimental disc.

The effect of the ribs locating the baffle holding rod is assumed negligible, to facilitate a two-dimensional treatment. Solutions were obtained with the upstream (inlet) boundary conditions specified in each of two ways. In the first, fully developed flow was imposed in a plane upstream of the leading tip of the holding rod, this being treated as square (conical in the experimental work) – the baffle/holding rod section was preceded by a straight section of 90 diameters in length in the experimental study. In the second, uniform profiles for all quantities were imposed for an inlet plane immediately downstream of the locating ribs *ie.* with the rod extending from the inlet plane. The differences in solutions obtained with each specification are negligible in the wake region of interest (< 1% in the magnitudes of axial velocities in the plane of the baffle); accordingly only solutions obtained with the latter specification are discussed.

Zero axial gradients in all variables were specified at the outlet boundary. Boundary conditions on pipe wall, baffle and rod faces were specified in terms of the wall functions described in section 4.10. SFCD was used, for the momentum equations only, for the reasons discussed in the foregoing chapter.

Predictions were obtained on progressively finer computational grids, and the finest, of 51×47 cells, used to obtain the results presented, is illustrated in figure 6.2.10a. At this level of refinement the results are sensibly grid independent – quantified as maximum differences in predicted axial velocity of < 4%, and in predicted turbulence kinetic energy of < 2%, compared with results obtained on a 42×38 cell grid.

The flow features are shown in figures 6.2.10 – these figures are self explanatory. Note will be taken of the range of values of the Kolmogorov time scale τ_k , and length scale η , which have been defined in section 5.3.6 and distributions of which are illustrated in figures 6.2.10f and 6.2.10g, respectively. The minimum value of τ_k in the region downstream of the baffle is 1.3×10^{-5} s, and the maximum, on the centreline at the outlet, 7.6×10^{-5} s. η ranges in value from 3.6×10^{-6} m to 8.8×10^{-6} m. These values will be compared in the following section to those in the flow of shear-thinning fluids.

From the comparison of predicted and experimental axial velocity on radial profiles, figure 6.2.11a, it is apparent that the predictions fail to reproduce the peak in axial velocity on the tip of the baffle. This is ascribed to the form of approximation of the baffle shape – from the foregoing, the influence of the specified variable distributions at the inlet, and of numerical diffusion, may be discounted. Perić (1985) presented predictions for flow in the similar configuration of a pipe with axially-mounted conical baffle with 25% area reduction, which successfully captured the axial velocity peak on the baffle tip also observed experimentally in that flow. Perić used a non-orthogonal grid, permitting exact representation of the geometry. The predictions of McGuirk, Taylor and Whitelaw (1982) for flow in both configurations took the plane of the baffle as the inlet plane, circumventing the geometry representation problem.

The comparison in planes downstream of the baffle shows that within the recirculation zone the calculated value of $\partial u / \partial r$ in the mixing layer is smaller than that measured, suggesting that calculated diffusion of axial momentum from larger to smaller radii is too great. The velocity deficit further downstream, particularly obvious from figure 6.2.12b showing centreline development of axial velocity, implies that radial diffusion of axial momentum is here too small. The length of the recirculation bubble is underestimated by $\sim 16\%$.

In figure 6.2.11d profiles of turbulence kinetic energy at successive locations downstream of the baffle are compared with the data of de Pinho (1990).^{*} The form of the distribution is well reproduced at $x = 42.5\text{mm} - 0.25D_{\text{disc}}$ downstream of the disc face – albeit with magnitudes overpredicted, by a factor of ~ 2 . At all locations further downstream, however, the peak in the shear layer is seriously underpredicted while the predicted near-axis values are close to the measured levels until the stagnation point (close to the $x = 72.4\text{mm}$ location – $1.91D_{\text{disc}}$

^{*} Because the three components of r.m.s. velocity were not measured at the same radial locations, some interpolation was necessary to calculate k from them.

downstream of the disc face) is reached, when turbulence levels are underpredicted here also.

This kind of disagreement has been reported by McGurk *et al* (1982) and Perić (1985), and may be attributed to the inadequacies of the $k - \epsilon$ model, as discussed by McGurk *et al*. Briefly, the strong streamline curvature in this kind of flow renders the eddy viscosity hypothesis invalid, as outlined in section 5.4.5 in connection with the mixing vessel flow. In addition an examination of the relative orders of magnitude of the terms in the k equation permitted McGurk *et al* to show that the shear flow is far from being in equilibrium immediately downstream of the baffle and that the forms of the production and dissipation distributions imply that it is also not self-preserving. This calls the adoption of the eddy viscosity hypothesis still further into question, given that its success is usually associated with flows which *are* self-preserving. Experiment indicates that the generation through normal stress/normal strain is important in the vicinity of the stagnation point; the eddy viscosity hypothesis is known, however, not to represent normal stresses adequately and McGurk *et al* showed that predicted production of k near the stagnation point is indeed very small. Finally, in the wake, dissipation comes to exceed production and convection is relatively more important; in such flows the eddy viscosity hypothesis can produce adequate results *provided* C_μ is made a function of the production/dissipation ratio.

6.2.4 Turbulent shear-thinning fluid flow in pipe with baffle

Predictions for the flow of shear-thinning aqueous solutions of CMC in the configuration of figure 6.2.9, are presented here. The bulk flow rate for the flow of the 0.1% CMC solution was 8.88m/s, and for the 0.2% CMC solution 8.94m/s. Defining a shear rate as

$$\dot{\gamma} = \left(\frac{u_{\max} - u_{\min}}{\Delta r} \right)_{\max}$$

which “represents an average value in the recirculation and shear layer regions in a plane close to the recirculation bubble”, where $u_{\max}$ and $u_{\min}$ are the maximum positive and negative velocities in the annular jet and recirculation regions, respectively, and Δr is the distance between them, and taking the value of a characteristic viscosity from this shear rate and the viscometric data, de Pinho quotes Reynolds numbers, based on disc diameter, of $\sim 42,000$ and $\sim 22,000$ for the 0.1% and 0.2% CMC solution cases, respectively. The concept of a characteristic viscosity is yet more tenuous for this type of flow than that in a straight pipe, for

shear-thinning fluids, however, and the level of turbulence which these Reynolds numbers represent is therefore extremely uncertain.

The computational details are as for the Newtonian case, and evidently the limitations on geometry representation imposed by the grid apply here also. The 51×45 cell computational grid used to obtain the results presented for the 0.1% aqueous solution is illustrated in figure 6.2.12a. At this level of refinement the results are sensibly grid independent – quantified as *maximum* differences in predicted axial velocity of $< 5\%$, and in predicted turbulence kinetic energy of $< 2\%$, compared with results obtained on a 57×50 cell grid.

The larger size of next-to-solid boundary cells in this grid compared to that used for the Newtonian study is necessitated by the thicker viscous sublayer associated with this fluid – in both dimensionless and dimensional terms. Even with this measure y^+ has a value $< y_{lt}^+$ on the pipe wall from the inlet to approximately 31mm from the inlet, and on the holding rod from approximately 22mm to the baffle; further grid refinement on these surfaces results in more than one node being located in the sublayer, outside the scope of the wall function treatment. A grid with next-to-wall cells of sufficient size, such that $y^+ < y_{lt}^+$ at all next-to-wall nodes, results in unsatisfactory resolution of gradients near the wall in the planes immediately downstream of the baffle, a consequence of using an orthogonal grid. Accordingly this grid represents what is considered to be the best compromise between the conflicting requirements of remaining within the scope of the wall functions in pipe sections of thick sublayer, and obtaining satisfactory gradient resolution in sections where the sublayer is thinner.

The features of the flow of the 0.1% solution are shown in figures 6.2.12, and it will be noted that normalised values of pressure, turbulence energy and length scale are sensibly the same as in the Newtonian fluid flow. The Kolmogorov time scale τ_k ranges in value from 1.9×10^{-5} s to 1.2×10^{-4} s, and the length scale η from 7.3×10^{-6} m to 2.0×10^{-5} m.

As in the case of the flow of the Newtonian fluid, the predictions fail to reproduce the peak in axial velocity on the tip of the baffle, for the same reasons. The discrepancies between the predicted and experimental axial velocities in planes downstream of the baffle are slightly larger (of the order of 2%) than in the Newtonian case; this is primarily a result of the use of a larger next-to-wall cell and the consequently poorer gradient resolution at the wall in the region immediately downstream of the baffle. The prediction of the peak reverse centreline velocity too close to the baffle, the underprediction of the extent of the recirculation zone,

and the underprediction of the rate of recovery of the centreline velocity – figure 6.2.13b – is qualitatively similar to the results for the Newtonian fluid flow case. The length of the recirculation is predicted as $< 2\%$ smaller than in the Newtonian case; the value measured by de Pinho is $> 6\%$ smaller.

The 51×45 cell computational grid used to obtain the results presented for the 0.2% aqueous solution is illustrated in figure 6.2.14a. At this level of refinement the results are sensibly grid independent – quantified as maximum differences in predicted axial velocity of $< 6\%$, and in predicted turbulence kinetic energy of $< 3\%$, compared with results obtained on a 57×50 cell grid.

The very much thicker viscous sublayer associated with this fluid necessitates next-to-solid boundary cells of considerable size in this grid. For the results presented here y^+ has a value $< y_{it}^+$ on the pipe wall from the inlet to approximately 34mm from the inlet, on the holding rod from the inlet to the baffle and on the upstream face of the baffle from the holding rod to 5mm from the axis; further grid refinement on these surfaces results in more than one node being located in the sublayer.

The features of the flow of the 0.2% solution are shown in figures 6.2.14, and some differences in normalised values of pressure, turbulence energy and length scale, by comparison with the flow of the Newtonian fluid, are identifiable. These may be attributed firstly to the larger next-to-wall cells used, and secondly to the contribution of the extra ϵ equation source terms, which will be addressed again momentarily. τ_k ranges in value from 2.0×10^{-5} s to 1.7×10^{-4} s, a ratio of 8.54 – this compares with a ratio of 6.32 in the 0.1% CMC case and 5.71 in the Newtonian case, and illustrates the effects of shear-thinning at the micro scale level. η ranges in value from 8.0×10^{-6} m to 3.1×10^{-5} m, a ratio of 3.85 – the equivalent values are 2.74 in the 0.1% CMC case and 2.44 in the Newtonian case.

The quite pronounced underprediction of radial gradient $\partial u / \partial r$ for ~ 40 mm *ie.* $\sim 2D$ downstream of the baffle is due in large measure to the poorer gradient resolution afforded by the near-wall grid – further downstream, however, the gradient prescription resulting from this next-to-wall node is accurate, while $y^+ < y_{it}^+$ at the last several next-to-wall cells before the outlet, reflecting the rate at which sublayer thickening takes place in the flow of this fluid as it recovers. The prediction of the rate of recovery of the centreline velocity* – figure 6.2.15b – is of the same accuracy as that achieved in the Newtonian flow case. The length of

* No measurements of axial velocity were made precisely on axis – those shown are the nearest available, at locations in the range $r/R = 0.008 - 0.024$.

the recirculation is predicted as 6% smaller than in the Newtonian case – this is coincident with the difference between the Newtonian and 0.2% CMC case values measured by de Pinho, though the predicted difference is probably due to the different velocity distribution in the pipe as a whole just mentioned.

Significant differences are apparent, however, in the comparison of predicted turbulence energy with experimental values, between the 0.1% CMC case, figure 6.2.13d, and the 0.2% CMC case, 6.2.15d. This is considered to be the most valid cross comparison in view of the uncertainty associated with Reynolds numbers (these are in any case dissimilar) – the bulk flow rates in these cases are similar (annular jet bulk velocities of 8.88m/s and 8.94m/s, respectively) and dissimilar to the water case (annular jet bulk velocity of 7.68m/s). Specific reference is then made to the second profile downstream of the baffle, at $x = 42.5\text{mm} - 0.25D_{\text{disc}}$ downstream, and it is noted that whereas at the radius of the blade tip the underprediction of the measured level is $\sim 50\%$ of the measured value in the 0.1% CMC case, it is $\sim 10\%$ of the measured value in the 0.2% CMC case, while the predicted levels are within 5% of each other. Referring to the profile at $x = 51.5\text{mm} - 1.5D_{\text{disc}}$ downstream, the overprediction on axis is $\sim 20\%$ of the measured value in the 0.1% CMC case, but $\sim 70\%$ in the 0.2% CMC case, and again the predictions agree to within 5%. The cited discrepancies between the predictions are typical of the solution domain as a whole, and are attributed to the non-negligible contribution of the extra source terms in the ϵ equation, quantified below. More important, however, in the context of comparison with experiment is the evidence in the data of significant differences in turbulence energy distributions, and differences in the turbulence structure *ie.* the relative magnitudes of the fluctuating velocity components, are even more marked.

De Pinho notes that centreline distributions of axial and cross-stream normal Reynolds stresses show reductions with increasing CMC concentration, but that the cross-stream values decrease much more rapidly, and comments that the very much increased anisotropy he observed in the flows of the CMC solutions (by comparison with that he observed in the flow of water) with preferential damping of tangential and radial Reynolds stresses, cannot be explained by the influence of viscous diffusion in these flows, but “must be the result of another property, such as elasticity”. While a Reynolds stress model might be expected to provide improved predictions for the flow of Newtonian fluids in this geometry, a separate effort to model the mechanism amplifying the anisotropy in this as in other flows of drag-reducing polymer solutions is required before accurate predictions might

be expected for flows of such fluids. Given the lack of consensus as to the nature of this mechanism, such modelling would of necessity be hypothetical, but predictions made with a turbulence model incorporating a model of elasticity might well yet prove to be the only means of establishing if it is indeed responsible for the effects discussed here.

Figure 6.2.16 shows the magnitude of the additional source terms in the ϵ equation, proposed in section 3.8.4 to model shear-thinning behaviour, as a proportion of the ‘standard’ source term, *viz.*

$$\frac{\rho \frac{\epsilon u_j}{\mu} \frac{\partial \mu}{\partial x_j}}{C_1 \frac{\mu_t \epsilon}{k} \frac{\partial u_i}{\partial x_j}^2} \quad (6.2.1)$$

and

$$\frac{\frac{\mu_t}{\sigma_\epsilon \mu} \frac{\partial \epsilon}{\partial x_j} \frac{\partial \mu}{\partial x_j}}{C_1 \frac{\mu_t \epsilon}{k} \frac{\partial u_i}{\partial x_j}^2} \quad (6.2.2)$$

In the case of the 0.1% solution, the maximum value of the first of these ratios in the region downstream of the baffle is $\sim 20\%$, and of the second $\sim 5\%$. In the case of the 0.2% solution, the maximum value of the first ratio in the downstream region is $\sim 100\%$, and of the second $\sim 10\%$. Comment on this result will be made in connection with consideration of these quantities for the mixing vessel prediction, in section 6.3.4.

6.3 Analysis of mixing vessel flow predictions

6.3.1 Case details

Hockey (1990) has measured the flow of a 0.2% aqueous solution of CMC, identical to that employed by de Pinho in the pipe flow cases considered in sections 6.2.2 and section 6.2.4, in the mixing vessel configuration used in the Newtonian fluid flow study considered in section 5.3 (figure 5.3.1). Hockey’s measurements were made at an impeller speed of 600 rpm; this corresponds to a power number N_P

$$N_P = \frac{P}{\rho N^3 D^5} \quad (2.4.15)$$

of 4.3. Using the Metzner-Otto procedure, outlined in section 2.4.3, for obtaining an average molecular viscosity and thus bulk Reynolds number

$$Re_{mv,st} = \frac{D_{imp}^2 N \rho}{\mu_{av}} \quad (2.4.16)$$

produces a value of $Re_{mv,st}$ of 9,600 – where Hockey (1990) found that to obtain an $N_P - Re_{mv,st}$ correlation equivalent to the Newtonian (including coincidence of the zone of transition) necessitated a value of the constant c in (2.4.17) of ~ 54 . Hockey also obtained measurements of the flow, at 600 rpm, of a high-viscosity Newtonian fluid – an aqueous solution of glycerine with $\mu = 1.14 \times 10^{-2}$ kg/m-s and $\rho = 1142$ kg/m³ – in this vessel. This corresponds also to values of N_P and $Re_{mv,st}$ of 4.3 and 9,600, respectively i.e. the glycerine and CMC cases (as they will be referred to from hereon) are power-matched, and by extension, bulk-Reynolds-number matched. A lid was found necessary in both cases to prevent troughing and air entrainment at the fluid surface.

The grid of 15,903 points employed for the water flow predictions presented in the previous chapter, figure 5.3.2, was initially employed in obtaining predictions for the CMC case also. It was, however, found that at many points along the baffle and the lid several grid nodes along a normal to the surface were located within the sublayer, as defined by the value of y^+ at such nodes being less than y_{lt}^+ ; and while a reduction of residuals of several orders of magnitude in a computation on this grid proved achievable, convergence to the point of sensible iteration-to-iteration invariance of field values did not.

Accordingly the $31 \times 26 \times 19 = 15,314$ point grid of figure 6.3.1 was adopted, with greatly increased node-to-wall distances on all solid boundaries, these being necessary to ensure that over the greater part of the area of solid surfaces the next-to-wall-node values of y^+ were less than y_{lt}^+ . In view of the size of next-to-wall cells further grid refinement was not considered worthwhile because of the amplification of truncation errors associated with excessively large ratios of successive inter-nodal distances.

While the comparison between the glycerine case and that of the water flow considered in chapter 5 is of interest insofar as they are characterised by different values of Re_{mv} , the primary purpose of the glycerine case predictions is to provide a basis for comparison with the CMC case. The 15,903-point grid of figure 5.3.2 was used for these predictions, as axial and radial node density is sufficiently close to that of the 15,314-point CMC case grid in regions removed from solid boundaries

that differences in the predictions attributable to discretisation may be considered negligible. Within the time constraints of this study it did not prove possible to obtain predictions for the flow of this fluid on a finer grid; in making comparisons with the water case the effects of grid refinement illustrated in chapter 5 must therefore be borne in mind.

6.3.2 Flow patterns in vertical ($x - r$) planes

Velocity vectors in successive planes are presented in figure 6.3.2, axial and radial velocity profiles in figures 6.3.3 and 6.3.4, respectively, and the complementary iso-bars in figure 6.3.5 – these illustrate the same flow pattern, in qualitative terms, as shown in the 87,000-point grid predictions for the flow of water (hereafter referred to as the water case) already considered in section 5.3.2, as expected. Discussion here will accordingly focus on the quantitative differences between the predictions for the CMC case and those for the water and glycerine cases, in an attempt to determine which may be ascribed to numerical and/or modelling factors and which are reproductions of shear-thinning behaviour. In the glycerine case, velocity vectors are not presented in view of qualitative similarity of the flow field to that of the other fluids; rather comparison with the CMC flow field, in the 0° plane, is made on a profile-by-profile basis in figures 6.3.6 to 6.3.10. The experimental data on figures 6.3.6 to 6.3.10 have been included here to avoid later duplication of the figures – discussion of the comparison with these measurements will be made in section 6.4.

The impeller jet

It is apparent from the velocity vectors in all planes that the upward inclination of the impeller jet is much less pronounced than in the water case predictions. It is noted, however, that the degree of jet asymmetry predicted for the water flow increased with grid refinement – compare the 16,000 point and 87,000 point predictions at $r = 0.748R$, figure 5.4.9 – and it is thus reasonable to ascribe the flatter prediction for the CMC case to grid coarseness also.

Figure 6.3.6 illustrates that while the velocity profiles across the impeller jet, for the CMC and glycerine cases, are coincident at the blade tip ($r = 0.340R$), reflecting the employment of the same values of the empirical data in the impeller treatment in both cases, the magnitudes of the glycerine flow velocities are $\sim 3.5\%$ greater at the jet peak at $r = 0.544R$ and $r = 0.748R$, due to the 14% higher

density (and hence greater momentum) of the glycerine solution. The jet shape is similar in both cases, however, indicating that turbulent diffusion continues to govern cross-stream redistribution, as might be expected since $Re_t = 1330$ at $r = 0.544R$ and $= 860$ at $r = 0.748R$ in the CMC case, and $= 1170$ at $r = 0.544R$ and $= 1000$ at $r = 0.748R$ in the glycerine case. The greater radial gradient in Re_t in the CMC case is a reflection of shear-thinning, the molecular viscosity being lower than that of the Newtonian glycerine solution in the impeller jet at the blade tip and immediately downstream, of approximately the same magnitude in the impeller jet at the radius of the baffle edge, and higher elsewhere in the vessel – compare figures 6.3.11 and 6.3.12.

The below-impeller region

The predicted strength of the downward wall jet is greater in the CMC than the glycerine case, and increasingly so as the vessel bottom is approached – figure 6.3.7. The jet width in the CMC case is also increasingly narrower from $x = 0.170H$ down. Significant discrepancies are also evident in the upflow region, across the complete radius up to $x = 0.119H$ and in the vicinity of the axis up to the impeller. Re_t is a minimum in both cases in the region immediately inboard of and below the toroidal vortex, figures 6.3.11 and 6.3.12, but while never less than 250 in the glycerine case, it is less than 100 in the CMC case for $r > 0.4R$ at $x = 0.068H$ and in a narrowing region up to $x \sim 0.2H$ and $r \sim 0.5R$. This is clearly not the high-Reynolds-number regime on which the assumptions incorporated in the $k - \epsilon$ model are predicated. In the region of lowest Re_t just identified the steeper predicted gradient in the flow of CMC is particularly marked, a direct result of lower turbulent diffusion.

The predicted radial velocities at all radial locations below the impeller, with the exception of that at $r = 0.272R$, are smaller in magnitude in the CMC than the glycerine case, near the bottom and more particularly near the impeller ($r < 0.3R$) and the impeller jet ($r > 0.3R$) – figure 6.3.8. This prediction of a more abrupt switch from floor jet to upward flow, and the later entrainment of the upflow in the impeller jet (the latter being particularly obvious in the narrower impeller jet profiles for the flow of CMC at $r = 0.544R$ and $r = 0.748R$) must be attributed to the lower Re_t obtaining in the CMC case, with the associated reduction in turbulent diffusion.

The above-impeller region

The predicted axial velocity in the inflow region above the impeller is virtually identical for both CMC and glycerine cases – $x = 0.408H$, figure 6.3.9 (where $Re_t \approx 400$ in the CMC case and ≈ 1000 in the glycerine case) and the discrepancy in the wall jet at this height is attributable to the grid used in the CMC case. The difference in the downflow velocities at $x = 0.180H$, however, is of the order of 10% of the glycerine case values, and in the width of the upflow region $\sim 25\%$ of the glycerine case value. This is considered to reflect less the predicted level of turbulence at this level than the large discrepancy propagated from the $x = 0.240H$ level, which is of the order of 50% of the Newtonian values. Here Re_t is in the range 100 – 200 for the CMC case, as compared to 200 – 1200 for the Newtonian case, and a sharper wall jet is thus observed in the former, resulting from the much lower levels of turbulent diffusion.

Differences in predictions of radial velocities between the CMC and glycerine cases are substantially greater above the impeller than below – it, as a proportion of these velocities – figure 6.3.10. This, however, reflects the fact that the above-impeller velocities are an order of magnitude smaller than those below and thus the discrepancies are no greater in absolute terms than before. The one qualitative discrepancy is the outward flow in the CMC case as opposed to the inward flow in the glycerine case at $r = 0.408R$ and $0.476R$ – this is associated with differences in the location and direction of rotation of the downward vortex which will be considered in the following section.

6.3.3 Flow patterns in horizontal ($r - \theta$) planes

Velocity vectors for the CMC case in successive planes are presented in figure 6.3.13 and swirl velocity profiles in figure 6.3.14, with a few representative pressure distributions in figure 6.3.15. Comparison of predicted swirl velocities with those for the glycerine case, in the 0° plane, is made in the below- and above-impeller regions in figures 6.3.16 and 6.3.17, respectively. Again, consideration of the comparison with the experimental data in figure 6.3.16 will be made in section 6.4.

The below-impeller region

Comparison of the velocity vectors for the CMC and water cases (figures 6.3.13 and 5.3.7, respectively) shows similarity of flow patterns in the near-bottom re-

gion (essentially radial inflow, with a similar vortical structure at $\theta \approx 70^\circ$), and nearer the impeller, at $x = 0.25H$ (radial outflow near the baffle plane, strong swirl between baffles). At the intermediate $x = 0.187H$ level the upflow vorticity downstream of the baffle has strengthened its twin contra-rotating structure in the CMC case; this twin structure was only evident at the lowest ($x = 0.054H$) level in the water case, and has been suppressed completely at $x = 0.187H$.

In the lower region of the vessel ($x = 0.068H$ and $0.170H$) the predicted co-rotational swirl in the vicinity of the axis, in the CMC case, is twice that in the glycerine case – figure 6.3.16. The steeper gradients cannot directly be attributed to low Re_t values in the former case, however, as these are comparable in both, from bottom to impeller for $r < 0.05m = 0.34R$ (eg. at $r = 0.025m = 0.170R$, $(Re_t)_{glc} \approx 420$ and $(Re_t)_{CMC} \approx 390$ at $x = 0.05m = 0.170H$, and $(Re_t)_{glc} \approx 390$ and $(Re_t)_{CMC} \approx 460$ at $x = 0.08m = 0.272H$; see also figures 6.3.11 and 6.3.12). The difference in the predicted values between the CMC and water cases is still larger (a factor of ~ 4 – compare figures 5.4.19 and 6.3.16). It is noted that the near-axis swirl velocities in the glycerine case are approximately twice the magnitude of those in the water case, but when normalised by impeller tip speed the magnitudes are comparable. It is notable that little axial variation in swirl is predicted for both CMC and glycerine cases, from impeller to bottom, and it is thus possible that the CMC/glycerine case differences, to $r < 0.05m = 0.34R$, originate with the differences ‘seen’ by the equations on the impeller disc, and that these are maintained, in essentially solid-body rotation (to a radius of $0.02m$), to the lowest levels in the vessel.

The sharper swirl velocity gradients in the CMC case for $x > 0.119H$ and $r > 0.11m = 0.75R$ (figure 6.3.16) by comparison with both the glycerine and water cases (figures 6.3.16 and 5.4.19, respectively) *are* attributable to the low turbulent diffusivity already noted in this region in connection with consideration of the wall jet in the previous section.

The above-impeller region

The most substantial difference between the flow patterns evidenced by the velocity vectors, figure 6.3.13 for the CMC case and figure 5.3.7 for the water case, is the strongly co-rotational flow, at all levels from lid to impeller in the near-axis downflow, in the CMC case, compared to the counter-rotating flow, strong near the surface and weaker as the impeller is approached, in the water case. Consideration of the swirl velocity profiles on the various grids for the water case, figure 5.4.25,

indicates that this difference may be a grid dependency effect – the prediction for the flow of water on the 16,000 point grid is in fact in agreement with that for the flow of the CMC solution.

The upward vortex downstream of the baffle continues through the $x = 0.599H$ plane in the CMC case whereas it is no longer clearly defined at $x = 0.605H$ in the water case. While predictions on the various grids in the latter case have not been compared in the plane of the vortex, figure 5.2.27 makes the comparison just upstream, in the baffle plane, and this shows little grid dependence in the region immediately inboard of the baffle. Rather the greater vortex height in the CMC case is likely to be another reflection of the increased suppression of turbulence associated with the thicker boundary layer on the downstream face of the baffle and consequent reduced turbulent diffusion of the vortex.

The vortical structure at $x = 0.837H$ in the CMC case (figure 6.3.13), in the downflow region and downstream of the baffle, is but slightly upstream of that at $x = 0.850H$ in the water case (figure 5.3.7). In both cases also the locus of the vortex centre is in the downstream direction with progress toward the impeller; while the vortex is still identifiable at $x = 0.551H$ in the water case it has been absorbed into the overall impeller-induced swirling flow before reaching $x = 0.599H$ in the CMC case. The directions of rotation are, however, opposite, that in the CMC case being counter to that of the impeller. This is partly attributable to the differing directions of swirl in the region of the axis referred to above *ie.* to grid dependence, and partly to the lower levels of turbulent diffusion in the CMC case, which serve to exacerbate gradients – figure 6.3.17 illustrates this by comparing the swirl predictions for the flows of the CMC and glycerine solutions.

6.3.4 Turbulence energy and dissipation rate distributions

Distributions of turbulence energy, in normalised form, $\tilde{k}$, for the CMC case, are presented in $x - r$ and $r - \theta$ planes in figures 6.3.18 and 6.3.19, respectively; and for the glycerine case in $x - r$ planes in figure 6.3.20. The same contour values are used for the CMC and glycerine cases to facilitate comparison, though chosen with a view to optimum illustration of the distributions in the CMC case – this applies also to the length and time scale distributions presented in the following sections. The contour intervals are piecewise linear (contours A-C, then D-G) for the $\tilde{k}$ distributions, and pseudo-logarithmic scale for the $\tilde{\epsilon}$ distributions.

While impeller jet values of $\tilde{k}$ are comparable in both case in all planes, it is

immediately obvious that at all other locations values are substantially lower in the CMC case, and this primarily reflects the influence of the solid boundaries, and the prediction of very much thicker boundary layers.

Distribution patterns are broadly similar in the 3° plane, with minimum bulk flow values in both cases associated with the regions inboard of the toroidal vortices. Values in the vortices do not differ by more than a factor of 2, and are closer in the upflow region below the impeller; the discrepancy in the lowest and highest 10% of the vessel is greater than a factor of 3, however, and this applies over a still larger volume immediately upstream and downstream of the baffle, figures 6.3.18b and 6.3.20b. While the inward locus of the toroidal vortices is associated with the disappearance of the local minimum inboard of the vortices in planes adjacent to the baffle in both cases, the discrepancy in absolute values outboard of the radius of the baffle edge *ie.* $r > 0.8R$, is particularly marked.

The $r - \theta$ plane distributions, figure 6.3.19, for the CMC case serve to emphasise that the suppressive effect of the baffles is fully as great as that of the walls, bottom and lid; the extent to which this influence extends inward, in terms of giving rise to substantial circumferential gradients $\partial k / \partial \theta$, is particularly worthy of comment in the lowest plane for which distributions are shown, figure 6.3.19a.

It has been suggested in the previous chapter that Re_t is a measure of the relative importance of turbulent and molecular diffusion. To relate the quantity to the turbulence processes described in section 3.5 offers an further interpretation of the predicted levels of turbulence energy in the vessel. The energy spectrum, defined as the Fourier transform of the velocity autocorrelation, may be considered in terms of production, inertial and dissipation ranges – see Tennekes and Lumley (1972). It is only with the existence of an identifiable inertial range, in which no energy is added by the mean flow and none taken out by viscous dissipation, that a cascade mechanism is truly present, and Driscoll and Kennedy (1983) note that overlap between the production and dissipation ranges of the turbulence spectrum is significant for $Re_\lambda < 100$, where

$$Re_\lambda = \frac{u' \lambda}{\nu} \quad (6.3.1)$$

and

$$u' = \left(\frac{2k}{3} \right)^{3/2} \quad (6.3.2)$$

and λ is the Taylor microscale

$$\lambda^2 = \frac{10\nu k}{\epsilon} \quad (6.3.3)$$

Re_λ is thus related to Re_t as

$$Re_\lambda = \sqrt{10} \sqrt{Re_t} \quad (6.3.4)$$

This suggests that a transfer range cannot be identified in the spectrum for $Re_t < 1000$, which, it will be noted from figures 6.3.11 and 6.3.12, is the value which obtains at all locations outside the impeller jet.

The extra ϵ equation source terms

The relative magnitudes of the extra ϵ equation source terms, as defined by (6.2.1) and (6.2.2), for the CMC case predictions (these terms are obviously zero for the Newtonian cases) are presented in figure 6.3.23, in addition to the magnitude of their sum relative to the same 'standard' term. The first extra term has a maximum relative magnitude of $> 500\%$, associated with the regions immediately above and below the impeller; values in the impeller jet are in the range $10 - 100\%$. The second has a maximum relative magnitude of $> 100\%$, again in the regions immediately above and below the impeller; values in the impeller jet are $< 10\%$.

This result, of non-negligible terms in spatial gradients of molecular viscosity μ , is consistent with that for the pipe with axially-mounted baffle cases seen in section 6.2.4; it is difficult to justify in an equation representing inertially-dominated turbulence processes. The same level of rigour has been employed in the derivation of the exact equation with μ as a field variable as in its original derivation in which spatial gradients of μ did not have to be accounted for, and modelling of the extra terms has followed the same principles as the original modelling. Thus it is considered that this outcome reflects on the inadequacy of the assumptions made in the modelling of the ϵ equation as a whole, and/or the assumptions underlying the derivation of the exact equation (perhaps the most tenuous of these is that a single length scale constitutes an adequate characterisation of the local structure of turbulence).

6.3.5 Turbulence length and time scale distributions

The length scales are presented on the same normalised basis, as for the water case considered in the previous chapter *ie.* $\tilde{L} = L/r$. The distribution contours are presented in $x - r$ and $r - \theta$ planes as figure 6.3.24 and 6.3.25, respectively, for the CMC case and in $x - r$ planes as figure 6.3.26 for the glycerine case. As before, smaller contour intervals at the lower end of the scale in the $x - r$ plane figures are employed to illustrate the steeper gradients in the impeller jet.

The range of values of $\tilde{L}$ in the CMC and glycerine cases is broadly similar – the same contour values are used in the presentation in each case, but contours of equal value are seen to be approximately co-located, with exceptions which will be discussed momentarily. This is of course in accord with the expectation that the distributions of quantities characteristic of the macro scales should be similar *ie.* rheology independent. Equally encouraging, however, is the similarity of the distributions in the $Re_{mv} = 48,000$ water case and the $Re_{mv} = 9,600$ glycerine case *ie.* the predictions do indicate substantially independent-of- Re values of L when normalised by impeller radius.

Turning to specific comparisons, and making those between the water and glycerine cases – figures 5.3.14 and 6.3.26 – first, the 0.05 and 0.07 contours in the impeller jet are essentially coincident in all planes; impeller blade-tip to baffle-edge growth is a factor of 1.76 at $\theta = 1.5^\circ$ in the water case, and 1.66 at $\theta = 3.0^\circ$ in the glycerine case. Below-impeller values are in the range $\sim 0.07 - 0.14$ in the former case, $\sim 0.05 - 0.09$ in the latter; above the impeller the ranges are $\sim 0.11 - 0.20$ and $\sim 0.09 - 0.17$. The somewhat higher values in the water case are attributable to the higher levels of turbulence kinetic energy predictions obtained on a finer grid. The influence of the baffle is also similar in both cases – the near-coincidence of the 0.05 and 0.07 contours, throughout the flow, in the $\theta = 44^\circ$ plane in the water case and in the $\theta = 43^\circ$ plane in the glycerine case is in particular noteworthy.

The coincidence of impeller-blade-tip values in the CMC and Newtonian cases reflects the use of the same boundary conditions; the lower rate of growth in $\tilde{L}$ in the impeller jet (of a factor of 1.36) in the 3.0° plane, in the former case, reflects the more rapid fall-off in turbulence energy levels as the radius of the baffle edge is reached. This is less pronounced in planes near that of the baffle – compare the 42.3° (CMC) and 43.0° (glycerine) distributions – but is once more apparent on reaching the 54° plane.

Values below the impeller jet are in the same range (0.07 – 0.09) in both the

CMC and glycerine cases; on the inner side of the local toroidal vortex, however, the CMC case values are substantially lower, attributable to lower k values in this region (compare figures 6.3.18 and 6.3.20; see also the Re_t distributions, figures 6.3.11 and 6.3.12). The other noteworthy feature of the below-impeller region distributions is the *higher* value of $\tilde{L}$, in the CMC case, below the impeller disc.

Discrepancies in the above impeller region are only of significance at mid-radius in the upper region of the vessel ($r \approx 0.2 - 0.6R$ and $x > 0.6H$), where the glycerine case values are $\approx 10 - 25\%$ higher; reference to figures 6.3.11 and 6.3.12 will confirm that Re_t is here in the range 200-300 in the CMC case, as opposed to 700-1000 in the glycerine case. In the higher-turbulence-intensity region surrounding the upper vortex the values are in close agreement – as are the CMC and water case values here: consider the locations of the contours in the 0.075-0.12 range in the water case at $x = 0.442H$ (figure 5.3.15) with those in the 0.070-0.12 range in the CMC case at $x = 0.440H$ (figure 6.3.25).

Figures 6.3.27 and 6.3.28 present the normalised integral time scales $\tilde{\tau}$ in $x-r$ and $r-\theta$ planes, respectively, for the CMC case; figure 6.3.29 presents this quantity in $x-r$ planes for the glycerine case. The inverse of the impeller blade frequency (here = 0.1sec) is the normalising quantity, as before.

Comparison of the normalised time scales in the water and glycerine cases – figures 5.3.16 and 6.3.29, respectively – shows that this quantity is also sensibly independent of Re_{mv} over this Re_{mv} range. The most specific support for this conclusion is the locus of the 0.4 contour in the impeller jet, in all planes, but more generally, the range of values in various regions is close *eg.* 1.5 – 3.4 above the impeller in the 1.5° (water) and 3.0° (CMC) planes for $r < 0.8R$, and $\sim 1.0 - 2.0$ below the impeller in the 54° plane.

The range of values of $\tilde{\tau}$ in the CMC case is broadly coincident with those for the Newtonian cases, albeit with more pronounced local differences owing to low levels of turbulence energy. Impeller boundary conditions of course impose the same values of $\tilde{\tau}$ on the blade tip in the CMC and glycerine cases, of 0.126; the blade-tip to baffle-edge increase is 2.93 in the CMC case and 3.36 in the glycerine case (which seems to be a Re_t effect; the corresponding figure for the water case is 4.68). Wall-jet values are consistently in the range 0.6 – 1.3 in all planes in both cases; the significant discrepancies are in the zone below and immediately inside the lower toroidal vortex, and in the effect of the baffle over a greater circumferential interval in the CMC case. While the former discrepancy is probably largely due to the inability of the present methodology to predict adequately levels

of k , particularly near the vessel bottom (*cf.* experimental comparisons in section 5.4.4 and to follow in section 6.5.4), the latter is equally probably qualitatively in accordance with a reality of a very much thicker baffle boundary layer.

6.3.6 Kolmogorov length and time scale distributions

The characteristic length and time scales of the Kolmogorov eddies, η and τ_k respectively, have been defined in section 5.3.6, they are presented here in $x - r$ and $r - \theta$ planes for the CMC and glycerine cases in turn, as figures 6.3.30 to 6.3.34.

Values of η in the CMC case range from $\sim 5 \times 10^{-5} - 6 \times 10^{-4}$ m, and in the glycerine case from $\sim 7 \times 10^{-5} - 3.5 \times 10^{-4}$ m; impeller tip values in the plane of the disc are 4.4×10^{-5} m and 6.0×10^{-5} m, respectively. The greater range of η_{CMC} is a shear-thinning effect; thus it is lower than η_{glc} in the vicinity of the impeller due to lower molecular viscosity ($\mu_{\text{CMC}}/\mu_{\text{glc}} = 0.57$ on the blade tip), approximately equal at the radius of the baffle edge ($(\mu_{\text{CMC}}/\mu_{\text{glc}} = 0.84$ at $r = 0.8R$) and higher elsewhere in the vessel ($\mu_{\text{CMC}}/\mu_{\text{glc}}$ is of the order of 2 in much of the above-impeller region; the notional limiting value is 4.38, at a shear rate of 1s^{-1} , though this is not approached in these predictions). By comparison the range of η in the water case is $\sim 2 - 9 \times 10^{-5}$ m; the factor of ~ 5 being similar to the glycerine case. The extent of the ranges of η_{glc} and η_{water} are governed by that of ϵ alone, though of course the very much smaller magnitudes of η_{water} , particularly in regions removed from the impeller, reflect the order of magnitude difference in μ .

In addition to the greater radial gradient in η in the impeller jet in the CMC case – the ratio of baffle edge to blade tip values is 2.56, as opposed to 1.93 in the glycerine case – a qualitative as well as quantitative difference may be noted in planes removed from the baffle. Values in the jet impingement zone extend a greater distance away from the zone in the flow of the CMC solution, reflecting the relatively slower growth of μ_{CMC} in the locally high- ϵ wall jets, while steep gradients in the near-wall region reflect the collapse in ϵ values due to the thicker boundary layer (figures 6.3.21 and 6.3.22 may be compared in this context).

Values of τ_k in the CMC case range from $\sim 6 \times 10^{-4} - 2 \times 10^{-2}$ s, and in the glycerine case from $\sim 5 \times 10^{-4} - 1.15 \times 10^{-2}$ s; impeller tip values in the plane of the disc are 2.9×10^{-4} s and 3.6×10^{-4} s, respectively. Shear-thinning effects may again be identified by comparison of the ratios of blade tip and baffle edge values, in the plane of the impeller disc; this ratio is 4.47 in the CMC case and

3.71 in the glycerine case.

As for η , the significance which may be attached to distributions of τ_k in regions removed from the impeller jet and vortex vicinity is limited, in view of the reservations which must attach to the predictions of turbulence quantities as a whole in these zones.

The principal practical implication to be expected from the larger gradients in η and τ_k in the shear-thinning cases is that micromixing and reaction processes will be more localised *ie.* concentrations of reactants/products in regions of low η and τ_k will be more pronounced. Furthermore, processes governed by these scales are less likely to proceed more quickly as a result of increased impeller input power, as this is likely to be dissipated in the impeller region and intensify localisation – rather these are processes whose efficiency is most likely to be increased by multiple impeller configurations.

6.4 Comparison of mixing vessel flow predictions with experiment

The profile-by-profile discussion of the predictions for the CMC and glycerine cases, figures 6.3.6 to 6.3.10 and figure 6.3.16, is here extended to consideration of the experimental data of Hockey (1990). This is available in the 0° plane only.

6.4.1 Mean axial velocity comparisons

The discrepancies between Hockey's (1990) experimental values for axial velocity, for the CMC and glycerine cases, at all locations except $x = 0.828H$, are within the range of his estimated uncertainty, indicating that with the exception of the near-lid location the fluid rheology has no influence on the distribution of this quantity *ie.* turbulence levels are indeed sufficiently high for turbulent diffusion to be the dominant redistributive mechanism.

The below-impeller region, figure 6.3.7

The agreement between prediction and experiment for the glycerine case, at all axial locations for $r > 0.05m = 0.34R$, is as good or better than that for the water case – figure 5.4.1. The overprediction near the axis is attributed in part to truncation error, as it is noted that the predictions for the water case on the finest grid indicate a capturing of near-axis gradients at $x = 0.265H$ and $0.282H$ which is not in evidence in the coarser grid predictions – figure 5.4.1.

The predictions of sharper gradients for the CMC case, discussed in section 6.3.1, are confirmed to be incorrect by the experimental data, and the failure to adequately estimate levels of turbulent diffusion is considered to reflect the underprediction of turbulence kinetic energy using the $k - \epsilon$ model in this type of flow – consider the comparison with experiment in the water case, presented in section 5.4.4 (the degree to which the underprediction is repeated in the present case will be apparent in the discussion to follow in section 6.5.4). Thus the apparently accurate prediction in the vicinity of the axis at $x = 0.0272H$ is considered to be fortuitous, the cancellation of too-low turbulent diffusion by numerical diffusion (*cf.* the above comments for the glycerine case).

The above-impeller region, figure 6.3.9

The agreement with experiment in the glycerine case is of the same quality as in the water case. Thus at a level intermediate between impeller and surface – $x = 0.612H$ – the wall jet is predicted to within the bounds of experimental uncertainty, and the strength of the downflow is slightly underpredicted, a discrepancy which would be resolved by grid refinement – see the 16,000 and 87,000 point SFCD predictions for the water case at $x = 0.544H$ and $0.680H$, figure 5.4.6. Closer to the surface – $x = 0.828H$ – wall jet strength is underpredicted, and underprediction of downward velocity greater; this again accords with the comparison for the water case on this grid with SFCD, and the differences here are also chiefly attributable to grid coarseness. It is noted, however, that the prediction of a local minimum in downward velocity at $r \approx 0.06m \approx 0.4R$ is here well supported, in terms of both location and relative magnitude, by the experimental data, in contrast to the comparison with the water case, for which the experimental data is admittedly much sparser.

The agreement between prediction and experiment in the CMC case at $x = 0.408H$ and $0.612H$ is satisfactory, as might be expected given the strength and hence convection-dominated nature of the flow; underestimation of redistribution due to turbulence is again manifest in the region of lower Re_t at $r > 0.1m \approx 0.7R$ where the width of the wall jet is underpredicted and its peak strength overpredicted. At $x = 0.828H$ experiment indicates that velocities are an order of magnitude smaller for the CMC than the glycerine case, over the greater part of the radius ($r > 0.06m \approx 0.4R$), with the replacement in the near-wall region of the strong upward jet by a weak downflow. It is difficult to conceive of the very much flatter CMC profile at these radial locations as resulting from turbulent diffusion,

nor is there any evidence for it in terms of the r.m.s. velocity measurements to be presented in the course of the comparison with turbulence energy predictions in section 6.5.4. Accordingly it is concluded that this (experimental) profile reflects a very much thicker boundary layer associated with the lid, and wall in the upper region, in the flow of the CMC solution. The predictions fail to capture even the qualitative aspects of this behaviour, and continue to exhibit the pattern of a relatively strong upward wall jet, resulting from low turbulence level predictions, at this and higher locations, to the last node before the lid (at $x = 0.860H$).

Values of Re_t have been cited above in support of the argument that too-low predicted values of k are responsible for steeper gradients in the CMC case predictions, and a brief comment on the relative accuracy of the values of Re_t in the CMC case is thus appropriate. It would indeed be anticipated that $(Re_t)_{CMC}$ be somewhat lower than $(Re_t)_{glc}$: due in part to the higher mean molecular viscosities associated with the flow of the CMC solution (averaging $\sim 180\% - 200\%$ of the glycerine values according to the predictions) and also to the very much thicker boundary layer associated with flow of this solution. The above statements hinge, however, on the contention that the values of $(Re_t)_{CMC}$ are lower to a physically incorrect degree, and that this is due to underprediction of k . Any underprediction of k will, however, entail a lower value of ϵ and therefore a higher value of μ (calculated according to (3.7.36)). Thus while modelling of shear-thinning behaviour (plausibly) amplifies the underprediction of Re_t resulting from underpredicted k it is possible that the ratio of $(Re_t)_{CMC}$ to $(Re_t)_{glc}$ is exaggerated by the model for μ (through poor estimates of ϵ and/or the other parameters in (3.7.36), or more fundamentally because of invalidity of the model).

6.4.2 Mean radial velocity comparisons

The impeller jet, figure 6.3.6

The peak impeller jet velocity on the blade tip ($r = 0.340R$), in the CMC case, is underpredicted by 27%, with overpredictions of 14% at $x = 0.092m = 0.313H$ and 23% at $x = 0.104m = 0.354H$.

At the $r = 0.544R$ location both peak strength (92% of the experimental value) and asymmetry of the jet are reasonably well predicted in the CMC case; as in the water case, however, the rate of decay of the impeller jet is underpredicted, and this translates into an 18% overprediction of peak velocity at $r = 0.748R$. The corresponding figures for the glycerine case are 102% and 108% of the experimental

values, respectively. The discrepancy in the predicted strength of the impeller jet in the two cases is due to the differing values in the ‘wall functions’ used as boundary conditions on the impeller disc, which result in a difference in impeller tip values of radial velocity of $\sim 4\%$ of the CMC case values. The experimentally-observed behaviour is rather different for each of the solutions: the CMC solution has the stronger jet at $r = 0.544R$, but the weaker (by 16% of the glycerine case value) at $r = 0.728R$. A consistent feature of the experimental data for the flow of both solutions, however, is the shift in the location of the peak impeller velocity from $x = 0.333H$ at $r = 0.340R$ and $0.544R$ to $x = 0.350R$ at $r = 0.728R$: this is not reflected in the predictions but the water case study indicates that it would be on finer grids.

The below-impeller region, figure 6.3.8

Given the small magnitudes involved, a remarkable degree of mutual consistency is exhibited by the measurements of radial velocity between the vessel bottom and the impeller, well within the bounds of uncertainty in all cases, and consistent with the pattern of mutual agreement seen in the measurements of axial velocity in the same region.

At $r = 0.136R$ the prediction for the glycerine case is accurate to within experimental error bounds, with the flatter CMC profile attributed to lower turbulent diffusion of the principal (axial) velocity component, as discussed in section 6.3.2. The incorrect prediction of a zero axial gradient at $r = 0.272R$, in both cases, is attributable to inadequate grid refinement – note the improvement in gradient resolution from the 16,000 to the 87,000 point grid at $r = 0.340R$ in the water case, figure 5.4.9. At the locations further from the axis the agreement between the predictions and the experimental data for the flow of the glycerine solution is extremely good – much better than between the predictions on this grid and the measurements for the water case; this is particularly marked near the vessel bottom. Hockey’s (1990) measurement for the glycerine case is 75% of his water case value at $r = 0.612R$ and $x = 0.02m = 0.068H$, and 78% at $r = 0.680R$ at the same axial location, if the velocities are normalised by impeller tip speed. This data for the water case is not shown but is close to Yianneskis’ (1982) value at the intermediate $r = 0.646R$, $x = 0.02m = 0.068H$ location, figure 5.4.9. Thus the higher (normalised) velocity in the (higher Reynolds number) water case is a Reynolds number effect, not reproduced by the predictions. Furthermore the experimental corroboration of the glycerine case predictions emphasises that the predicted pro-

files for the CMC case are erroneously flat, again attributed to underestimation of turbulent diffusion of axial velocity.

The above-impeller region, figure 6.3.10

Differences between the measured values for the CMC and glycerine cases above the impeller are substantial in proportion to the magnitudes involved. These magnitudes are themselves sufficiently small in the near-axis region, however, ($r = 0.136R$ and $0.272R$) that the differences are within the bounds of experimental uncertainty. At all locations further from the axis magnitudes are sufficiently large that the differences cannot be so dismissed; furthermore they are sufficiently consistent as to be indicative of a genuine difference in flow pattern between the two cases. The higher velocities in the CMC case at $x = 0.12m = 0.408H$ (just above the impeller), for $r = 0.408R$ and $0.476R$, are indicative of a broader, more diffuse, impeller jet. At the $x = 0.18m = 0.612H$ level the non-negligible (of the order of 25% of the axial velocities) inward-directed flow in the CMC case contrasts with the very weak inward-directed flow in the glycerine case. This pattern is maintained at the $x = 0.24m = 0.816H$ level for $r = 0.408R$ and $0.476R$, but reversed for $r > 0.680R$; the inward flow of the glycerine solution is now relatively strong while the CMC solution is quiescent. This last is indicative of a much thicker boundary layer on the lid from mid-radius to wall in the CMC case; such an interpretation would also explain the discrepancy at the $x = 0.18m = 0.612H$ level as simply a downward shift in the inward flow, occasioned by the thicker layer. It is also consistent with the interpretation of the experimentally-measured axial velocity profile at the uppermost location, considered in the previous section.

6.4.3 Mean swirl velocity comparisons

The below-impeller region, figure 6.3.16

At $x = 0.068H$ the experimental measurements for the CMC and glycerine solutions are in close agreement with the exception of a much stronger wall jet in the CMC case, indicative of reduced turbulent diffusion in this flow. The disagreement evident at $r = 0.10m = 0.680R$ and $0.11m = 0.748R$ is of the order of experimental uncertainty but at the $x = 0.170H$ level the quantitative and qualitative discrepancies over most of the vessel radius are too great to be potentially due to experimental error. Given that closer to the impeller ($x = 0.221H$ and $x = 0.272H$) these differences are once more reduced, to within the bounds of

experimental uncertainty over the impeller radius, it is unlikely that they originate on the impeller disc (where fluid rheology might be expected to influence flow patterns); a conclusion that low levels of turbulence are responsible for allowing fluid rheology to play a rôle locally is equally tenuous, however, in view of the agreement already observed in the measured values of the other mean velocity components in the two flows.

The agreement between the predictions, particularly that for the glycerine case, and experiment is qualitatively very good indeed at all levels, in contrast to the water case. Particularly noteworthy is the experimental support for the predicted solid-body rotation in the near-axis region, with quantitatively satisfactory agreement in terms of magnitude and spatial extent from $x = 0.170H$ upwards. As the experimental data is self-consistent regarding this feature, and as Hockey's (1990) data is equally consistent with that of Yianneskis for the water case regarding its absence in that flow – see figure 5.4.19 – it must be regarded as a low bulk Reynolds number effect, which the present methodology incorrectly predicts to persist to too high a value of this parameter. Despite the discrepancies in the measurements they do confirm that the predicted gradients in this as in the other mean velocity components in the bulk flow, in the CMC case, are too large.

The near-wall gradient is well resolved at $x = 0.119H$, but underpredicted below this level and overpredicted above. This is indicative of large variations in sublayer thickness on the wall from the bottom to the jet region, and illustrates the difficulty in locating the next-to-wall node in an orthogonal grid (which implies that these nodes must be equidistant from the wall from bottom to jet) such that it is outside the sublayer where this is thickest but still within the logarithmic region where the sublayer is thinnest.

The baffle wake, figure 6.5.1

A limited number of measurements are available in the plane of the baffle (45°) and at 5° intervals in the downstream direction to the 65° plane, at a height $x = 0.221H$ and over the outer third of the vessel radius. Close correspondence is observed between the data for the CMC and glycerine cases in all planes; once more the CMC case predictions exhibit the relatively steeper gradients associated with low turbulence level predictions.

The prediction of strong swirl, in the glycerine case, inboard of and in the (45°) plane of the baffle, is contradicted by the experimental finding of radial flow, with the exception of the region adjacent to the baffle edge. Both experiment and

prediction are consistent with those at the nearest location for the water case – $x = 0.238H$, figure 5.4.22 – and grid refinement in the latter case was found to reduce the magnitude of the discrepancy but to maintain the overprediction of radial gradient $\partial w / \partial r$ and the too-close-to-baffle prediction of the local minimum. The comparisons in the wake region make clear that the strength of recirculation is very much underpredicted – particularly the near-wall reverse flow, not reproduced to any significant extent. Much better qualitative agreement is evident in the 60° and 65° planes; some reservation must however be expressed regarding the apparently good quantitative agreement in the glycerine case in the 65° plane in view of the deterioration in such agreement observed with grid refinement in the water case at the nearby location of $x = 0.238H$ and $\theta = 67.5^\circ$ – figure 5.2.24.

No measurements of swirl velocity are available in the above-impeller region.

6.4.4 Turbulence kinetic energy comparisons

The below-impeller region, figure 6.5.2

As measurements of all three components of r.m.s. velocity are available, the comparison made here is between turbulence kinetic energy calculated as $1/2(u'^2 + v'^2 + w'^2)$ and the predicted quantity k .

The overall level of agreement of the glycerine case predictions with experiment is comparable to that in the water case – figure 5.4.29 (where it should be remembered that the relevant comparison in the latter case is with the 16,000-point SFCD case predictions). Thus the k is fairly consistently underpredicted by a factor of ~ 3 at $x = 0.08m = 0.272H$ *ie.* immediately below the impeller, at locations from the axis to $r = 0.272R$, but agreement improves significantly from $r = 0.340R$ (reflecting the imposition of boundary conditions at $r = 0.333R$, the blade tip) to $r = 0.544R$, before deteriorating once more as the region of jet impingement on the wall is approached. Experiment indicates a very much less pronounced axial gradient $\partial k / \partial x$ in the glycerine than in the water case in the near-axis region, and accordingly the underprediction near the bottom, $x = 0.02m = 0.068H$ and $r = 0.136R$ is a factor of ~ 4 in the former case, whereas at the same height and $r = 0.116R$ the underprediction is a factor of > 5 in the latter case. This discrepancy is the largest in the solution domain, and Hockey's (1990) detailed data for the near-axis region for the glycerine case indicate that the r.m.s. values incorporate a considerable degree of 'pseudo-turbulence' due to vortex processing. This conclusion is based on the fact that the axial r.m.s. veloc-

ity component shows little radial gradient over the radius of the vessel as a whole, whereas the near-axis increase in the radial and tangential r.m.s. velocity components is substantial, yet if this were attributable to true turbulence the increase would be expected to be apparent in all three components, and certainly to be manifest in the direction of flow (here almost perfectly axial). Of the potential sources of error in prediction of true turbulence the reasonable agreement in mean swirl obtained for the glycerine case, figure 6.3.16, discounts underprediction of mean strain as a cause of underprediction of generation, and isolates the inadequacies of the eddy viscosity hypothesis (given the strong streamline curvature and the normal stresses due to 'floor' jet impingement).

The experimental data shows little significant difference between the CMC and glycerine cases, while the predictions show lower values in the CMC case near the vessel bottom and at all locations from $r = 0.408R$ outward; this is explicable primarily in terms of the very much thicker sublayer predicted to obtain on the vessel wall and bottom. Higher values are predicted for the CMC case at $x > 0.03\text{m} = 0.102H$, for $r \leq 0.340R$, and these are partly attributable to the contributions of the extra ϵ equation source terms, acting here as sinks – the relative influence of these terms on the predictions is more marked in this than in the baffle case because of the order-of-magnitude higher Re_t obtaining in the latter.

The above-impeller region, figure 6.5.3

As measurements of all only two components of r.m.s. velocity are available, the comparison made here is between the average of these and the quantity $\sqrt{2/3k}$ obtained from the predictions. It should also be noted that at most radial locations the reference value of the ordinate is non-zero.

Agreement in both cases in the region immediately above the impeller and jet is to within 25% until the radius of the baffle edge is approached ($r = 0.748R$ and $0.816R$). At intermediate levels ($x = 0.2\text{m} \approx 0.7H$) agreement is within 30% in the downflow region ($r \leq 0.272R$) and in the vicinity of the upper toroidal vortex ($r \geq 0.748R$); the discrepancy, particularly in the CMC case, widens to a factor of ~ 2 at intermediate radial locations, becoming more pronounced near the lid – $r = 0.544R$, $r = 0.646R$ and $r = 0.680R$. The discrepancy between the predictions is again in large measure attributable to the suppression of turbulence near solid boundaries – particularly so at the lid where, despite the size of the next-to-lid cells, $y^+ < y_{lt}^+$ for $r < 0.3R$ and $r > 0.7R$.

6.5 Summary of findings

Predictions of fully-developed turbulent pipe flow of Newtonian show that

- The $k - \epsilon$ model used with wall functions results in underprediction, of the order of 25%, of near-wall turbulence energy levels in Newtonian fluid flow – this is a weakness which is not generally recognised in the literature.

For the fully-developed turbulent pipe flow of shear-thinning fluids

- Prediction of the velocity distribution for a shear-thinning fluid with ‘log law’ slope equal to the Newtonian is to the same level of accuracy as obtained for Newtonian fluid flow.
- Predicted distributions for flows of shear-thinning fluids with ‘log law’ slope steeper than the Newtonian do not fully capture the measured velocity gradients.

The data against which predictions of turbulence energy are compared were obtained in the flow of a drag-reducing fluid, and show a very much steeper wall-to-axis distribution, and very much higher levels of near-wall turbulence energy when normalised by friction velocity, than characteristic of Newtonian fluid flow; anisotropy is more pronounced than observed in flow of Newtonian fluids. These are not shear-thinning effects; it can, however, be concluded that

- Correct prediction of turbulence energy levels in the flow of drag-reducing fluids, which is apparently an effect of elasticity, requires, as a first approximation, modification of $k - \epsilon$ constants and/or low-Reynolds-number modifications to the model.

Predictions of turbulent flow, in a pipe with an axially-mounted baffle, of water (Newtonian) and shear-thinning fluids show that

- Little difference in flow pattern is evidenced by predictions of flow of Newtonian and shear-thinning fluids; modest differences in turbulence energy levels are due to the extra ϵ equation source terms.
- Little difference in Kolmogorov length and time scale distribution patterns is evident between Newtonian and shear-thinning fluid flow; the range of these parameters, however, increases as a result of shear-thinning – by a factor of ~ 1.5 when the shear-thinning index is 0.73.
- Since the wall function approach requires location of next-to-wall nodes outside the viscous sublayer, and since this is thicker in the straight pipe flow of the fluids of interest, considerably coarser near-wall grid distributions are necessary with the use of wall functions. It must be emphasised, however, that

the degree to which the sublayers are thicker is largely due to phenomena other than shear-thinning.

- The first of the extra ϵ equation source terms is of the same order as the 'standard' terms, the second an order of magnitude smaller.

The level of agreement of these predictions, for the Newtonian fluid flow, with experiment is similar, to that obtained in previous work, with discrepancies being chiefly attributable to known deficiencies of the $k-\epsilon$ model. The data for the shear-thinning flow cases show differences in both flow pattern and turbulence structure which cannot be attributed to variations in molecular viscosity at the levels of turbulence intensity involved; this gives rise to greater discrepancies between the predictions and data, in both mean velocity and turbulence energy, than for the Newtonian case. The phenomena responsible are insufficiently well understood to enable recommendation of alternative modelling strategies with confidence but more pronounced anisotropy suggests that Reynolds stress models will be required.

Predictions for the flow of a shear-thinning solution in a mixing vessel have been analysed in conjunction with those for a 'power-matched' flow of a high-viscosity Newtonian fluid. Differences between the two sets of results are non-negligible, in contrast to experimental observation, and this is attributed in part to the inadequacies of the 'wall function' approach with the flow of these fluids, because of the thickness of the viscous sublayers involved, and partly to inadequacies in the turbulence model, which combine to result in too-low levels of turbulence energy and accordingly turbulent diffusion. This is further borne out by qualitatively similar, but lower in magnitude, distributions of k and ϵ . The following specifics are noted:

- The range of Kolmogorov scales is greater in the flow of the shear-thinning than the Newtonian fluids, with higher gradients in the impeller jet – this is a shear-thinning effect and as such expected.
- Both of the extra ϵ equation source terms are of the same order as the 'standard' terms.

The non-negligible relative magnitude of the extra ϵ equation source terms is difficult to justify in an equation representing inertially-dominated turbulence processes. Given, however, that the same level of rigour has been employed in the derivation of the exact equation with μ as a field variable as in that of the 'Newtonian' equation, and that modelling of the extra terms has followed the same principles as the original modelling, it is considered that this outcome reflects on the inadequacy of the assumptions made in the modelling of the ϵ equation as a

whole, and/or the assumptions underlying the derivation of the exact equation.

The low levels of turbulent diffusion in the case of the shear-thinning fluid are reflected in the comparison with experiment, which confirms the qualitative correctness of the predicted mean flow pattern, but shows that velocity gradients are overpredicted.

From the predictions for the flow of water and a high-viscosity Newtonian fluid

- Distributions of turbulence length and time scale have been found to agree, on a normalised basis, for flows of different Newtonian fluids at different bulk Reynolds numbers.

Comparison of the high-viscosity Newtonian fluid flow predictions with experiment has shown the same level of agreement of mean axial and radial velocity, and turbulence kinetic energy, as obtained on the same grid for the water flow, but also in particular that

- Agreement of mean swirl velocity in the below-impeller region is satisfactory, in contrast to that for the water case.

7 Conclusions

7.1 Achievements and findings

An existing methodology for the prediction of turbulent flow of Newtonian fluids in ducts and mixing vessels has been refined, and extended to enable prediction of such flows of shear-thinning fluids.

Experimental data in the literature for turbulent pipe flows of shear-thinning fluids indicates that a thicker laminar sublayer obtains than in such flows of Newtonian fluids *ie.* velocity profiles plotted on ‘law of the wall’ terms, with viscosity at the wall taken as the characteristic viscosity, are shifted upward. The degree of upward shift appears to be a function of the ‘power law’ index of the fluid; definitive conclusions require very much more experimental data than currently available. Such data would have to be for a range of flow rates at each of a range of ‘power law’ indices; the invalidity, or at best greater reliability than for Newtonian fluid flow, of flow comparisons on a Reynolds number basis alone has been made clear. A consensus has been identified in the literature that drag reduction is probably caused by elasticity and/or other normal stress mechanisms; while this places reproduction of the phenomenon outside the scope of this study the fact that pipe flows of many shear-thinning fluids exhibit such behaviour makes isolation of phenomena attributable to shear-thinning difficult.

The $k - \epsilon$ model of turbulence and the associated boundary conditions have been modified to account for shear-thinning fluid behaviour. The transport equation for rate of dissipation of turbulence kinetic energy ϵ has been rigorously re-derived, with mean molecular viscosity a field variable, and on the basis of an order-of-magnitude analysis two of the four terms additional to those in the ‘standard’ form of the equation which arise are retained in the modelled form. Wall functions have been employed as boundary conditions for solid boundaries; the values of the empirical coefficients are, however, chosen for each shear-thinning fluid on the basis of experimental data for the fully-developed pipe flow of that fluid. In addition a model for the mean molecular viscosity, based on ϵ , has been implemented.

A novel differencing scheme, Self-Filtered Central Differencing (SFCD), is employed in the discretisation of the convection terms of the transport equations; it guarantees boundedness while offering second-order accuracy. An explicit implementation *ie.* deferred flux correction is employed, with the correction updated after each iteration of the TDMA solution method employed for the sets of trans-

port equations.

The ratio of the computing effort in the solution of the pressure correction set to that in the solution of a representative transport equation set has been shown to be large; and conjugate gradient algorithm adopted in the solution of the pressure correction equation sets as a result. The reduction in computing effort occasioned by its use, by comparison with the use of the TDMA algorithm, has been quantified as a factor of > 20 on an 87,000 point grid, for solution to a final/initial residual ratio of 5%, and it has also been shown that the relative advantage increases as this convergence criterion is tightened.

For the case study of laminar flow in a pipe with a step contraction the use of SFCD has been shown to result in much more accurate predictions on a particular grid than the use of Upwind Differencing (UD), and to offer substantial savings in computing effort and storage compared to the latter scheme if solutions to the same level of accuracy are sought with each scheme.

Predictions of the flow of a Newtonian fluid in a mixing vessel, on a considerably finer – 87,000-point – grid than employed in previous work and using SFCD, have been analysed in detail, and the chief features identified as:

- The impeller jet has an upward inclination, reduced in the plane of the baffle.
- The lower toroidal vortex changes from an elliptical to circular cross section in travelling inward and downward past the baffle; the upper vortex has a pronounced inward tilt where squeezed by the baffles and is also shifted downward.
- Secondary vortices are predicted within the radius of the impeller near the vessel bottom, in the baffle wake extending from the impeller jet upward and downward, and in association with the downward flow extending from near the fluid surface to half the vessel height.
- The distribution of k and ϵ is characterised by rapid decay from the impeller blade tip region, with locally high values associated with the vortices and the downflow region immediately above the impeller.
- Turbulence length and time scales increase from minimum values in the blade tip region to maxima on solid boundaries – the increase in the vicinity of the baffle is marked. Minimum values of the former quantity in the jet are associated with the periphery, and of the latter with the jet core.
- Distributions of Kolmogorov length and time scales are qualitatively similar to those of the turbulence scales, but do not exhibit the dependence on vessel geometry of the latter. Blade tip values of Kolmogorov length scale are three

orders of magnitude smaller than those of turbulence length scale, those of Kolmogorov time scale two orders of magnitude smaller than the turbulence time scale.

Comparison of mean velocity and turbulence energy predictions on three grids and using UD and SFCD has shown that:

- Predictions obtained on each of the coarser grids with SFCD are for the most part much closer to the finest grid solution than those obtained with UD.
- Finest grid results are for most variables in the greater part of the vessel close to grid independence.
- The swirl velocity shows the greatest grid/discretisation sensitivity.

Comparison of the fine grid results with measurements has shown that:

- The flow field is well characterised, particularly in terms of axial and radial mean velocity components, though prediction of the swirl component is less satisfactory.
- Deficiencies in the prediction of impeller jet strength have been attributed to the impeller boundary condition treatment.
- Turbulence energy is underpredicted, though by a factor of < 2 in most of the vessel, more severely near the vessel bottom. Gradients in k are also underpredicted. These failings have been attributed in part to the inadequacies of the $k - \epsilon$ model and in part to ensemble averaging in the impeller region; they have been cited as in large measure responsible for the deficiencies in the mean flow predictions.

Predictions of fully-developed turbulent pipe flow of Newtonian and shear-thinning fluids show that:

- The $k - \epsilon$ model used with wall functions results in underprediction, of the order of 25%, of near-wall turbulence energy levels in Newtonian fluid flow.
- Prediction of the velocity distribution for a shear-thinning fluid with 'log law' slope equal to the Newtonian is to the same level of accuracy as obtained for Newtonian fluid flow; predicted distributions for flows of shear-thinning fluids with 'log law' slope steeper than the Newtonian do not fully capture the measured velocity gradients.
- Correct prediction of the very much higher turbulence energy levels in the near-wall region in the flow of drag-reducing fluids, which is not apparently a shear-thinning effect, is beyond the scope of the model/boundary conditions.

For predictions of turbulent flow of Newtonian and shear-thinning fluids in a pipe with an axially-mounted baffle

- The macro-scale parameters are seen to be sensibly independent of fluid rheology, and micro-scale parameters to reflect shear-thinning, to a limited extent.
- Considerably coarser near-wall grid distributions are necessary with the use of wall functions, due to the thicker viscous sublayers associated with these fluids, though the degree to which they are thicker is largely due to phenomena other than shear-thinning.
- The first of the extra ϵ equation source terms is of the same order as the 'standard' terms, the second an order of magnitude smaller.

The agreement of these predictions with experiment is similar, for the Newtonian case, to that obtained in previous work. Greater quantitative discrepancies are found in the flow of the shear-thinning fluid which are due to experimentally observed non-shear-thinning effects. These include greater anisotropy and are believed to be due to elasticity.

Predictions for the flow of a shear-thinning solution in a mixing vessel have been analysed in conjunction with those for a 'power-matched' flow of a high-viscosity Newtonian fluid. Differences between the two sets of results are non-negligible, in contrast to experimental observation, and this is attributed in part to the inadequacies of the 'wall function' approach with the flow of these fluids, because of the thickness of the viscous sublayers involved, and partly to inadequacies in the turbulence model, which combine to result in too-low levels of turbulence energy and accordingly turbulent diffusion. The following specific points are noted:

- The range of Kolmogorov scales is greater in the flow of the shear-thinning than the Newtonian fluids.
- Both of the extra ϵ equation source terms are of the same order as the 'standard' terms.

The non-negligible relative magnitude of the extra ϵ equation source terms in both the baffle-in-pipe and mixing vessel cases, is inconsistent with expectation for an equation representing inertial processes. This is considered to reflect on the assumptions made in the modelling of the ϵ equation as a whole, and/or the assumptions underlying the derivation of the exact equation, given that the rederivation and modelling of the extra terms are on the same principles as the whole.

The comparison with experiment for the mixing vessel flow of the shear-thinning fluid has confirmed the qualitative correctness of the predicted mean

flow pattern, but shown that velocity gradients are overpredicted, for the reasons mentioned above.

From the predictions for the flow of water and a high-viscosity Newtonian fluid

- Distributions of turbulence length and time scale have been found to agree, on a normalised basis, for flows of different Newtonian fluids at different bulk Reynolds numbers.

Comparison of the high-viscosity Newtonian fluid flow predictions with experiment has shown the same level of agreement of mean axial and radial velocity, and turbulence kinetic energy, as obtained on the same grid for the water flow, but also in particular that

- Agreement of mean swirl velocity in the below-impeller region is satisfactory, in contrast to that for the water case.

Finally, then, it is considered that the refinements to the methodology make quantitatively accurate flow pattern predictions in mixing vessels realisable with currently available computing resources, and the model for turbulent flow of shear-thinning fluids provides hitherto unavailable guidance to the values of parameters affected by such rheology and which are of significance in mixing processes. Comparison with experiment has highlighted the shortcomings of the present methodology, and thus provided guidance to those aspects meriting further work.

7.2 Suggestions for further work

Physical modelling

In both the baffle-in-pipe and mixing vessel cases the inadequacies of the turbulence model have been obvious, and centre on the inadequacy of the eddy viscosity hypothesis in the presence of streamline curvature and/or anisotropy. This indicates a necessity to investigate the Reynolds stress model alternative, particularly as computing resources now becoming available should make it a feasible proposition for three-dimensional flow prediction. Anisotropy has been noted to be more pronounced in the flow of certain non-Newtonian fluids, but modelling of the causes of such anisotropy is probably necessary before a Reynolds stress model might be expected to be of benefit – this will be mentioned again momentarily.

The ϵ transport equation, the weakest link in the $k - \epsilon$ and any higher-order closure, is a separate issue equally deserving of attention. Given that most of the

parameters of significance in relation to mixing processes are strong functions of the dissipation rate, the multiple-scale approaches reviewed by Launder (1984a) would appear to be a potentially fruitful avenue of exploration. In addition, while the inclusion of terms which are functions of fluid properties would be no easier to justify in ϵ equations for two (or more) intervals of the turbulence spectrum, the model for shear-thinning fluid viscosity based on dissipation rate would be more firmly grounded in physical argument with the employment of a multiple-scale model, since the assumption of a log-normal distribution is yet more plausible for a dissipation rate characteristic of a higher-wavenumber interval of the spectrum than of the spectrum as a whole.

It seems clear that alternatives to wall functions must be evaluated in connection with flow of shear-thinning fluids, particularly in view of the untenability of the Couette flow assumption in sublayers of the thickness apparently associated with such flows – this is a still greater problem where drag reduction is involved. It cannot be emphasised too strongly, however, that the single most pressing need in the formulation of boundary conditions for the turbulent flow of such fluids is more data. The particular requirement is for (both mean velocity and turbulence energy distribution) data for the flow of fluids not exhibiting rheological effects other than shear-thinning; moreover the requirement for data for a large number of combinations of flows at different Reynolds numbers/flow rates, and fluids of different ‘power law’ indices, bears repetition.

In view of the difficulty in identifying shear-thinning fluids which do not also exhibit other non-Newtonian forms of behaviour, the possibility of modelling elastic mechanisms in turbulent flow should be considered – this may be a route to determination of the vexed question of the cause of drag reduction.

Indirect validation of the model for mean molecular viscosity is worthy of investigation – qualitative corroboration may be obtainable from mixing/reaction rate measurements for processes known to be governed by the microscales of turbulence.

The impeller model

The most obvious aspect of the current methodology requiring improvement is the treatment of the impeller region – a satisfactory solution will involve the detailed prediction of the flow between successive blades, the results of which can be matched to the flow in the vicinity of the impeller *ie.* act as boundary conditions for the present method. Prescriptions of mean velocity and turbulence

energy reflecting periodicity, vortex shedding *etc.* are required before evaluation of the relative merits of alternative turbulence models can be made with confidence, and in particular before the expense associated with higher-order closures can be justified.

The second reason for requiring such a model is the removal of the restriction on the methodology to consideration of the Rushton turbine alone – this is but one of a number of impeller types employed in industrial processes.

Numerical methodology

The aspect of the numerical methodology for which investigation of alternatives is most merited is the treatment of the $x-r$ plane boundaries of the solution domain; the cyclic boundary treatment employed here is believed to be the primary cause of the large number of iterations required to obtain convergence, a problem which will become relatively more important as increasing computing resources permit further grid refinement.

Appendices

Appendix A

The scalar invariants of the strain tensor

The three scalar invariants of the strain tensor $\dot{\gamma}$ are given by

$$\begin{aligned} I_{\dot{\gamma}} &= \text{tr } \dot{\gamma} = (\dot{\gamma} : \delta) = \sum_i \dot{\gamma}_{ii} \\ II_{\dot{\gamma}} &= \text{tr } \dot{\gamma}^2 = (\dot{\gamma} : \dot{\gamma}) = \sum_i \sum_j \dot{\gamma}_{ij} \dot{\gamma}_{ji} \\ III_{\dot{\gamma}} &= \text{tr } \dot{\gamma}^3 = \det \dot{\gamma} = \sum_i \sum_j \sum_k \epsilon_{ijk} \dot{\gamma}_{1i} \dot{\gamma}_{2j} \dot{\gamma}_{3k} \end{aligned}$$

where

$$\begin{aligned} \delta &= \text{unit tensor} = \sum_i \sum_j \delta_i \delta_j \delta_{ij} \\ \delta_{ij} &= \text{Kronecker delta} \\ \delta_i, \delta_j &= \text{unit vectors} \\ \epsilon_{ijk} &= +1 \text{ if } ijk = 123, 231 \text{ or } 312 \\ &= -1 \text{ if } ijk = 321, 132 \text{ or } 213 \\ &= 0 \text{ if any two indices are alike} \end{aligned}$$

$I_{\dot{\gamma}}$, $II_{\dot{\gamma}}$ and $III_{\dot{\gamma}}$ are independent of the choice of coordinate system to which the components of $\dot{\gamma}$ are referred ie. they transform as scalars under a rotation of the coordinate system.

$I_{\dot{\gamma}}$ can be shown to be $2(\nabla \cdot \mathbf{v})$, where $\mathbf{v}$ is the velocity vector, and this, the divergence of the velocity field, is zero for an incompressible fluid. $III_{\dot{\gamma}}$ is zero for shearing flows, where such flows are defined as having a set of shearing surfaces, and (i) the distance between any two neighbouring particles in such a surface is constant (ii) the separation of any two neighbouring shearing surfaces is constant.

$II_{\dot{\gamma}}$ is given, in cylindrical polar coordinates, by

$$\begin{aligned} II_{\dot{\gamma}} &= 4 \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial r} \right)^2 + \left(\frac{1}{r} \frac{\partial w}{\partial \theta} + \frac{v}{r} \right)^2 \right] + \\ &\quad 2 \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial r} \right)^2 + 2 \left(r \frac{\partial}{\partial r} \left(\frac{w}{r} \right) + \frac{1}{r} \frac{\partial v}{\partial \theta} \right)^2 + 2 \left(\frac{1}{r} \frac{\partial u}{\partial \theta} + \frac{\partial w}{\partial x} \right)^2 \end{aligned}$$

Appendix B

Determination of the Carreau model parameters

The simplified Carreau model for the apparent viscosity of a shear-thinning fluid is given by

$$\tilde{\mu} = \mu_0 [1 + (\lambda \dot{\gamma})^2]^\alpha \quad (\text{B.1})$$

and the resultant constitutive equation is

$$\tau = \mu_0 [1 + (\lambda \dot{\gamma})^2]^\alpha \dot{\gamma} \quad (\text{B.2})$$

This may be written in logarithmic form as

$$y = A + \alpha \log[1 + (\lambda \dot{\gamma})^2] + \log \dot{\gamma} \quad (\text{B.3})$$

where $y = \log \tau$ and $A = \log \mu_0$. Using the method of least squares to fit the best curve $y = f(\dot{\gamma})$ to the data involves minimising S , where

$$\begin{aligned} S &= \sum_{i=1}^N (y - y_i)^2 \\ &= \sum_{i=1}^N y^2 + \sum_{i=1}^N y_i^2 - 2 \sum_{i=1}^N y y_i \end{aligned} \quad (\text{B.4})$$

subject to conditions

$$\frac{\delta S}{\delta \Phi_i} = 0$$

Thus

$$\begin{aligned} S &= \sum_{i=1}^N \left\{ A + \alpha \log[1 + (\lambda \dot{\gamma}_i)^2] + \log \dot{\gamma} \right\} + \sum_{i=1}^N y_i^2 \\ &\quad - 2 \sum_{i=1}^N \left\{ A + \alpha \log[1 + (\lambda \dot{\gamma}_i)^2] + \log \dot{\gamma} \right\} y_i \end{aligned} \quad (\text{B.5})$$

ie.

$$\begin{aligned} S &= N A^2 + \sum_{i=1}^N (\log \dot{\gamma})^2 + \alpha^2 \sum_{i=1}^N \left\{ \log[1 + (\lambda \dot{\gamma}_i)^2] \right\}^2 \\ &\quad + 2 A \sum_{i=1}^N \log \dot{\gamma} + 2 A \alpha \sum_{i=1}^N \log[1 + (\lambda \dot{\gamma}_i)^2] \\ &\quad + 2 \alpha \sum_{i=1}^N \log \dot{\gamma} \log[1 + (\lambda \dot{\gamma}_i)^2] + \sum_{i=1}^N y_i^2 - 2 A \sum_{i=1}^N y_i \\ &\quad - 2 \alpha \sum_{i=1}^N \left\{ \log[1 + (\lambda \dot{\gamma}_i)^2] \right\} y_i - 2 \sum_{i=1}^N y_i \log \dot{\gamma} \end{aligned} \quad (\text{B.6})$$

Differentiating

$$\frac{\delta S}{\delta A} = 2NA + 2 \sum_{i=1}^N \log \dot{\gamma} + 2\alpha \sum_{i=1}^N \log[1 + (\lambda \dot{\gamma}_i)^2] - 2 \sum_{i=1}^N y_i \quad (\text{B.7})$$

$$= 0$$

from which

$$A = \frac{\sum_{i=1}^N y_i - \sum_{i=1}^N \log \dot{\gamma} - \alpha \sum_{i=1}^N \log[1 + (\lambda \dot{\gamma}_i)^2]}{N} \quad (\text{B.8})$$

Similarly

$$\begin{aligned} \frac{\delta S}{\delta \alpha} &= 2\alpha \sum_{i=1}^N \left\{ \log[1 + (\lambda \dot{\gamma}_i)^2] \right\}^2 + 2A \sum_{i=1}^N \log[1 + (\lambda \dot{\gamma}_i)^2] \\ &\quad + 2 \sum_{i=1}^N (\log \dot{\gamma}) \log[1 + (\lambda \dot{\gamma}_i)^2] - 2 \sum_{i=1}^N \left\{ \log[1 + (\lambda \dot{\gamma}_i)^2] \right\} y_i \\ &= 0 \end{aligned} \quad (\text{B.9})$$

from which

$$\begin{aligned} \alpha &= \left\{ \sum_{i=1}^N \left\{ \log[1 + (\lambda \dot{\gamma}_i)^2] \right\} y_i - \sum_{i=1}^N (\log \dot{\gamma}) \log[1 + (\lambda \dot{\gamma}_i)^2] - \right. \\ &\quad \left. A \sum_{i=1}^N \log[1 + (\lambda \dot{\gamma}_i)^2] \right\} / \sum_{i=1}^N \log[1 + (\lambda \dot{\gamma}_i)^2] \end{aligned} \quad (\text{B.10})$$

The derivative with respect to λ may also be obtained, but as it is not possible to obtain an explicit expression for λ in A and α an iterative procedure is necessary.

From (B.8) and (B.10)

$$\begin{aligned} A &= \left\{ \left(\sum_{i=1}^N y_i - \sum_{i=1}^N \log \dot{\gamma} \right) \sum_{i=1}^N \left\{ \log[1 + (\lambda \dot{\gamma}_i)^2] \right\}^2 - \right. \\ &\quad \left(\sum_{i=1}^N \left\{ \log[1 + (\lambda \dot{\gamma}_i)^2] \right\} y_i - \sum_{i=1}^N (\log \dot{\gamma}) \log[1 + (\lambda \dot{\gamma}_i)^2] \right) \\ &\quad \left. \sum_{i=1}^N \log[1 + (\lambda \dot{\gamma}_i)^2] \right\} / \\ &\quad \left\{ N \sum_{i=1}^N \left\{ \log[1 + (\lambda \dot{\gamma}_i)^2] \right\}^2 - \sum_{i=1}^N \log[1 + (\lambda \dot{\gamma}_i)^2] \right\} \end{aligned} \quad (\text{B.11})$$

A, α and the sum S are calculated from (B.11), (B.10) and (B.6) respectively, from an initial value of λ . The procedure is repeated for successive values of λ . The most accurate values of A, α and λ are those corresponding to the smallest sum, S .

Appendix C

The Reynolds number for the pipe flow of power-law fluids of Metzner and Reed

Metzner and Reed (1955) expressed the Rabinowitsch-Mooney equation for the fully developed flow of a purely viscous fluid in a pipe

$$\left(\frac{-du}{dr}\right)_w = \frac{3}{4}\left(\frac{8V}{D_P}\right) + \frac{1}{4}\left(\frac{8V}{D_P}\right) \frac{d \ln(8V/D_P)}{d \ln(D_P \Delta P / 4L_P)} \quad (C.1)$$

in the form

$$\left(\frac{-du}{dr}\right)_w = \frac{3n' + 1}{4n'} \frac{8V}{D_P} \quad (C.2)$$

where

$$\frac{1}{n'} = \frac{d \ln(8V/D_P)}{d \ln(D_P \Delta P / 4L_P)} \quad (C.3)$$

Then over any range of shear stresses for which n' is a constant

$$\frac{D_P \Delta P}{4L_P} = K' \left(\frac{8V}{D_P}\right)^{n'} = \tau_w \quad (C.4)$$

where K' is a constant of integration. Then substituting the Fanning friction factor

$$f = \frac{\tau_w}{\rho V^2 / 2} \quad (C.5)$$

into C.4 gives

$$\begin{aligned} f &= \frac{K'}{\rho V^2 / 2} \left(\frac{8V}{D_P}\right)^{n'} \\ &= \frac{16K' 8^{n'-1}}{\rho V^{2-n'} D_P^{n'}} \end{aligned} \quad (C.6)$$

By defining $f = 16/Re_{\text{gen}}$ as for Newtonian fluids Metzner and Reed defined the generalised Reynolds number for the pipe flow of a shear-thinning fluid

$$Re_{\text{gen}} = \frac{\rho V^{2-n'} D_P^{n'}}{K' 8^{n'-1}} \quad (C.7)$$

If the $\ln(8V/D_P) - \ln(\tau_w)$ relationship is linear over the range of shear stresses obtaining for the problem, the power law is valid ie. n' and n are identical. Substitution of (C.2) into the power law then gives

$$\tau_w = -K \left(\frac{du}{dr}\right)_w^n = K \left(\frac{3n+1}{4n}\right)^n \left(\frac{8V}{D_P}\right)^n \quad (C.8)$$

Comparison between (C.4) and (C.8) shows that

$$K' = K \left(\frac{3n+1}{4n} \right)^n \quad (\text{C.9})$$

The Reynolds number (C.7) then takes the form, for the pipe flow of power law fluids

$$Re_{pl} = \frac{\rho V^{2-n} D_p^n}{K 8^{n-1} \left(\frac{3n+1}{4n} \right)^n} \quad (\text{C.10})$$

Appendix D

Friction factor - Reynolds number relationship for fully developed turbulent pipe flow of inelastic fluids

The fully developed turbulent flow of a Newtonian fluid in a pipe may be represented by the logarithmic expression (Schlichting, 1960)

$$u^+ = A \ln y^+ + B \quad (D.1)$$

This may be integrated over the cross-sectional area to obtain the dimensionless bulk flow velocity

$$\begin{aligned} V^+ &= \frac{2}{(R^+)^2} \int_0^{R^+} (R^+ - y^+) (A \ln y^+ + B) dy^+ \\ &= \frac{2}{(R^+)^2} \left\{ R^+ A (y^+ \ln y^+ - y^+) + R^+ B y^+ \right. \\ &\quad \left. - A \left(\frac{(y^+)^2}{2} \ln y^+ - \frac{(y^+)^2}{4} \right) - \frac{B(y^+)^2}{2} \right|_0^{R^+} \} \end{aligned}$$

ie.

$$V^+ = A \ln R^+ - \frac{3A}{2} + B \quad (D.2)$$

Here

$$V^+ = \frac{V}{u_*} = \frac{V}{\sqrt{\tau_w/\rho}} = \sqrt{\frac{2}{f}} \quad (D.3)$$

and

$$R^+ = \frac{\rho R u_*}{\mu} = \frac{\rho R V}{\mu} \sqrt{\frac{f}{2}} \quad (D.4)$$

From (D.2), (D.3) and (D.4)

$$\begin{aligned} \frac{1}{\sqrt{f}} &= \frac{A}{\sqrt{2}} \ln \left(\frac{\rho 2 R V}{\mu} \frac{1}{2} \sqrt{\frac{f}{2}} \right) + \frac{1}{\sqrt{2}} \left(B - \frac{3A}{2} \right) \\ &= \frac{A}{\sqrt{2}} \ln (Re \sqrt{f}) + \frac{1}{\sqrt{2}} \left(B - \frac{3A}{2} - A \ln 2\sqrt{2} \right) \end{aligned} \quad (D.5)$$

(D.1) may be derived from Prandtl's mixing length theory and the constant A then represents the inverse of the mixing length. As a function of flow field rather than fluid this would be expected to have the same value for shear-thinning fluid

flows as for Newtonian fluid flows, i.e. $A \approx 2.5$. The velocity data of Bogue for Carbopol solutions, figure 2.4, provides tentative supporting evidence for such a conclusion, in the form of profiles of equal slope. The apparent viscosity at the wall, μ_w , may be chosen as characteristic of the flow of a shear-thinning fluid in a pipe, on the basis that viscosity forces dominate in the wall region only, that this region dominates the structure of such a flow, and that the shear stress is nearly uniform in this region. (D.5) may then be written in a form valid for both Newtonian and shear- thinning fluids

$$\frac{1}{\sqrt{f}} = 4 \log(Re_{\mu_w} \sqrt{f}) + \frac{1}{\sqrt{2}}(B - 6.35) \quad (D.6)$$

Here

$$Re_{\mu_w} = \frac{\rho V D}{\mu_w} \quad (D.7)$$

- this reduces to the conventional Reynolds number for pipe flow in the case of Newtonian fluids. μ_w is given by

$$\mu_w = \frac{\tau_w}{(du/dr)_w} \quad (D.8)$$

and thus

$$\mu_w = \tau_w^{(n-1)/n} K^{1/n} \quad (D.9)$$

in the case of the power law (which is generally accurate in the near-wall region due to the high shear rates obtaining).

Appendix E

The friction factor - Reynolds number correlation and logarithmic velocity profile expression of Dodge and Metzner

For the flow of Newtonian fluids in smooth pipes it is established that

$$u = (R, \rho, \tau_w, \mu, y) \quad (\text{E.1})$$

from which Dodge and Metzner (1959) assumed that, if the power law constitutive equation (2.2.4) holds

$$u = (R, \rho, \tau_w, K, n, y) \quad (\text{E.2})$$

for the flow of a shear-thinning fluid. Non-dimensionalising by the friction velocity gives

$$\frac{u}{u_*} = f_1(Z, y/R, n) \quad (\text{E.3})$$

where

$$Z = \frac{R^n \rho (u_*)^{2-n}}{K} \quad (\text{E.4})$$

The velocity defect ($u_{\max} - u$) in the turbulent core is determined by the random turbulent fluctuations, which have been shown to be independent of the viscosity for Newtonian fluids. Dodge and Metzner claimed that the equivalent assumption in a power law fluid analysis is that the velocity defect is independent of K , though not of n , which gives

$$u_{\max} - u = f(\tau_w, \rho, R, y, n) \quad (\text{E.5})$$

or, in non-dimensional form

$$\frac{u_{\max} - u}{u_*} = f_2(y/R, n) \quad (\text{E.6})$$

This is strictly only applicable in the turbulent core, but if assumed to apply right across the pipe diameter the expression

$$\begin{aligned} V &= \frac{2}{R^2} \int_0^R u r dr \\ &= \frac{2}{R^2} \int_0^R u_{\max} r dr - \frac{2u_*}{R^2} \int_0^R f_2(y/R, n) r dr \end{aligned} \quad (\text{E.7})$$

is obtained for the bulk velocity, which for a given n is

$$V = u_{\max} - C_1 u_* \quad (\text{E.8})$$

where C_1 is a constant. (E.3) written for the pipe centreline is

$$\frac{u}{u_*} = F_1(Z, n) \quad (\text{E.9})$$

which may be combined with (E.3) and (E.8) to give

$$\sqrt{\frac{2}{f}} = F_1(Z, n) - C_1 \quad (\text{E.10})$$

Since within the laminar sublayer the pipe radius plays no part in determining u , one has

$$u = f(\rho, \tau_w, K, n, y) \quad (\text{E.11})$$

which becomes

$$\frac{u}{u_*} = f_3(Z, (y/R)^n, n) \quad (\text{E.12})$$

in non-dimensional form. In the outer part of the turbulent core both (E.6) and (E.12) are assumed to be valid, and combining these expressions with (E.9) gives

$$f_{3n}(Z(y/R)^n) = F_{1n}(Z) - f_{2n}((y/R)^n) \quad (\text{E.13})$$

for any fixed value of n . Dodge and Metzner determined $F_{1n}(Z)$ by a partial differentiation procedure involving (E.13) to obtain

$$F_{1n}(Z) = A_n \ln(Z) + B_n \quad (\text{E.14})$$

where A_n and B_n are functions of n since (E.13) is for a fixed n . Then substituting (E.4) and (E.14) in (E.10) gives

$$\frac{1}{\sqrt{f}} = A_{1n} \log \left[\frac{\rho V^{2-n} D^n}{K} f^{1-n/2} \right] + C_{2n} \quad (\text{E.15})$$

where the constants have been modified to account for the conversion to common logarithms. Dodge and Metzner introduced the Reynolds number for pipeflow of power law fluids (2.4.12) at this point, along with the shear-thinning index n' , obtaining the relationship

$$\frac{1}{\sqrt{f}} = A_{1n} \log \left[Re_{pl}(f)^{1-n'/2} \right] + C_{2n} \quad (\text{E.16})$$

where

$$C'_{2n} = A_{1n} \log \left[\frac{1}{8} \left(\frac{6n' + 2}{n'} \right)^{n'} \right] + C_{2n} \quad (\text{E.17})$$

Dodge and Metzner held this to be valid, provided that K' and n' are evaluated at the wall shear stress, on the grounds of their demonstration that 74% of the contribution to V is attributable to shear rates occurring at shear stresses between τ_w and $0.96\tau_w$.

By the same partial differentiation procedure as used in deriving (D.14) Dodge and Metzner established that

$$f_{3n}((y/R)^n) = -A_n \ln(y/R)^n + E_n \quad (\text{E.18})$$

While (E.14) and (E.18) were both derived from consideration of the transition region between the laminar and fully turbulent regions, (E.14) is independent of y , as is also evident from (E.9). If (E.18) is written as

$$\frac{u_{\max} - u}{u_*} = -nA_n \ln(y/R) + g(y/R, n) \quad (\text{E.19})$$

where g is an unknown function intended to generalise (E.18), making it valid for the entire turbulent core, the combination with (E.14) yields

$$\frac{u}{u_*} = A_n \ln Z(y/R)^n + B_n - g(y/R, n) \quad (\text{E.20})$$

Comparison with the Newtonian logarithmic profile (2.5.1) for fully developed pipe flow shows that it may be regarded as a special case of (E.20), for which $n = 1$, and accordingly that

$$g(y/R, 1) = 0 \quad (\text{E.21})$$

Since for $n = 0$ the turbulent profile must be perfectly flat, *ie.* $u_{\max} - u = 0$

$$g(y/R, 0) = 0 \quad (\text{E.22})$$

Dodge and Metzner then concluded that

$$g(y/R, n') = 0, \quad 0 \leq n' \leq 1 \quad (\text{E.23})$$

and thus that

$$\frac{u_{\max} - u}{u_*} = -n'A_n \ln(y/R) \quad (\text{E.24})$$

and

$$\frac{u}{u_*} = A_n \ln Z(y/R)^{n'} + B_n \quad (\text{E.25})$$

ie.

$$u^+ = A_n \ln y_{pl}^+ + B_n \quad (E.26)$$

represent velocity distributions in fully-developed turbulent pipe flow of shear-thinning fluids.

In the laminar sublayer the same assumption is made as in the Newtonian case, namely that the velocity distribution is linear, and τ therefore constant and equal to τ_w :

$$\tau_w = K \left(\frac{u}{y} \right)^n \quad (E.27)$$

which may be expressed as

$$u^+ = (y_{pl}^+)^{1/n} \quad (E.28)$$

Appendix F

Derivation of the transport equation for ϵ

The equation of motion for u'_i is obtained as the difference between the instantaneous

$$\frac{\partial}{\partial x_j}(\rho \hat{u}_j \hat{u}_i) = -\frac{\partial \hat{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \hat{\tau}_{ij} \quad (\text{F.1})$$

and mean

$$\rho \frac{\partial}{\partial x_j}(\bar{u}_j \bar{u}_i) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}(\bar{\tau}_{ij} - \overline{\rho u'_i u'_j}) \quad (\text{F.2})$$

momentum equations; it reads

$$\frac{\partial}{\partial x_j} \rho (\underbrace{\bar{u}_i u'_j}_A + \underbrace{\bar{u}_j u'_i}_B + \underbrace{u'_i u'_j}_C - \underbrace{\overline{u'_i u'_j}}_D) = -\underbrace{\frac{\partial p'}{\partial x_i}}_E + \underbrace{\frac{\partial}{\partial x_j} \left(\mu \left(\frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right) \right)}_F \quad (\text{F.3})$$

(F.3) is differentiated with respect to x_l , multiplied by $\mu \partial u'_i / \partial x_l$ and time-averaged to obtain an equation in $\bar{\epsilon}$, where

$$\bar{\epsilon} = \frac{\mu}{\rho} \overline{\left(\frac{\partial u'_i}{\partial x_j} \frac{\partial u'_i}{\partial x_j} \right)} \quad (\text{F.4})$$

It is noted that due to isotropy

$$\overline{\mu \frac{\partial u'_i}{\partial x_l} \frac{\partial u'_j}{\partial x_m}} = 0 \quad \text{when } i = j \text{ \& } l \neq m$$

$$i \neq j \text{ \& } l = m \quad (\text{F.5})$$

With μ maintained inside differential operators as a field variable terms A – F in (F.3) become

$$\overline{\mu \frac{\partial u'_i}{\partial x_l} \frac{\partial}{\partial x_l} \left(u'_j \frac{\partial \bar{u}_i}{\partial x_j} \right)} = \frac{\partial \bar{u}_i}{\partial x_j} \overline{\mu \frac{\partial u'_i}{\partial x_l} \frac{\partial u'_j}{\partial x_l}} + \overline{\mu u'_j \frac{\partial u'_i}{\partial x_l} \frac{\partial^2 \bar{u}_i}{\partial x_l \partial x_j}}$$

$$= \mu u'_j \overline{\frac{\partial u'_i}{\partial x_l} \frac{\partial^2 \bar{u}_i}{\partial x_l \partial x_j}} \quad (\text{F.6})$$

$$\overline{\mu \frac{\partial u'_i}{\partial x_l} \frac{\partial}{\partial x_l} \left(\bar{u}_j \frac{\partial u'_i}{\partial x_j} \right)} = \frac{\partial \bar{u}_j}{\partial x_l} \overline{\mu \frac{\partial u'_i}{\partial x_l} \frac{\partial u'_i}{\partial x_j}} + \overline{\bar{u}_j \mu \frac{\partial u'_i}{\partial x_l} \frac{\partial^2 u_i}{\partial x_l \partial x_j}}$$

$$= \overline{\bar{u}_j \frac{\mu}{2} \frac{\partial}{\partial x_j} \left(\frac{\partial u'_i}{\partial x_l} \right)^2}$$

$$= \frac{1}{2} \frac{\partial}{\partial x_j} \bar{u}_j \epsilon - \frac{\bar{u}_j}{2} \overline{\frac{\partial \mu}{\partial x_j} \left(\frac{\partial u'_i}{\partial x_l} \right)^2} \quad (\text{F.7})$$

$$\begin{aligned} \overline{\mu \frac{\partial u'_i}{\partial x_l} \frac{\partial^2 u'_i u'_j}{\partial x_l \partial x_j}} &= \overline{\frac{\partial u'_i}{\partial x_l} \frac{\partial}{\partial x_j} \left(u'_i \frac{\partial u'_j}{\partial x_l} + u'_j \frac{\partial u'_i}{\partial x_l} \right)} \\ &= \overline{\frac{\partial u'_i}{\partial x_l} \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_j}{\partial x_l}} + \overline{u'_i \mu \frac{\partial u'_i}{\partial x_l} \frac{\partial}{\partial x_j} \left(\frac{\partial u'_i}{\partial x_l} \right)} + \overline{u'_j \mu \frac{\partial}{\partial x_j} \left(\frac{\partial u'_i}{\partial x_l} \right)^2} \end{aligned} \quad (\text{F.8})$$

$$\begin{aligned} &= \overline{\mu \frac{\partial u'_i}{\partial x_l} \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_j}{\partial x_l}} + \overline{\frac{\partial}{\partial x_j} \frac{u'_j \epsilon}{2}} - \overline{\frac{u'_j}{2} \frac{\partial \mu}{\partial x_j} \left(\frac{\partial u'_i}{\partial x_l} \right)^2} \\ &\quad - \overline{\mu \frac{\partial u'_i}{\partial x_l} \frac{\partial^2 u'_i u'_j}{\partial x_l \partial x_j}} \end{aligned} \quad (\text{F.9})$$

$$- \overline{\mu \frac{\partial u'_i}{\partial x_l} \frac{\partial^2 \rho'}{\partial x_l \partial x_i}} = - \overline{\frac{\partial}{\partial x_i} \left(\mu \frac{\partial u'_i}{\partial x_l} \frac{\partial p'}{\partial x_l} + \frac{\partial p'}{\partial x_l} \frac{\partial u'_i}{\partial x_l} \frac{\partial \mu}{\partial x_i} \right)} \quad (\text{F.10})$$

$$\begin{aligned} \overline{\mu \frac{\partial u'_i}{\partial x_l} \frac{\partial^2}{\partial x_l \partial x_j} \mu \left(\frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right)} &= \overline{\mu \frac{\partial u'_i}{\partial x_l} \frac{\partial}{\partial x_j} \left(\frac{\partial \mu}{\partial x_l} \frac{\partial u'_i}{\partial x_j} - \frac{\partial \mu}{\partial x_j} \frac{\partial u'_i}{\partial x_l} \right)} - \\ &\quad \overline{\left(\frac{\partial}{\partial x_j} \mu \frac{\partial u'_i}{\partial x_l} \right)^2} + \overline{\frac{1}{2} \frac{\partial}{\partial x_j} \left(\frac{\partial \mu \epsilon'}{\partial x_j} \right)} \end{aligned} \quad (\text{F.11})$$

Thus on substitution of (F.6) to (F.11) back into (F.3) and multiplication through by 2, with diffusive-like terms grouped for subsequent modelling, the time-averaged exact equation for ϵ reads

$$\begin{aligned} \frac{\partial(\rho \bar{u}_j \bar{\epsilon})}{\partial x_j} &= - \frac{\partial}{\partial x_j} \left(- \frac{\partial \bar{\mu} \epsilon'}{\partial x_j} + \overline{u'_j \epsilon'} + 2\nu \frac{\partial u'_i}{\partial x_l} \frac{\partial p'}{\partial x_l} \right) - 2\overline{\mu \frac{\partial u'_i}{\partial x_l} \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_j}{\partial x_l}} - \\ &\quad 2\overline{\left(\frac{\partial}{\partial x_j} \left(\mu \frac{\partial u'_i}{\partial x_l} \right) \right)^2} - 2\overline{\mu u'_j \frac{\partial u'_i}{\partial x_l} \frac{\partial^2 \bar{u}_i}{\partial x_l \partial x_j}} + \overline{\bar{u}_j \frac{\partial u'_i}{\partial x_l} \frac{\partial u'_i}{\partial x_l} \frac{\partial \mu}{\partial x_j}} + \\ &\quad \overline{u'_j \frac{\partial u'_i}{\partial x_l} \frac{\partial u'_i}{\partial x_l} \frac{\partial \mu}{\partial x_j}} + 2\overline{\mu \frac{\partial u'_i}{\partial x_l} \frac{\partial^2 u'_i u'_j}{\partial x_l \partial x_j}} + 2\overline{\frac{\partial p'}{\partial x_l} \frac{\partial u'_i}{\partial x_l} \frac{\partial \mu}{\partial x_i}} \end{aligned} \quad (\text{F.12})$$

The last 4 terms, in spatial gradients of μ , are zero where this quantity is a constant *ie.* in the case of a Newtonian fluid where dependence of μ on temperature and/or concentration is unimportant.

Appendix G

Determination of the empirical coefficients in the $k - \epsilon$ model

The modelled forms of the k and ϵ transport equations for Newtonian fluid flows are

$$\rho \frac{\partial}{\partial x_j} (\bar{u}_j k) = \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_j} \right) + \mu_t \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \frac{\partial \bar{u}_i}{\partial x_j} - \rho \epsilon \quad (\text{G.1})$$

and

$$\rho \frac{\partial}{\partial x_j} (\bar{u}_j \epsilon) = \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial x_j} \right) + C_1 \frac{\mu_t \epsilon}{k} \frac{\partial \bar{u}_i}{\partial x_j}^2 - C_2 \frac{\rho \epsilon^2}{k} \quad (\text{G.2})$$

where

$$\mu_t = \frac{C_\mu \rho k^2}{\epsilon} \quad (\text{G.3})$$

The empirical coefficients C_1 , C_2 , and C_μ are determined as follows.

C_μ

The boundary layer is assumed to be a simple shear layer in local equilibrium *ie.* transport of k is negligible and production of k due to shear equals viscous dissipation, thus:

$$\mu_t \left(\frac{\partial u}{\partial y} \right)^2 = \rho \epsilon \quad (\text{G.4})$$

ie.

$$\left[\mu_t \frac{\partial u}{\partial y} \right]^2 = \rho \epsilon \frac{C_\mu \rho k^2}{\epsilon} \quad (\text{G.5})$$

ie.

$$C_\mu^{1/2} = \frac{1}{\rho k} \mu_t \frac{\partial u}{\partial y} = \frac{\tau_t}{\rho k} \quad (\text{G.6})$$

Assuming constant shear stress across the viscous sublayer *ie.* $\tau_w = \tau_t$ gives

$$C_\mu^{1/2} = \frac{\tau_w}{\rho} \frac{1}{k} = \frac{u_*^2}{k} = \frac{1}{k^+} \quad (\text{G.7})$$

An experimental value of 3.3 for k^+ implies a value of C_μ of 0.09. The value of k^+ in pipe flow is $\sim 25\%$ higher than this figure.

C_1

The 'law of the wall'

$$\frac{u}{u_*} = \frac{1}{\kappa} \ln\left(\frac{yu_*}{\nu}\right) + C \quad (\text{G.8})$$

may be differentiated to obtain

$$\frac{\partial u}{\partial y} = \frac{u_*}{\kappa y} \quad (\text{G.9})$$

From (G.3) and (G.4)

$$\epsilon = C_\mu^{1/2} k \left(\frac{\partial u}{\partial y} \right) \quad (\text{G.10})$$

From (G.9) and (G.10)

$$\epsilon = \frac{C_\mu^{1/2} k u_*}{\kappa y} \quad (\text{G.11})$$

Thus

$$\frac{\partial \epsilon}{\partial y} = -\frac{C_\mu^{1/2} k u_*}{\kappa y^2} \quad (\text{G.12})$$

Now the transport equation for ϵ in a two-dimensional boundary layer reduces to

$$\frac{\partial}{\partial y} \left(\frac{\mu_t}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial y} \right) + C_1 \frac{\mu_t \epsilon}{k} \left(\frac{\partial u}{\partial y} \right)^2 - C_2 \frac{\rho \epsilon^2}{k} = 0 \quad (\text{G.13})$$

if convection (but not diffusion) is neglected. From (G.3), (G.11), (G.12) and (G.13)

$$-\frac{\partial}{\partial y} \left(\frac{k^2}{\sigma_\epsilon y} \right) + C_1 k \left(\frac{u_*}{\kappa y} \right)^2 - C_2 k \left(\frac{u_*}{\kappa y} \right)^2 = 0 \quad (\text{G.14})$$

and upon integration

$$\frac{k^2}{\sigma_\epsilon} + C_1 k \left(\frac{u_*}{\kappa} \right)^2 - C_2 k \left(\frac{u_*}{\kappa} \right)^2 = 0 \quad (\text{G.15})$$

From (G.7) and (G.15)

$$C_1 = C_2 - \frac{\kappa^2}{\sigma_\epsilon C_\mu^{1/2}} \quad (\text{G.16})$$

indicating a value of C_1 of approximately 1.5, for $C_2 = 1.9$ (see below).

C_2

The turbulence generated by a grid in a stream of uniform velocity u is as close to homogeneous turbulent flow as may be obtained experimentally.

In this case the transport equation (G.1) for k may be written exactly as

$$\rho u \frac{dk}{dx} = -\rho \epsilon \quad (\text{G.17})$$

ie. convection and dissipation only, while that for ϵ , (G.2), may be written as

$$u \frac{d\epsilon}{dx} = -C_2 \frac{\epsilon^2}{k} \quad (\text{G.18})$$

The solutions are of the form

$$k \propto x^n, \quad \epsilon \propto x^m$$

where

$$m = n - 1, \quad C_2 = 1 - \frac{1}{n}$$

Rodi (1972) summarised the experimental findings as indicating a range of -1 to -1.35 in the values of the exponent n , with the majority close to -1.2 . This indicates a value of C_2 of approximately 1.9.

Appendix H

The conjugate gradient algorithm

The conjugate gradient (CG) method may be regarded as a modification of the method of steepest descent – see, for instance, Hageman and Young (1981). This is an iterative procedure for determining the solution of the linear system

$$Ax = b \quad (\text{H.1})$$

Since the quadratic

$$Q(x_i) = \frac{1}{2}(x_i, Ax_i) - (x_i, b) \quad (\text{H.2})$$

has an absolute minimum for $x_i = x$, the exact solution (for proof of this theorem see, for instance, Noble (1969)) where $(\ , \)$ denotes the scalar product, the correction to the approximation x which will decrease $Q(x_i)$ most rapidly is sought, and this may be proved to be parallel to the residual vector

$$r_i = b - Ax_i \quad (\text{H.3})$$

– the line of steepest descent. From the given initial approximation x_0

$$x_{i+1} = x_i + \alpha r_i \quad (\text{H.4})$$

are determined in succession, where

$$\alpha_i = \frac{(r_i, r_i)}{(r_i, Ar_i)} \quad (\text{H.5})$$

The rate of convergence depends on the spread of the eigenvalues of A (for a geometric explanation of the reasons for this see, for example, Noble (1969)). If the direction of search for the improved estimate x_{i+1} is taken, not parallel to the residual vector, but such that successive direction vectors are conjugate ie.

$$(p_i, Ap_i) = 0 \quad (\text{H.6})$$

the CG method is obtained. From an arbitrary initial approximation x_0 , the initial residual and direction are computed as

$$r_0 = p_0 = b - Ax_0 \quad (\text{H.7})$$

Successive updates to x_0 are given by the recursive sequence of Hestenes and Stiefel (1952):

$$\alpha_i = \frac{(r_i, r_i)}{(p_i, Ap_i)} \quad (\text{H.8})$$

$$x_{i+1} = x_i + \alpha_i p_i \quad (\text{H.9})$$

$$r_{i+1} = r_i - \alpha_i p_i \quad (\text{H.10})$$

$$\beta_i = \frac{(r_{i+1}, r_{i+1})}{(r_i, r_i)} \quad (\text{H.11})$$

$$p_{i+1} = r_{i+1} + \beta_i p_i \quad (\text{H.12})$$

Due to the mutual orthogonality of the residual vectors and the associated conjugacy of the direction vectors demonstrated by Hestenes and Stiefel the method converges, in the absence of rounding errors, in at most N iterations. When solving large systems when rounding errors are present in the calculation, however, the mutual conjugacy of the sequence $p_i, p_{i+1}, p_{i+2} \dots$ becomes degraded and consequently so too does the finite termination property. In practice the rate at which the solution is refined depends mainly on the conditioning of A – ie. the ratio of the largest and smallest eigenvalues of A , or more precisely, on all of the ratios of the eigenvalues. If the eigenvalues are clustered around a small number of distinct values, then the use of conjugate gradients will significantly reduce the residual in a number of steps equal to the number of clusters.

However for the coefficient matrices of interest here, arising from a difference representation of the pressure correction equations, the eigenvalues generally have a wide range of values. The ratio of the largest to the smallest eigenvalue has been found to be of the order of 10^4 in this study. Hence preconditioning is necessary, to transform the system of equations into a form for which a conjugate gradient method ‘converges’ faster – one in which the eigenvalues are clustered.

The Cholesky factorisation

$$A = LL^T \quad (\text{H.13})$$

where L is lower triangular, makes the preconditioned system

$$x = (L^T)^{-1}(L^{-1}b) \quad (\text{H.14})$$

much easier to solve iteratively. A is large and sparse, but in such a factorisation the sparseness is lost. The calculation of L is time and storage consuming due

to fill-in, ie. due to many of the zero elements of A becoming non-zero in the corresponding locations in L . Incomplete Cholesky (IC) factorisation, described by Kershaw (1978) among many others, requires the prior definition of L . Undesirable fill-in is discarded. Only those elements which are to be non-zero in the final L are allowed to fill-in the intermediate factorisation steps. Thus the factorisation is performed as

$$B = (\tilde{L} + D^{-1})D(D^{-1} + \tilde{L}^T) \quad (\text{H.15})$$

where $\tilde{L}$ contains the subdiagonal elements of A , and D is chosen such that A and B agree on their main diagonals :

$$D_{ii} = (A_{ii} - \sum_{k=1}^{i-1} \tilde{L}_{ik}^2 D_{kk})^{-1} \quad (\text{H.16})$$

The modified CG algorithm is then given by the recursive sequence (from the arbitrary initial approximation x_0):

$$r_0 = b - Ax_0 \quad (\text{H.17})$$

$$s_i = (\tilde{L} + D^{-1})^{-1} r_i \quad (\text{H.18})$$

$$B^{-1} r_i = (D^{-1} + \tilde{L}^T)^{-1} D^{-1} s_i \quad (\text{H.19})$$

$$\beta_{i-1} = \frac{(r_i, (B^{-1} r_i))}{(r_{i-1}, (B^{-1} r_{i-1}))} \quad (\text{H.20})$$

$$p_i = B^{-1} r_i + \beta_{i-1} p_{i-1} \quad (\text{H.21})$$

$$\alpha_i = \frac{(r_i, B^{-1} r_i)}{(p_i, Ap_i)} \quad (\text{H.22})$$

$$x_{i+1} = x_i + \alpha_i p_i \quad (\text{H.23})$$

$$r_{i+1} = r_i - \alpha_i p_i \quad (\text{H.24})$$

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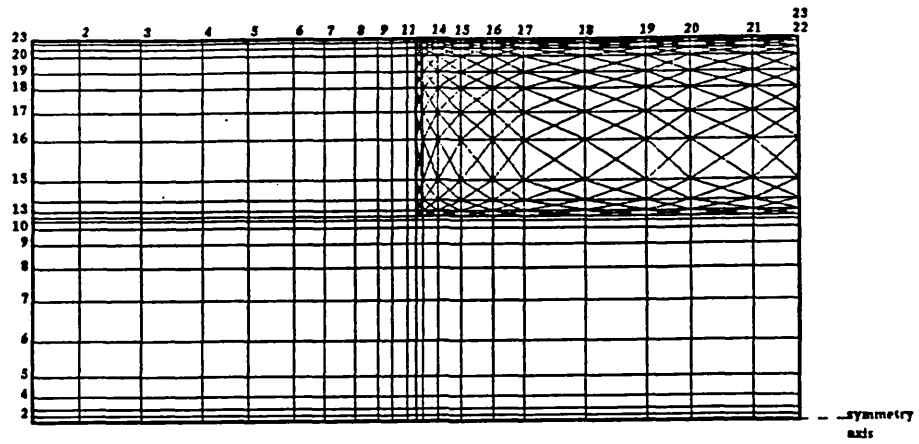
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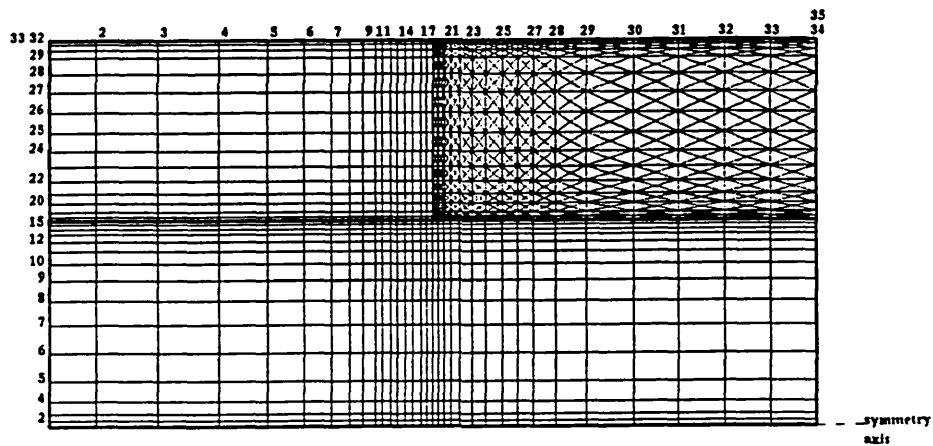
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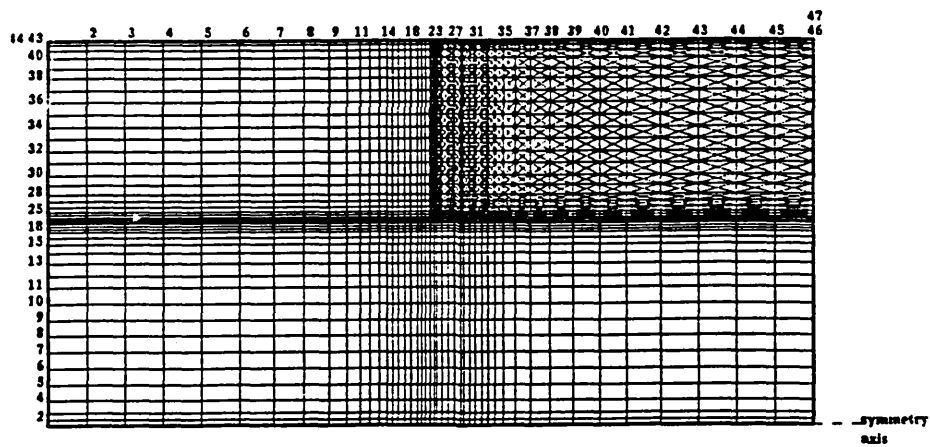
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a) 23 x 24

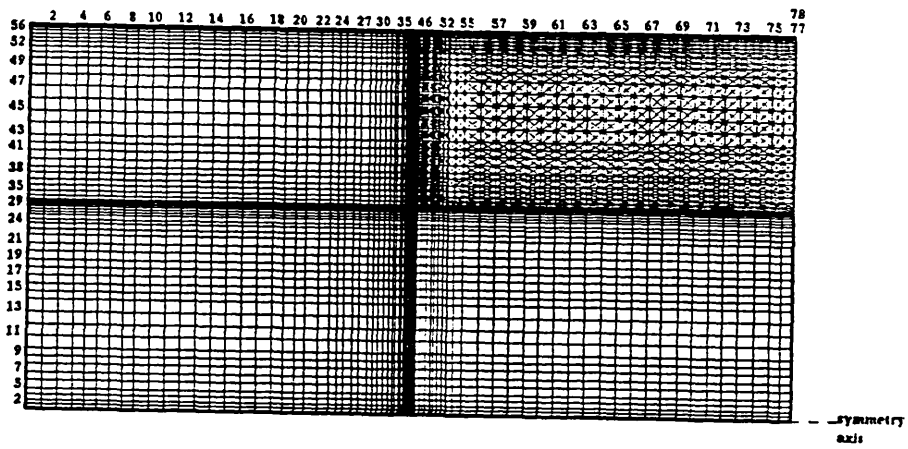


b) 35 x 33



c) 47 x 44

Figure 5.2.1 Computational grids, laminar flow, pipe with step contraction



d) 78 x 60

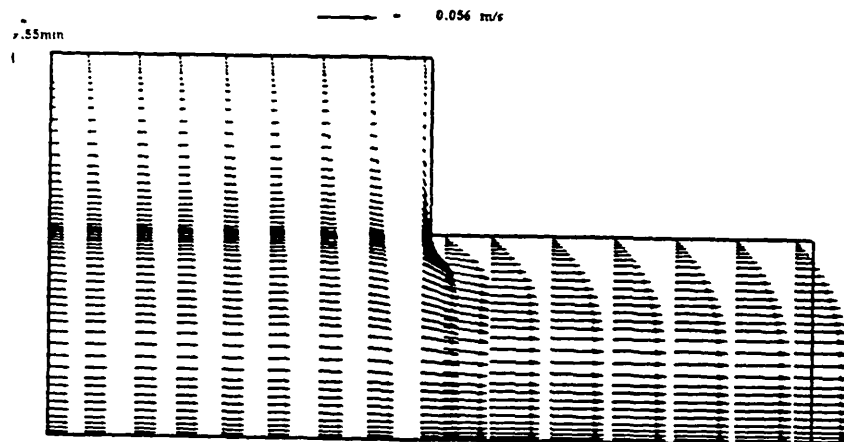


Figure 5.2.2 Velocity vectors, laminar flow, pipe with step contraction

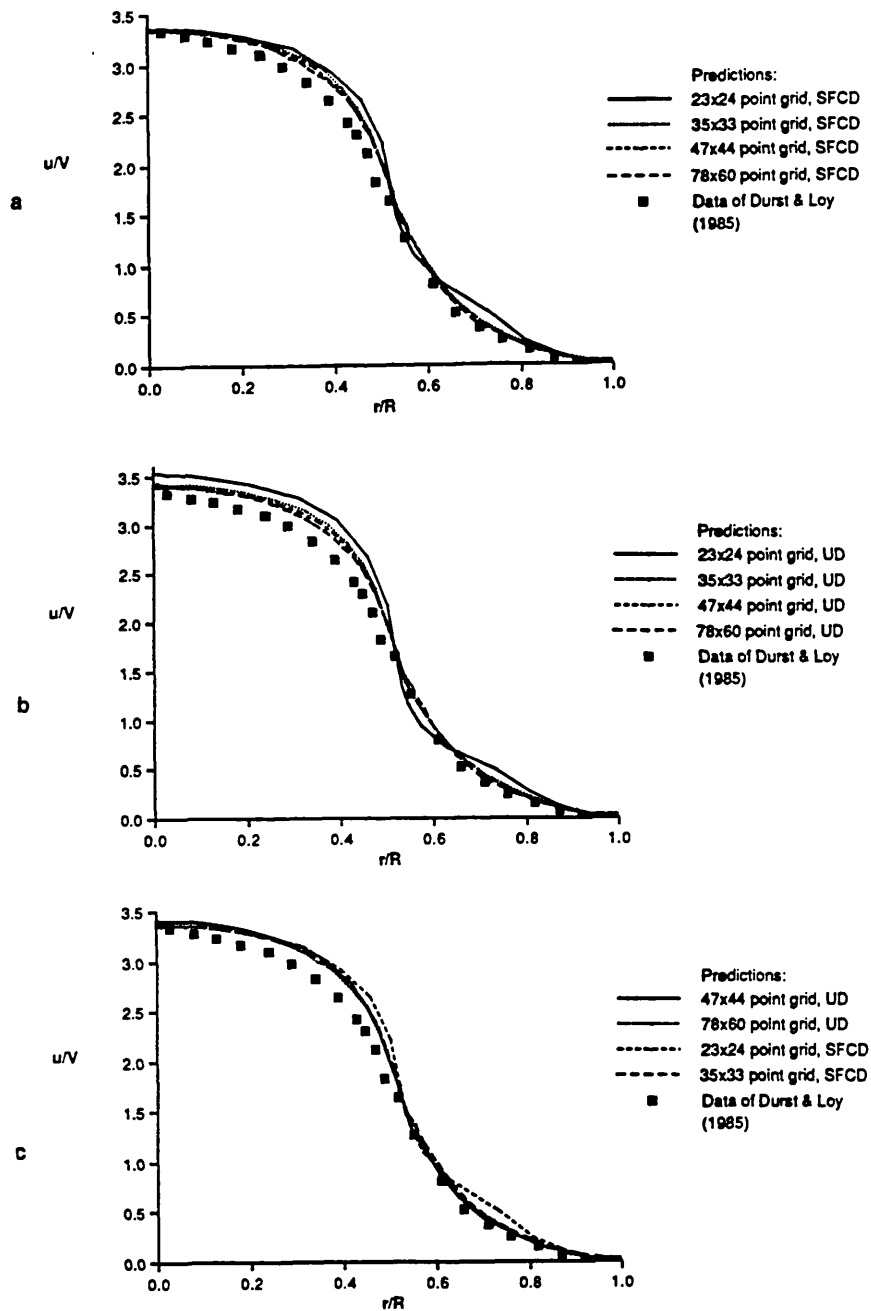


Figure 5.2.3 Comparison of UD and SFCD predictions, and of predictions with experiment, 0.039D upstream of contraction

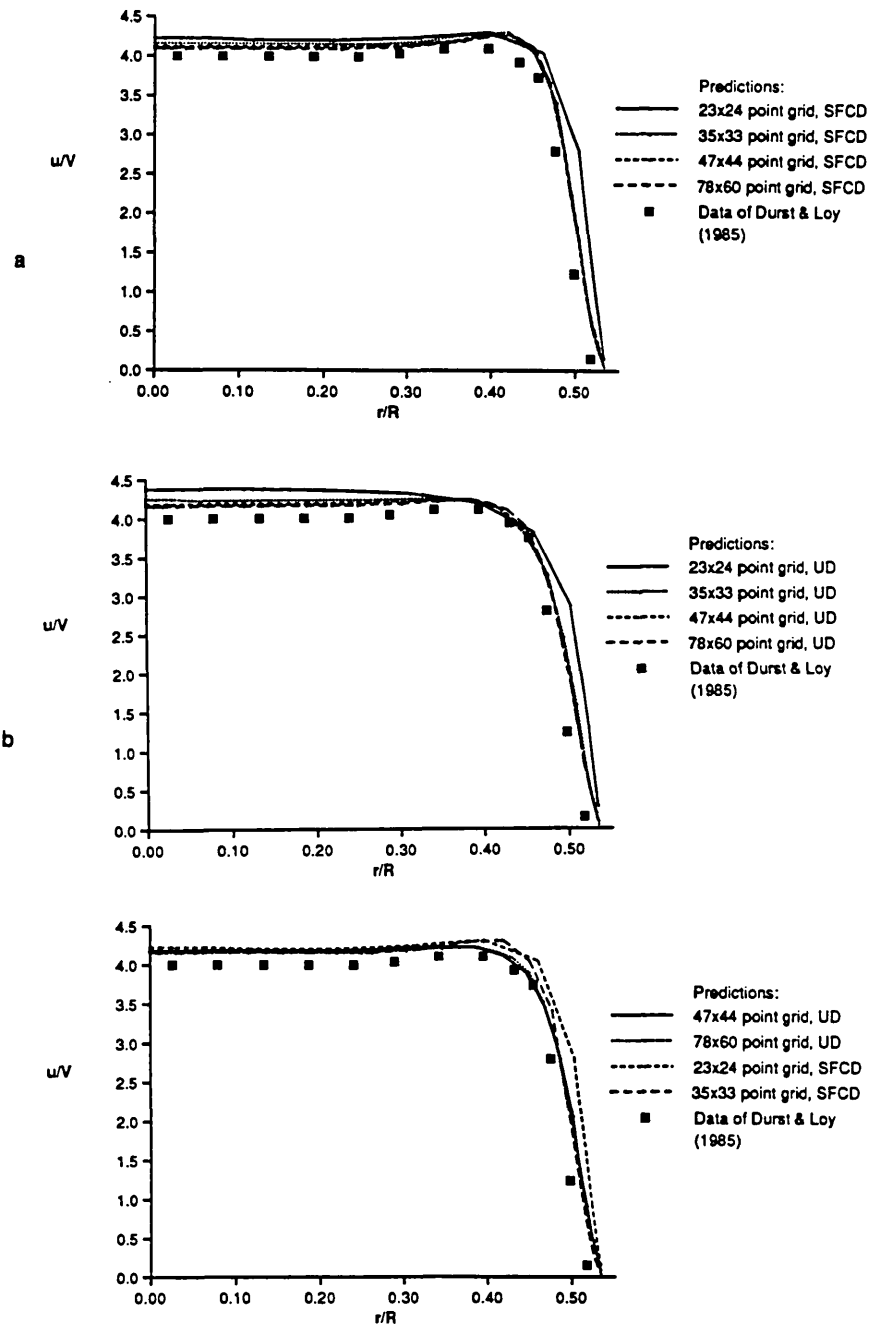


Figure 5.2.4 Comparison of UD and SFCD predictions, and of predictions with experiment, 0.052D downstream of contraction

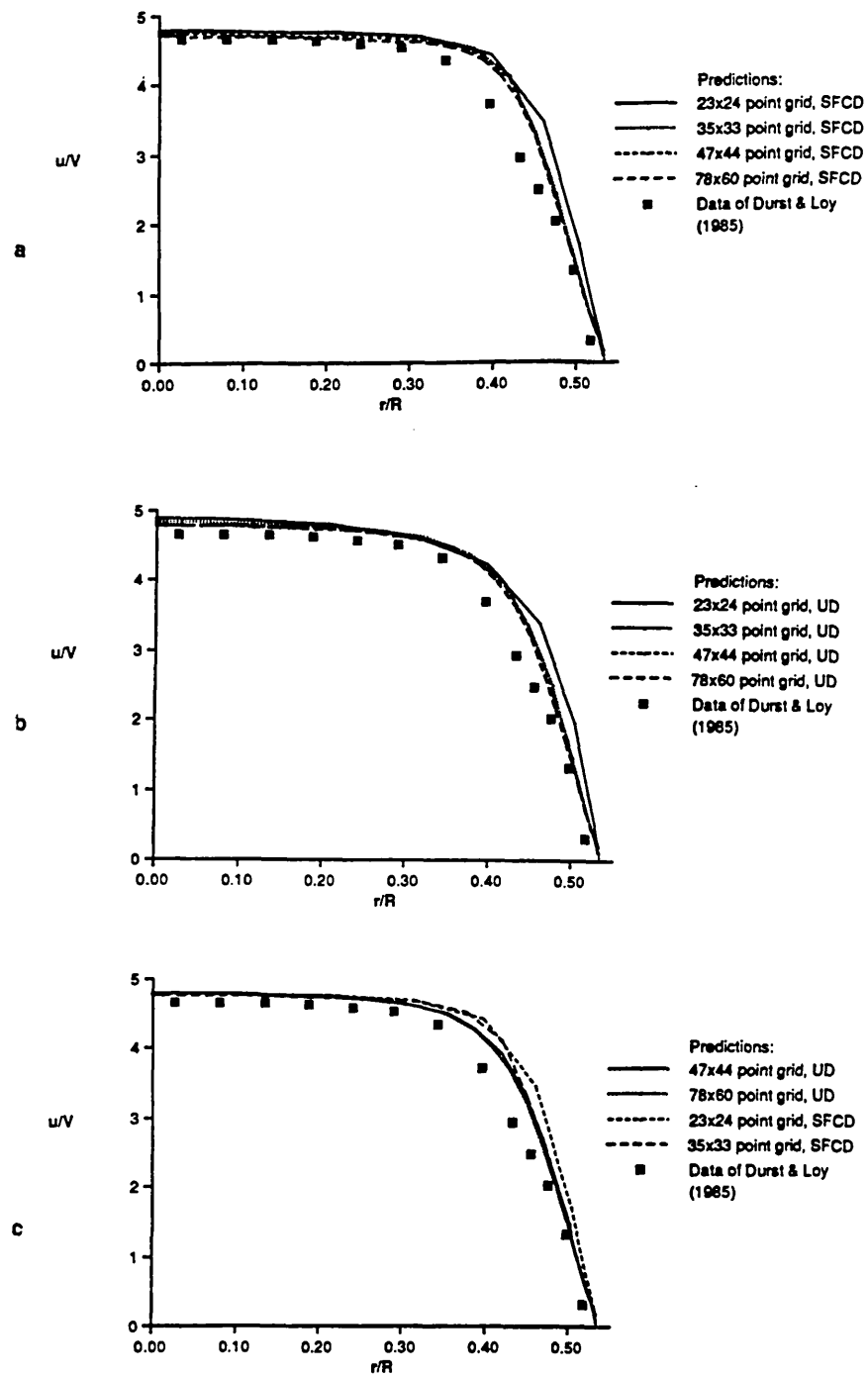


Figure 5.2.5 Comparison of UD and SFCD predictions, and of predictions with experiment, 0.209D downstream of contraction

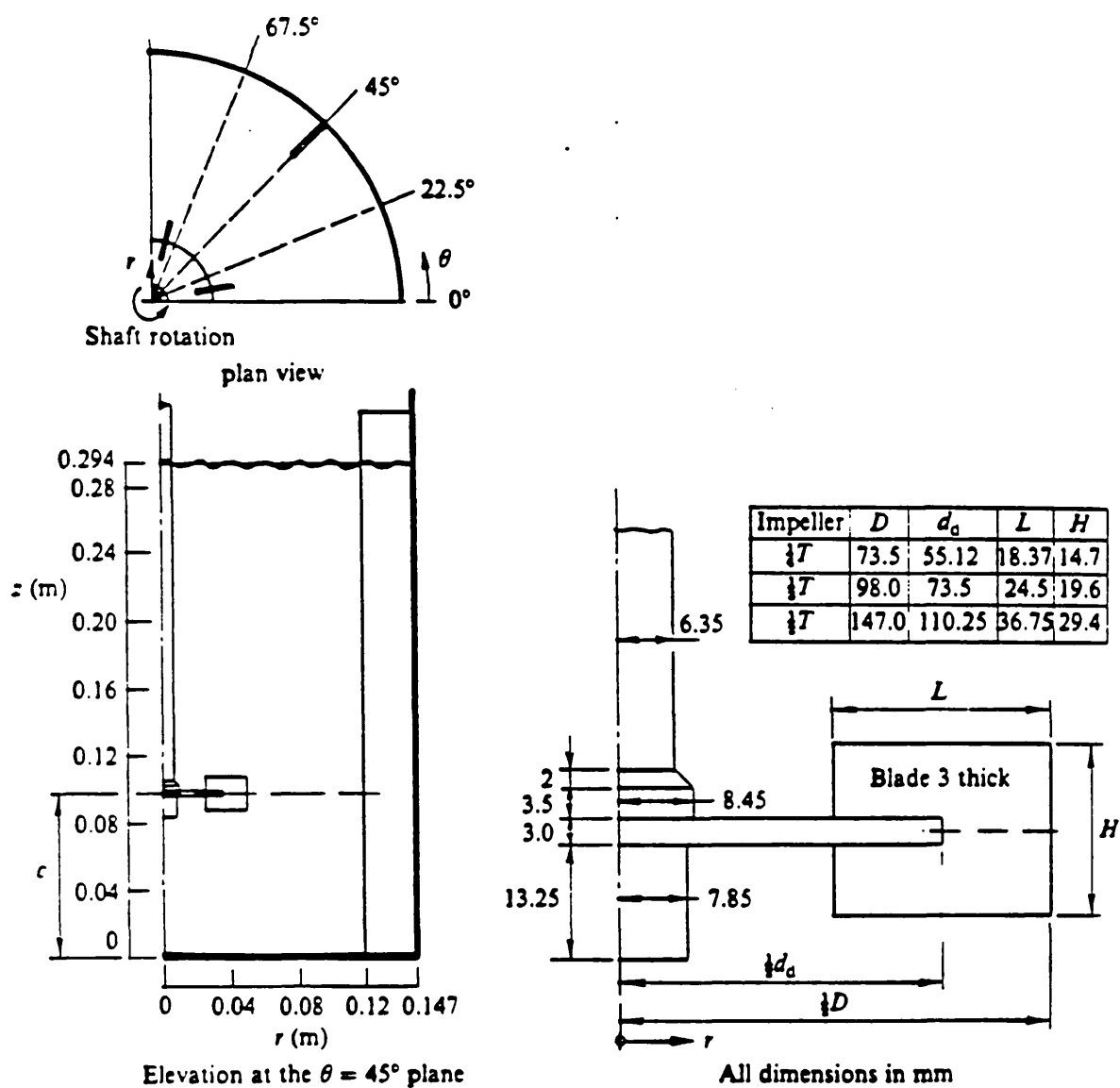
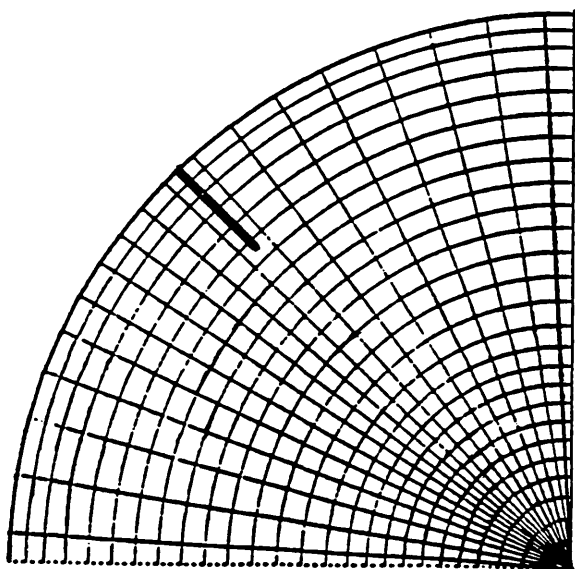
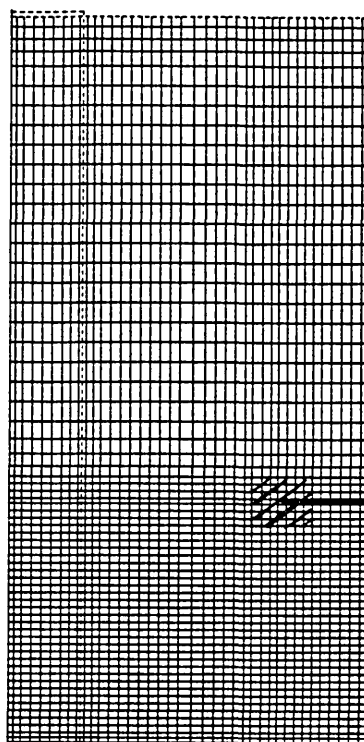
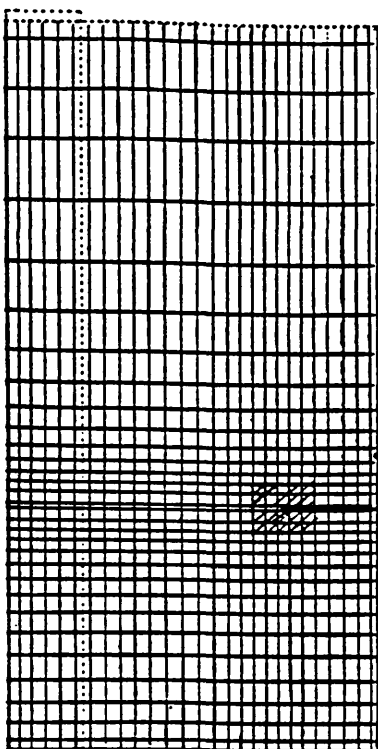
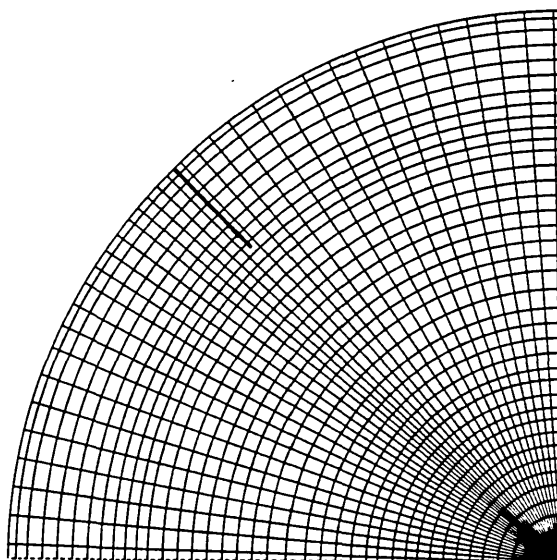


Figure 5.3.1 Mixing vessel geometry



31x27x19



62x39x36

Figure 5.3.2 Computational grids, mixing vessel

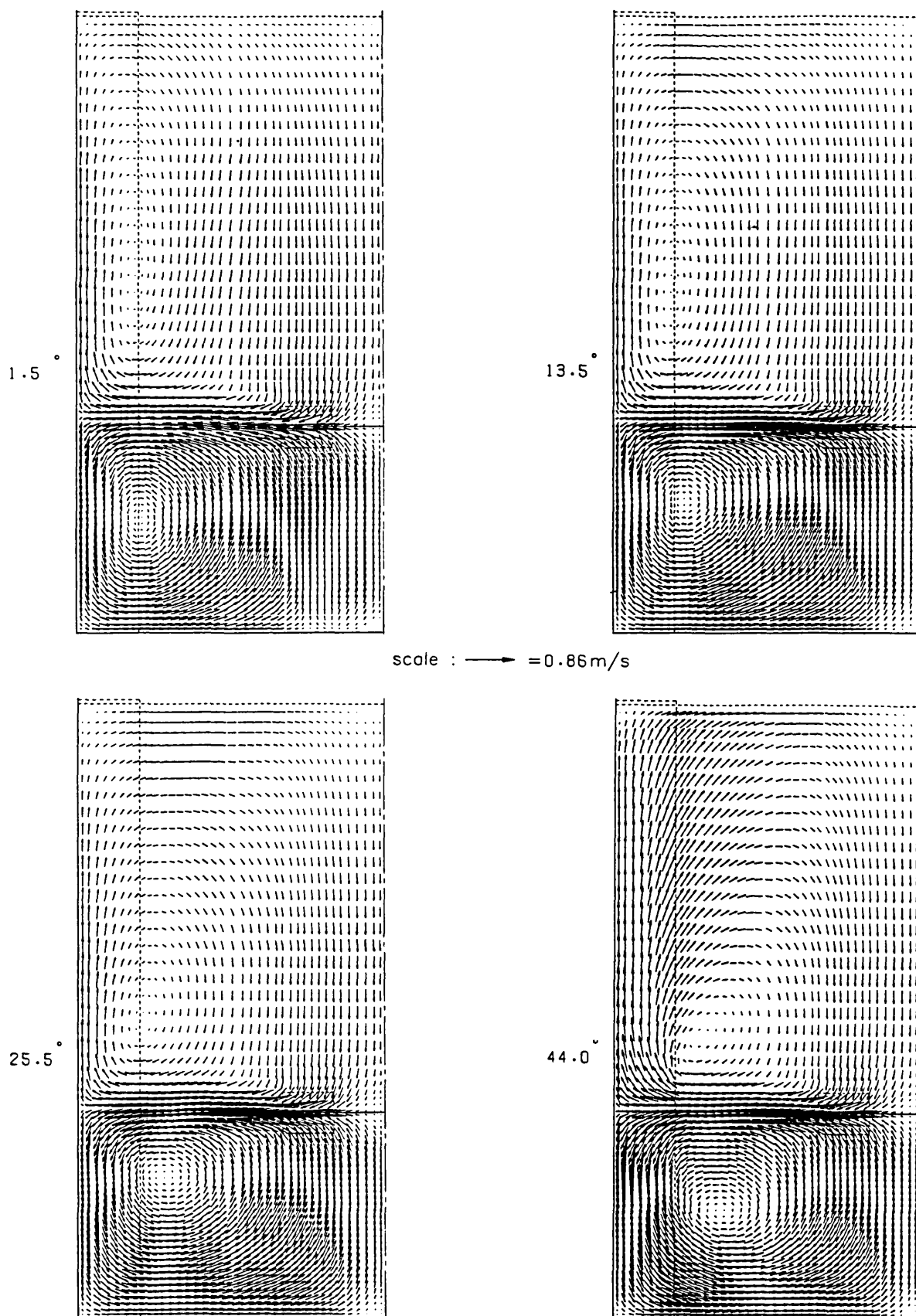


Figure 5.3.3 Velocity vectors in $x - r$ planes, finest grid, water in mixing vessel

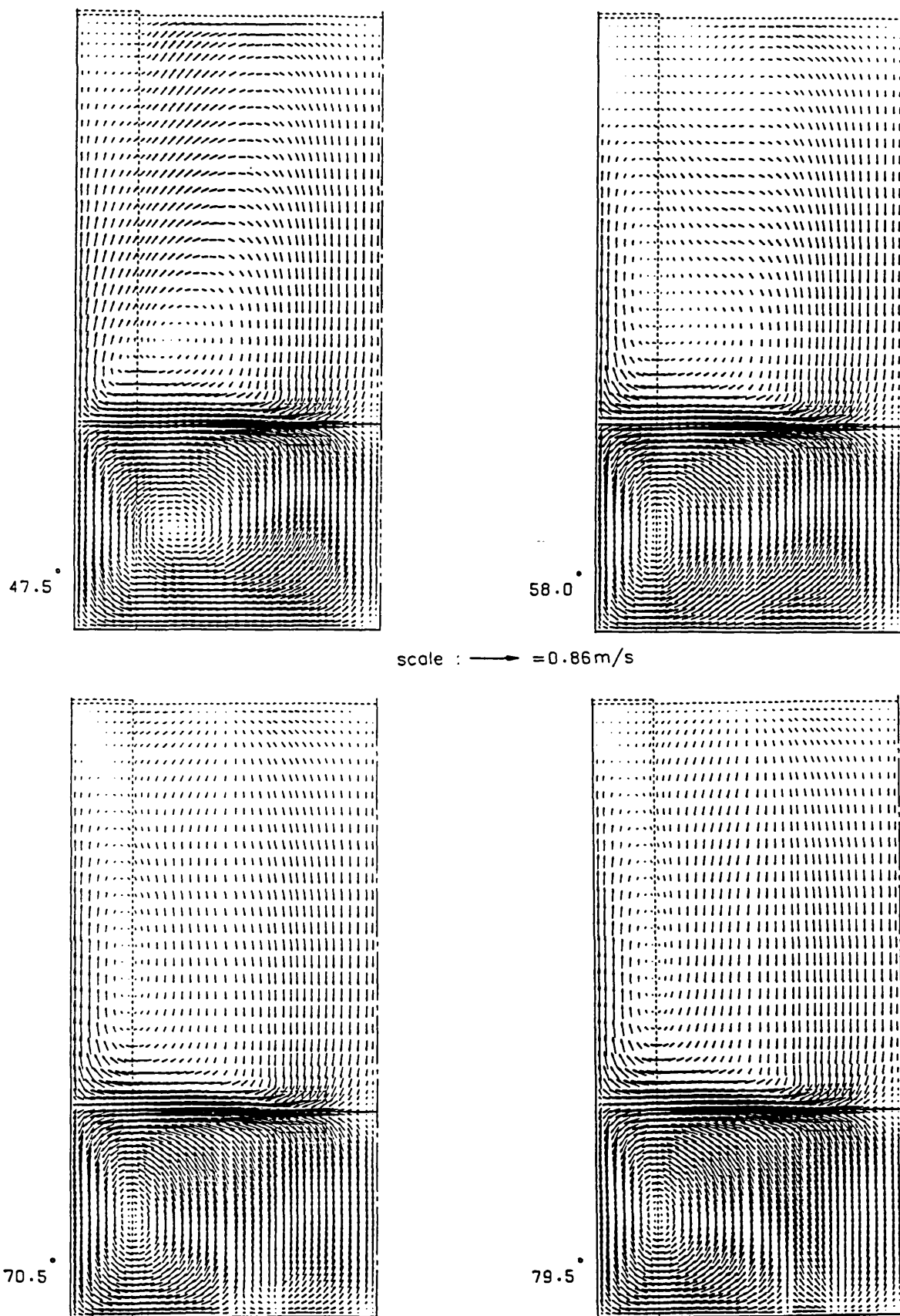


Figure 5.3.3 Velocity vectors in $x-r$ planes, finest grid, water in mixing vessel

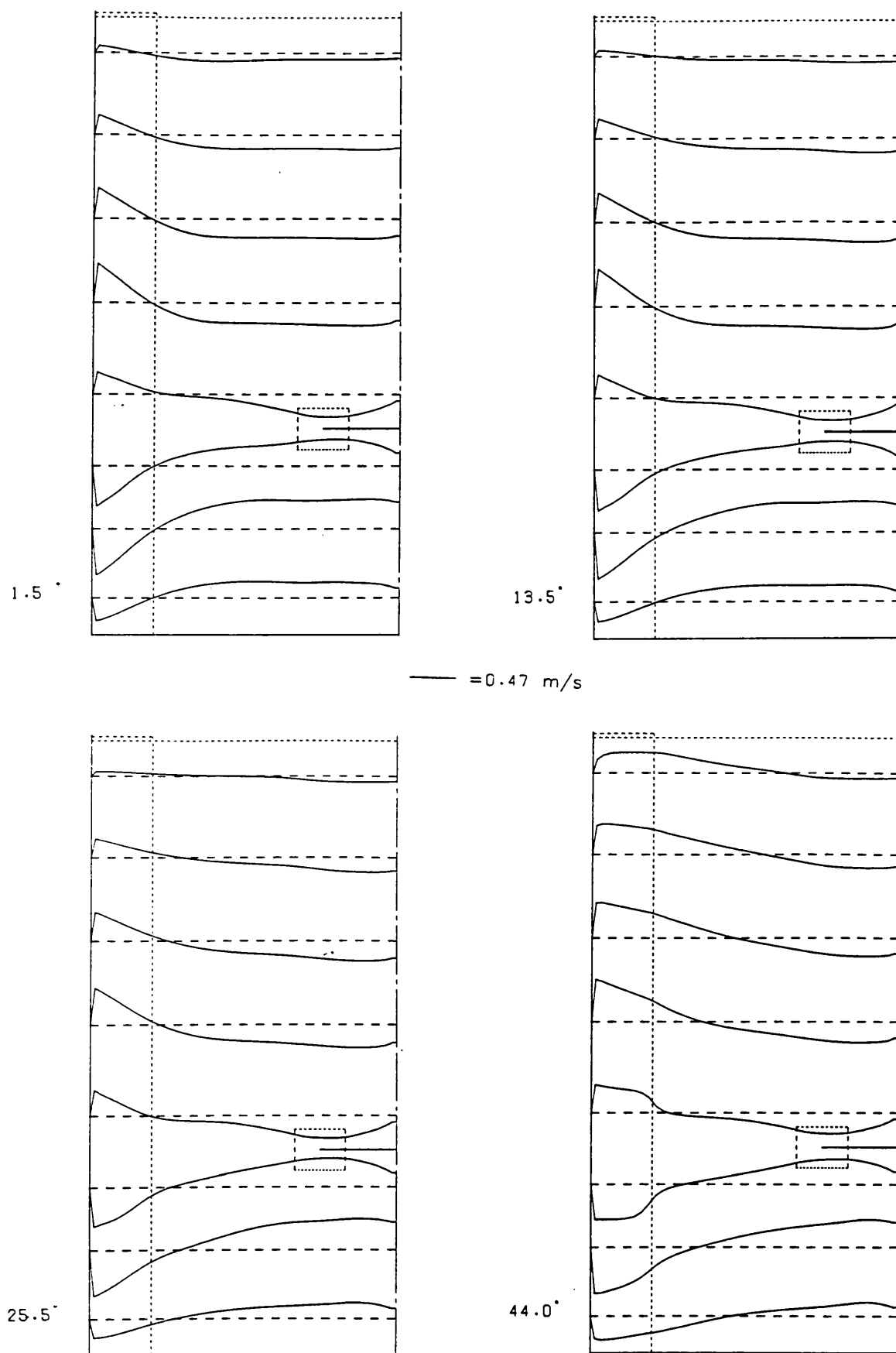


Figure 5.3.4 Axial velocity profiles in $x-r$ planes, finest grid, water in mixing vessel

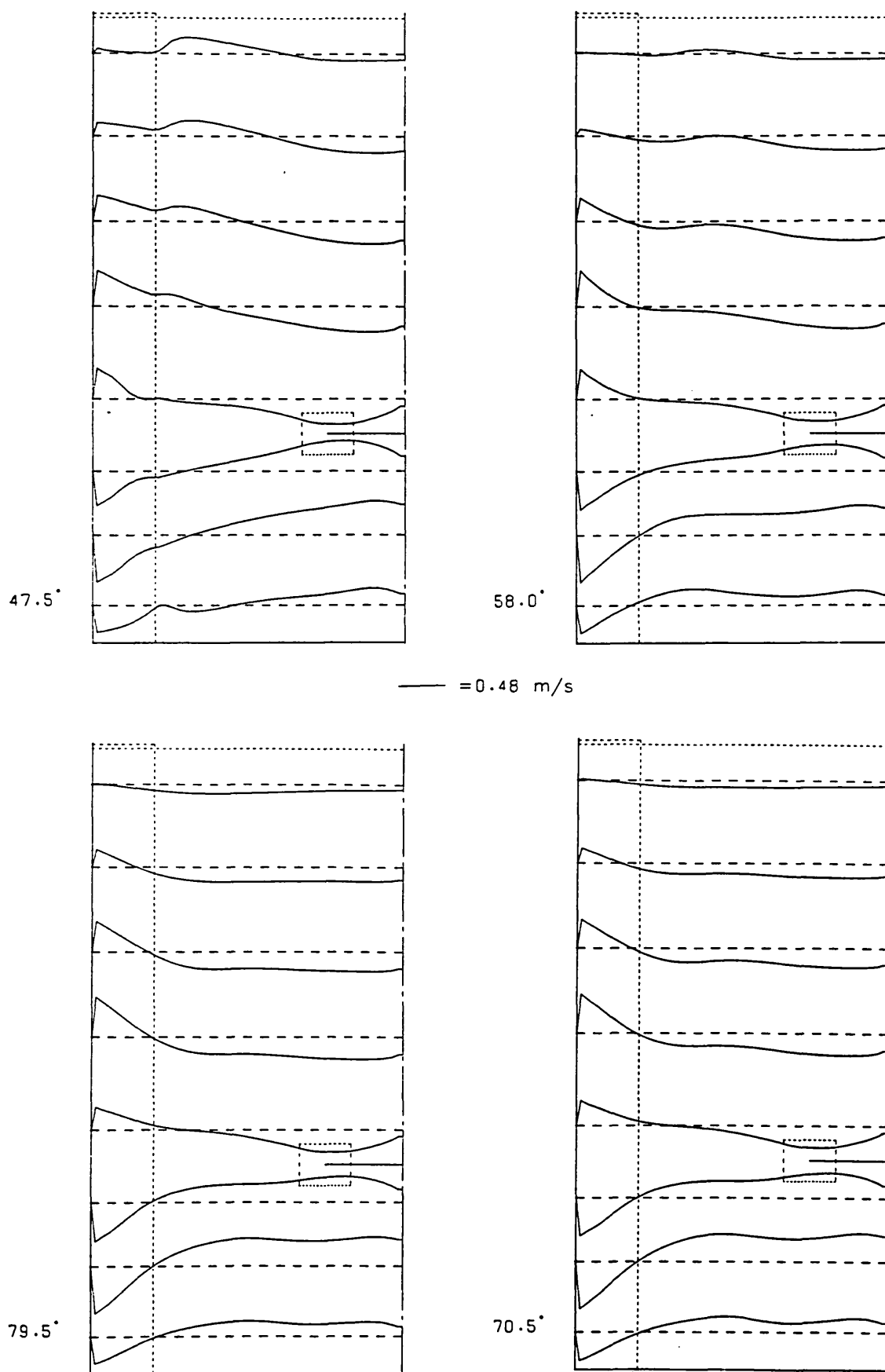


Figure 5.3.4 Axial velocity profiles in $x-r$ planes, finest grid, water in mixing vessel

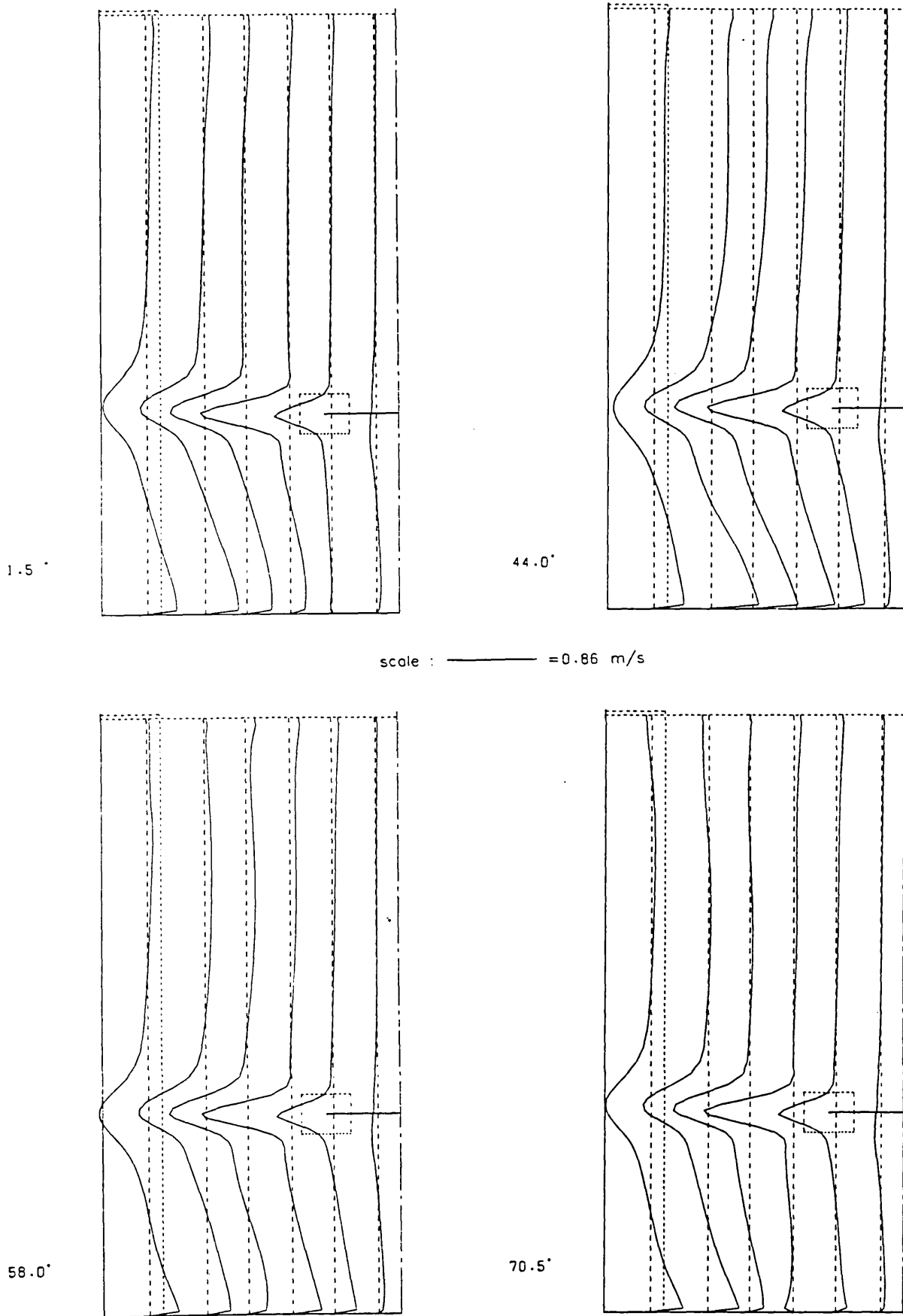


Figure 5.3.5 Radial velocity profiles in $x - r$ planes, finest grid, water in mixing vessel

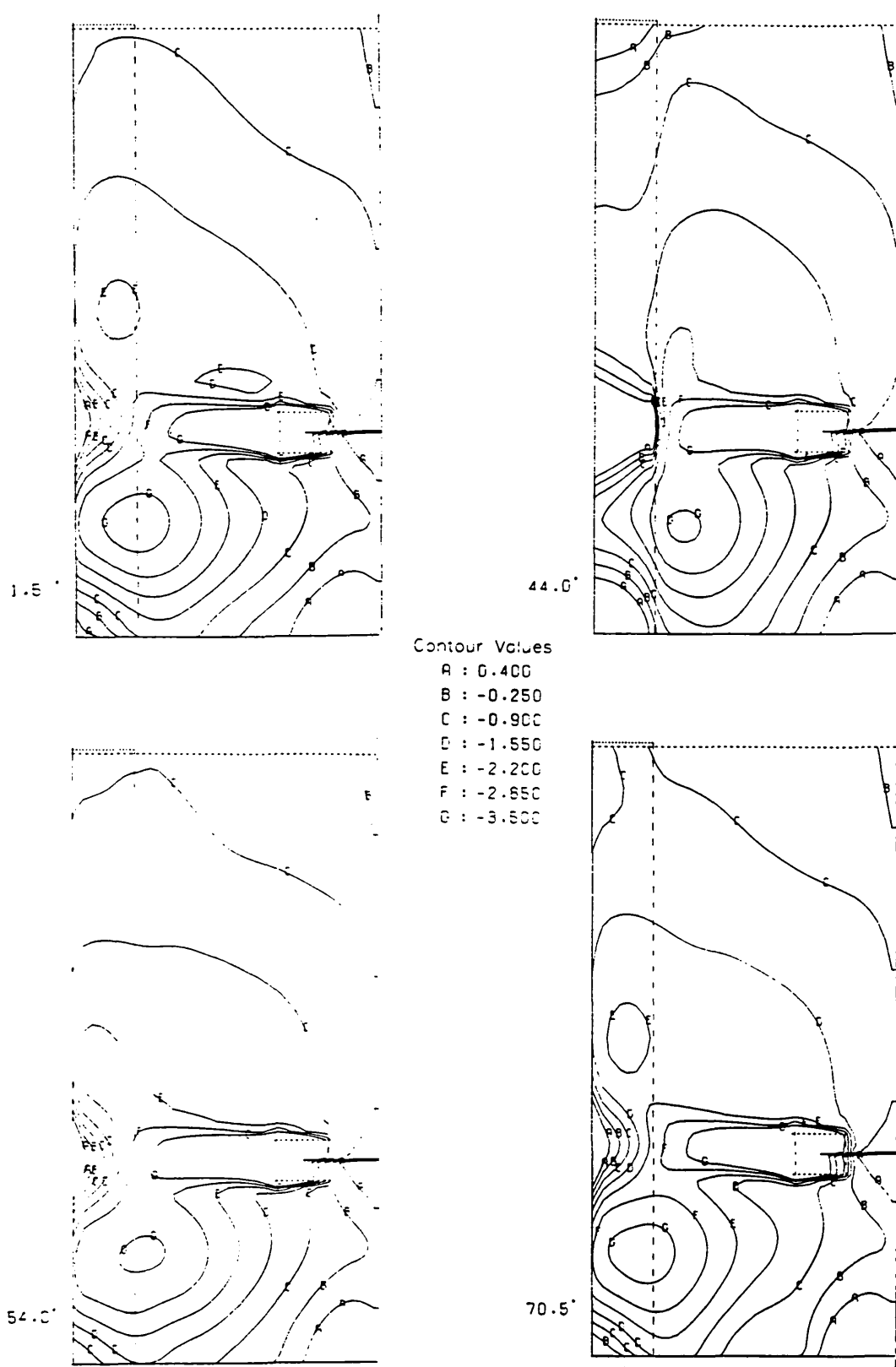


Figure 5.3.6 Normalised pressure in $x - r$ planes, finest grid, water in mixing vessel

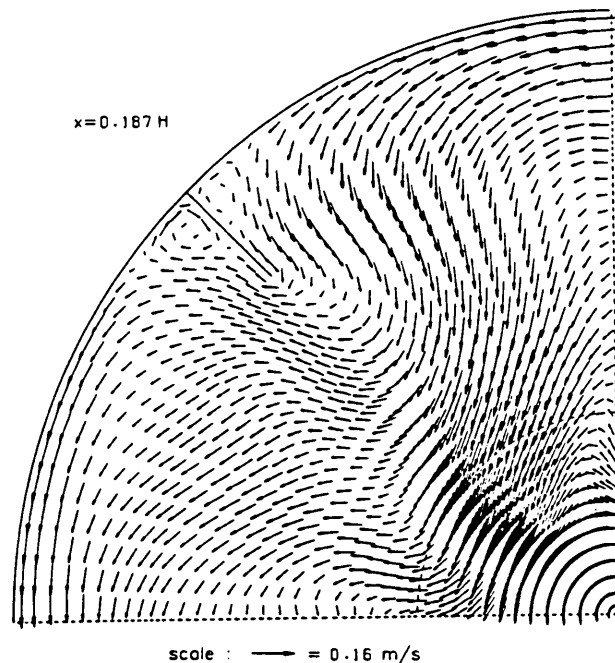
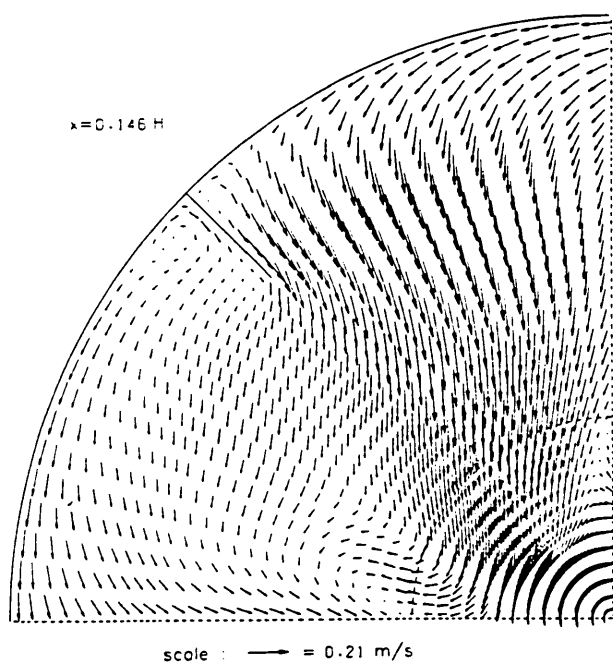
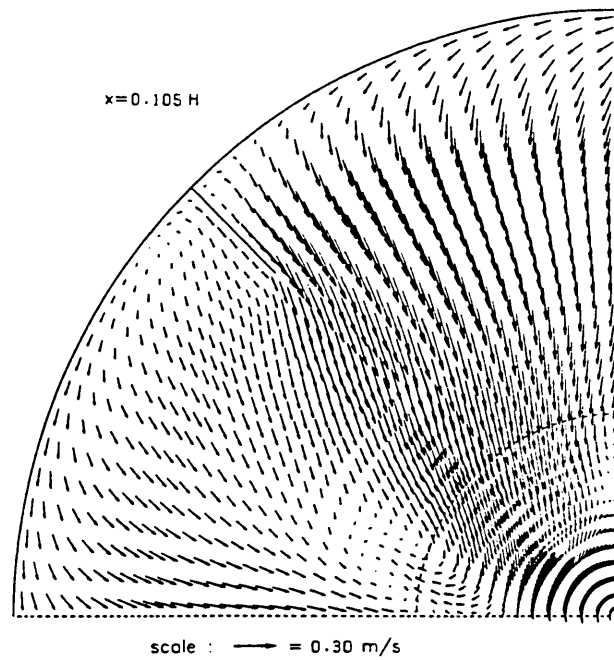
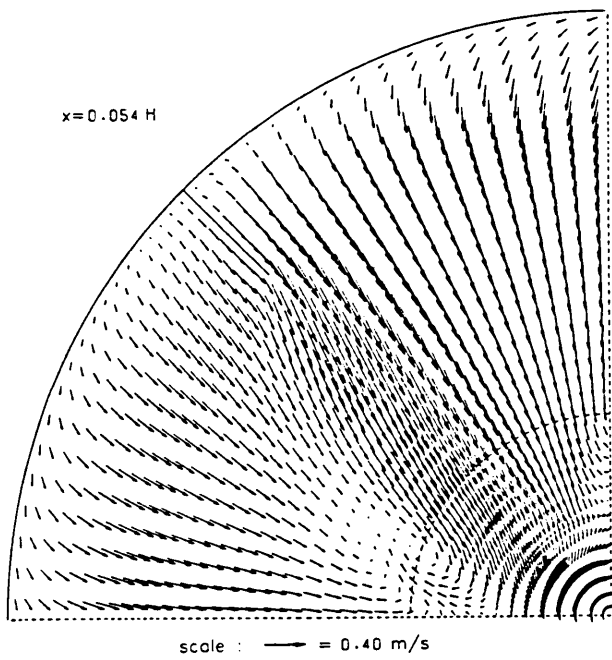


Figure 5.3.7 Velocity vectors in $r - \theta$ planes, finest grid, water in mixing vessel

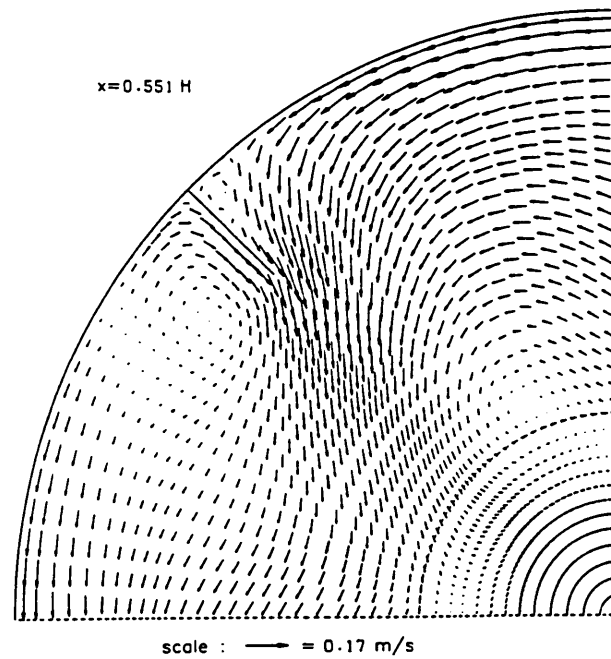
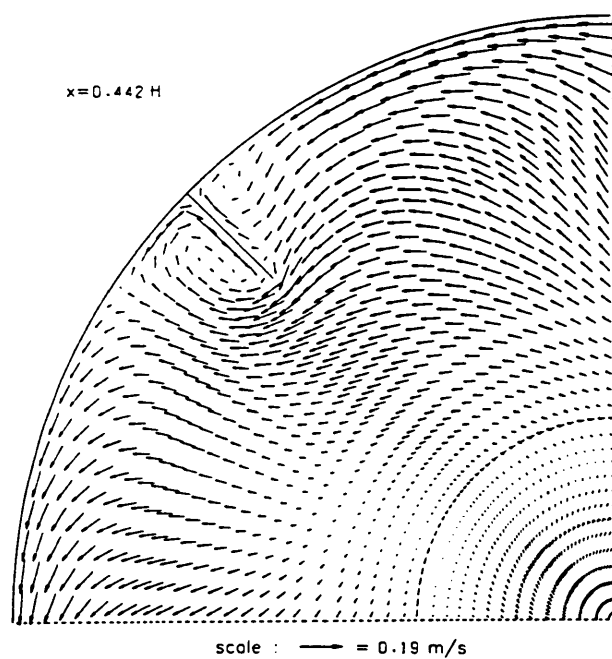
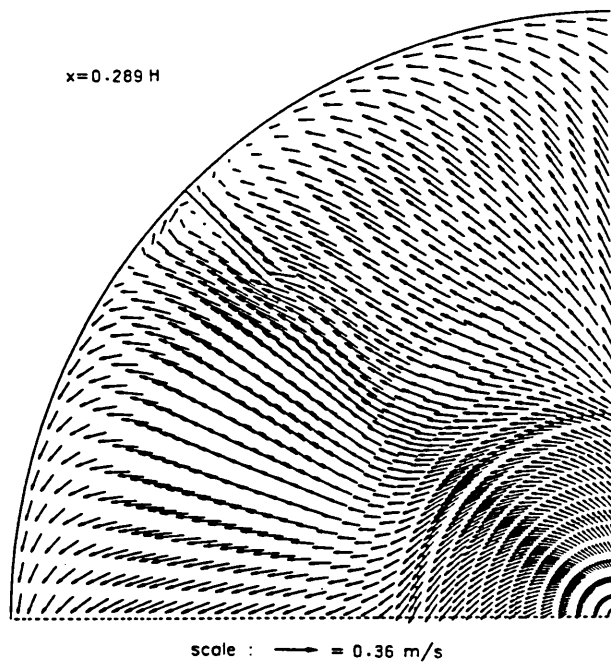
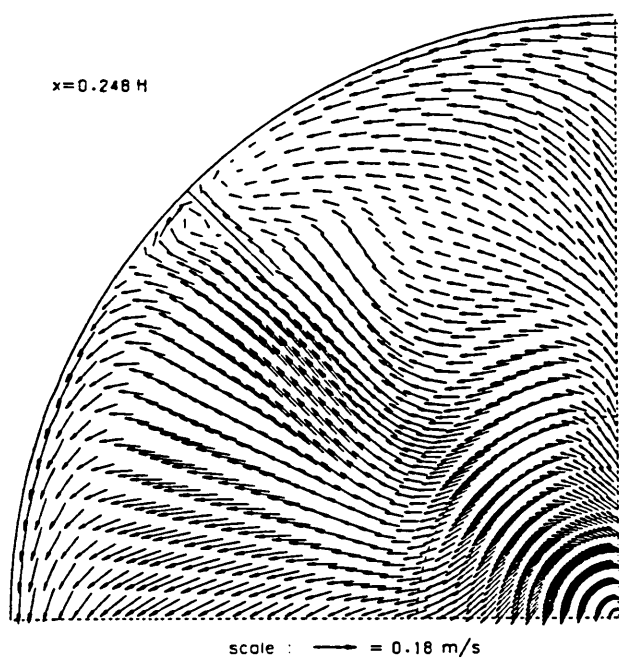


Figure 5.3.7 Velocity vectors in $r - \theta$ planes, finest grid, water in mixing vessel

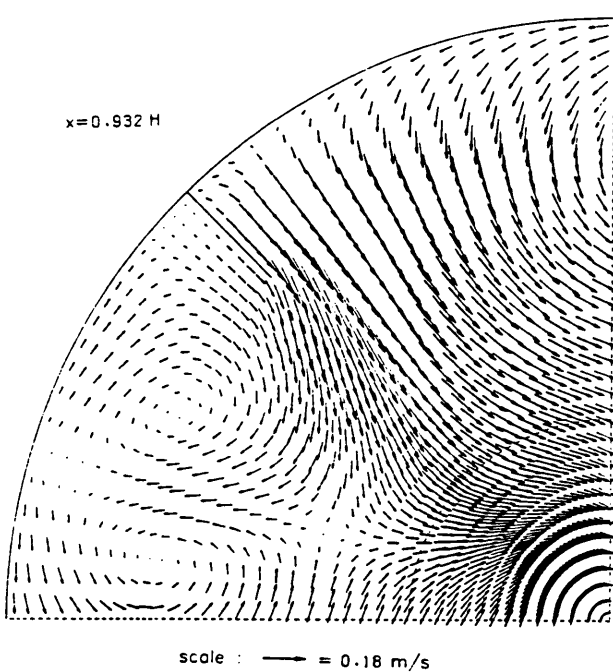
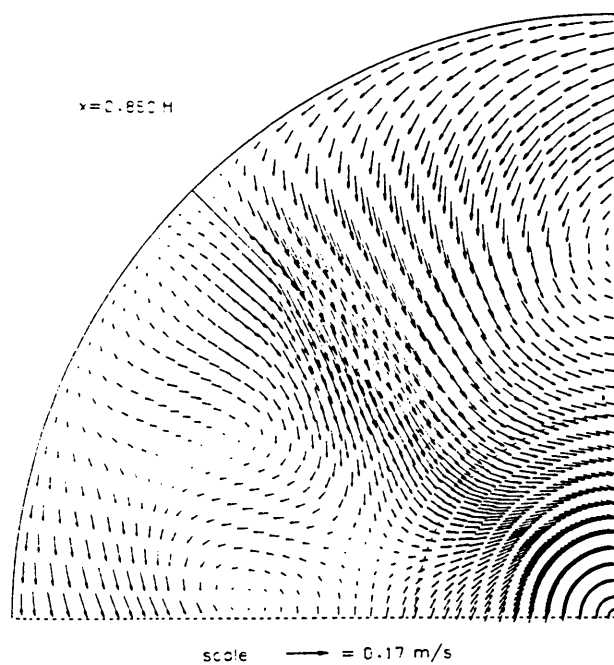
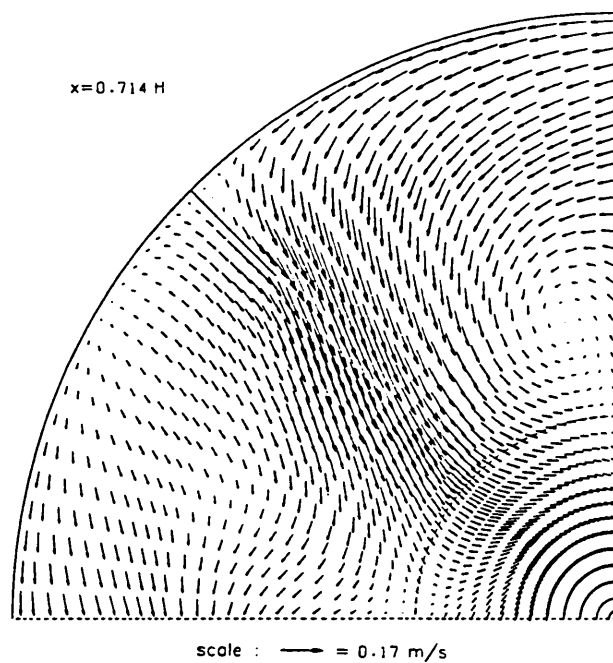
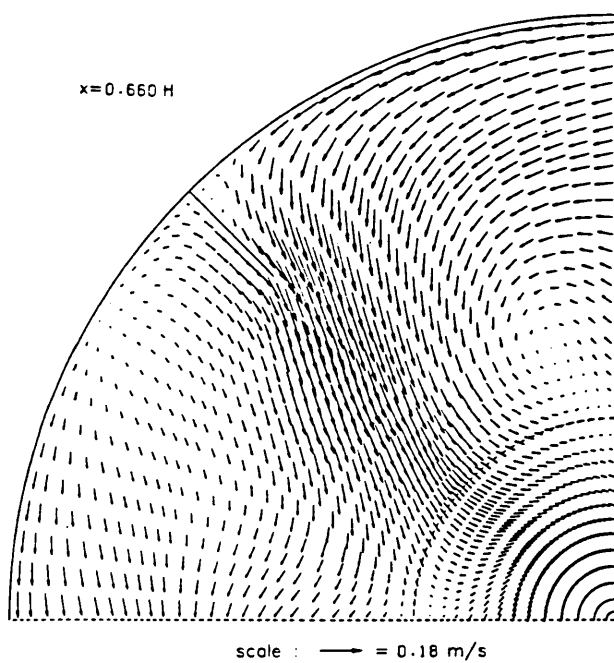


Figure 5.3.7 Velocity vectors in $r - \theta$ planes, finest grid, water in mixing vessel

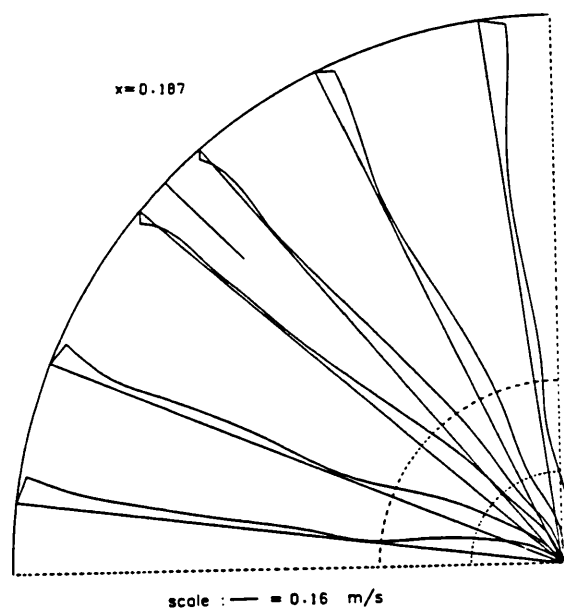
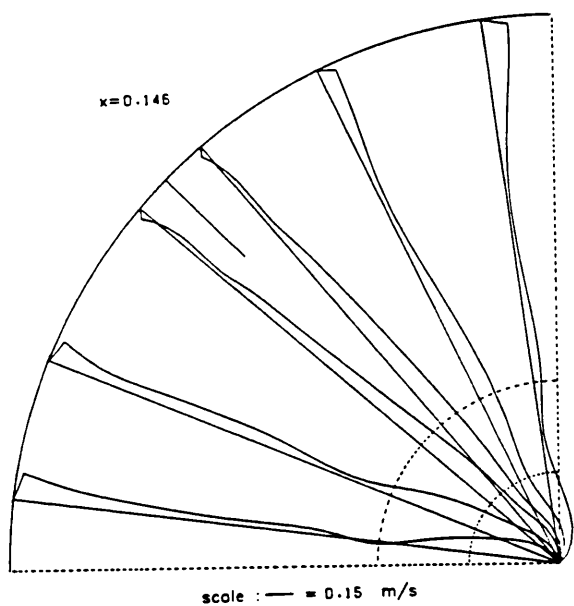
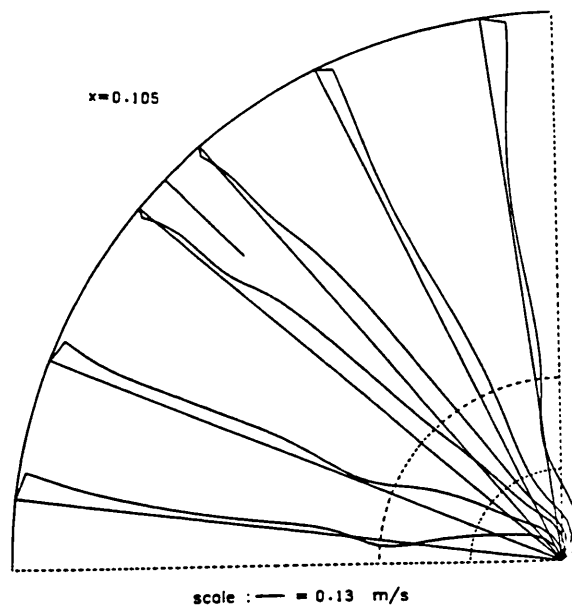
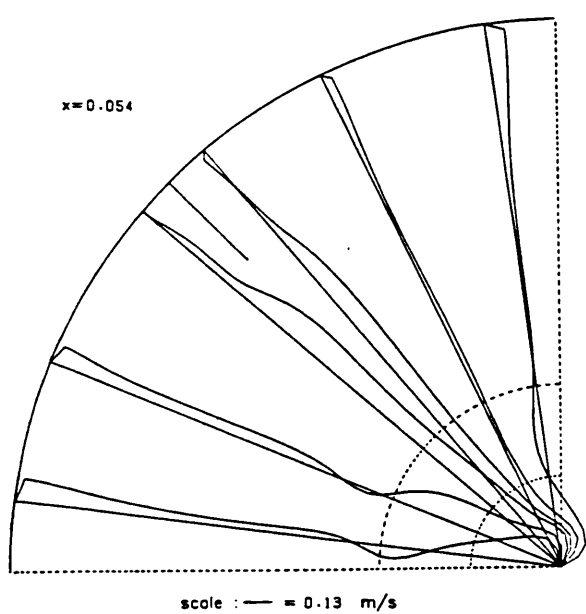


Figure 5.3.8 Swirl velocity profiles in $r - \theta$ planes, finest grid, water in mixing vessel

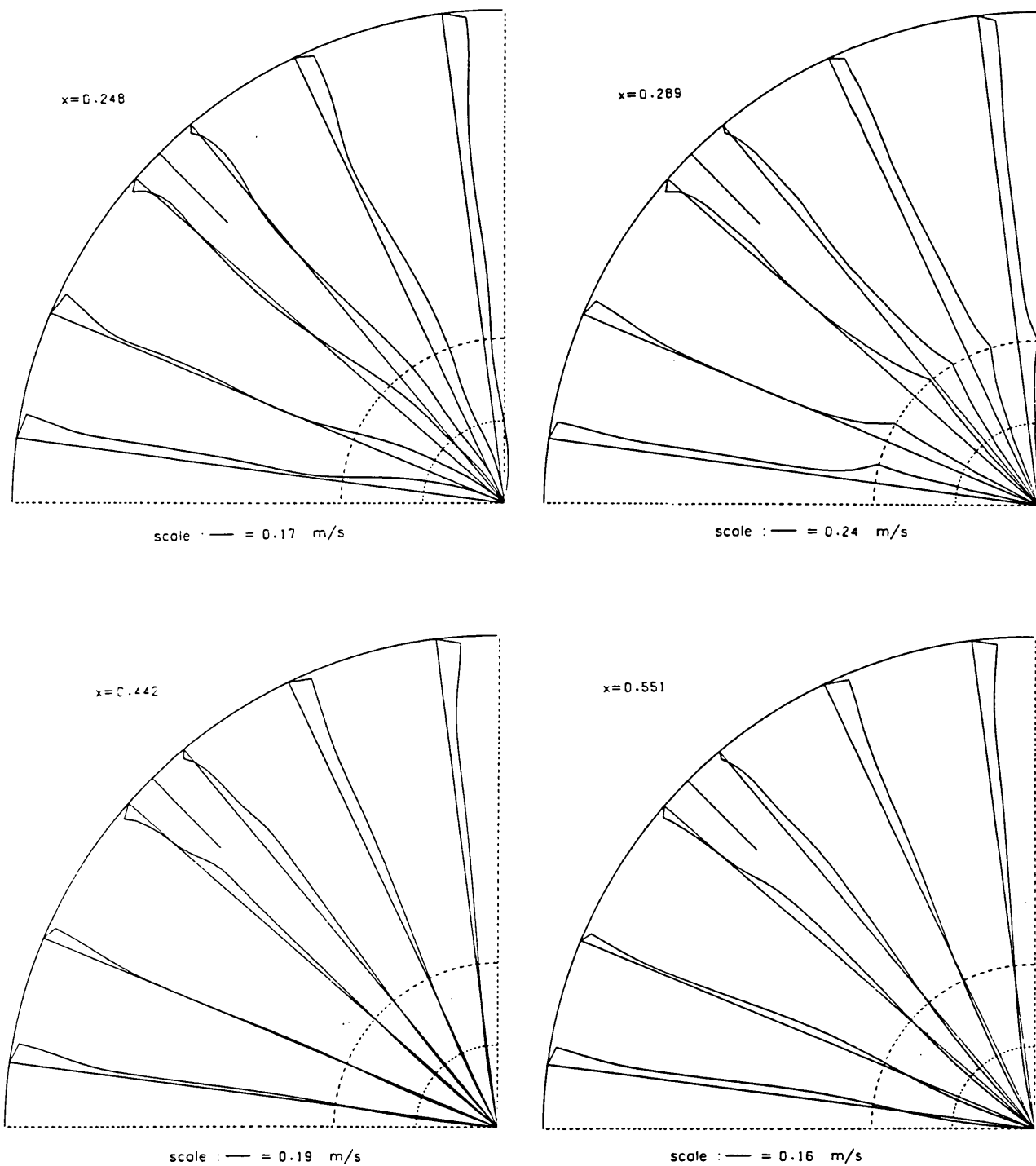


Figure 5.3.8 Swirl velocity profiles in $r - \theta$ planes, finest grid, water in mixing vessel

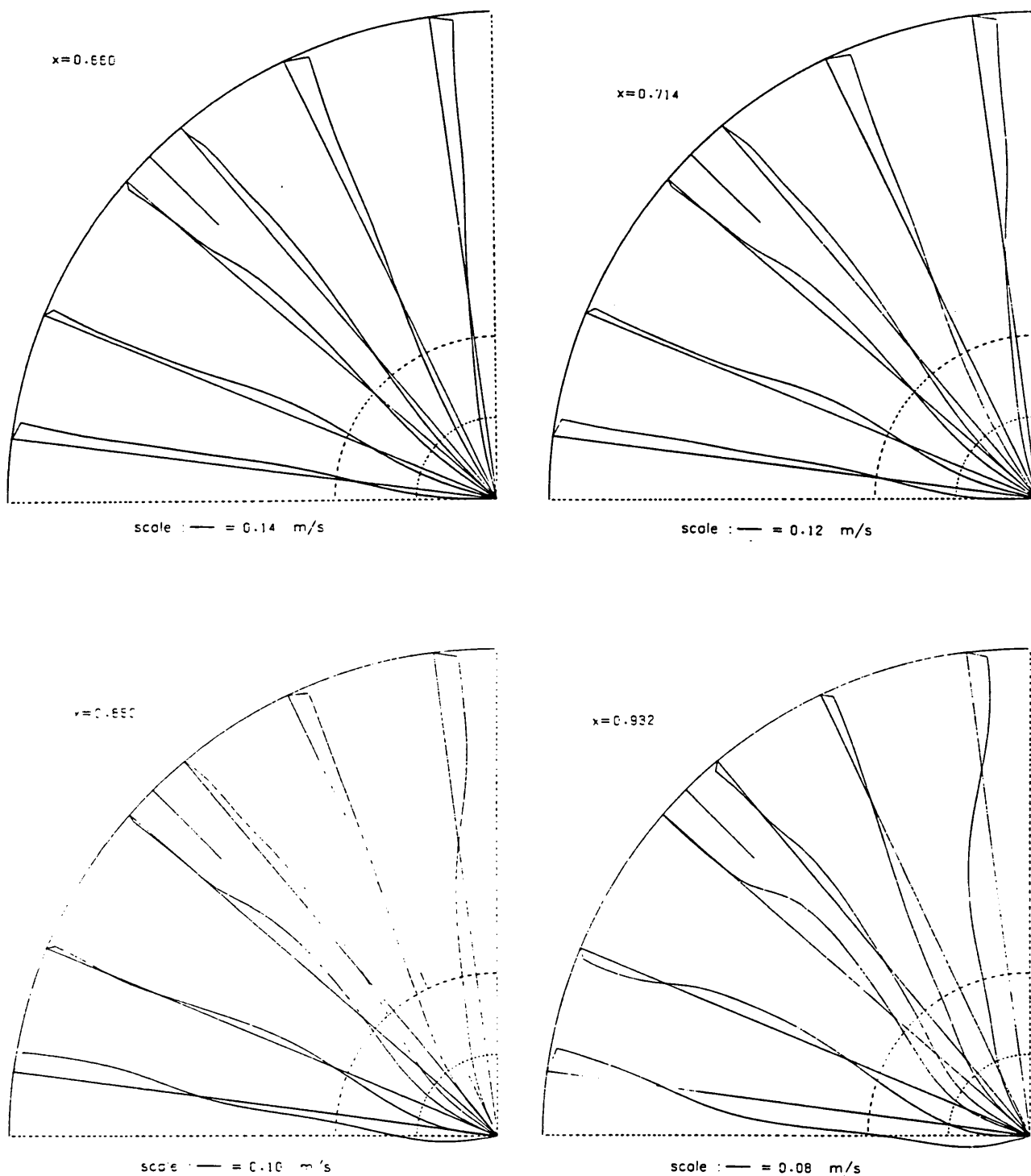


Figure 5.3.8 Swirl velocity profiles in $r - \theta$ planes, finest grid, water in mixing vessel

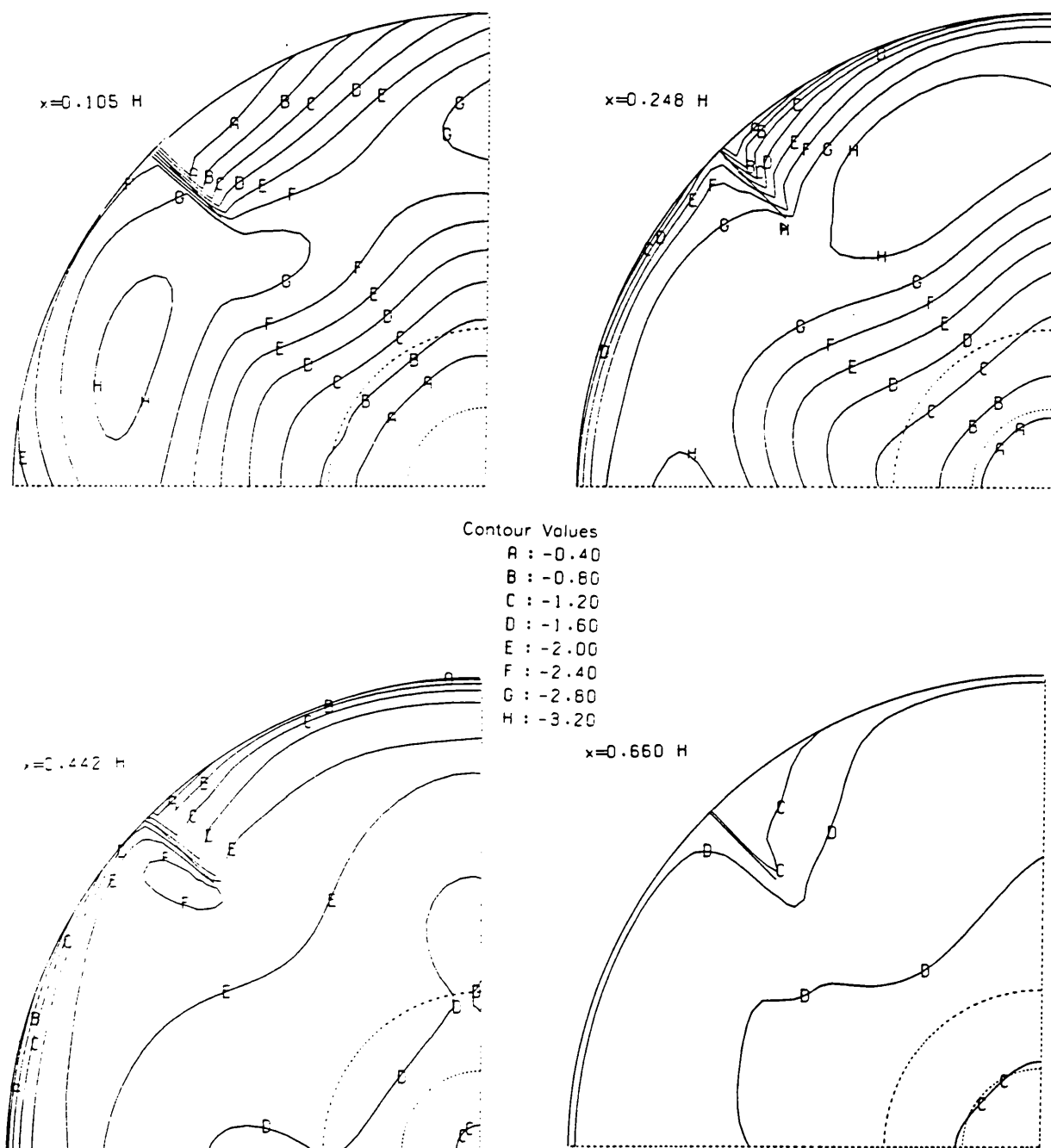
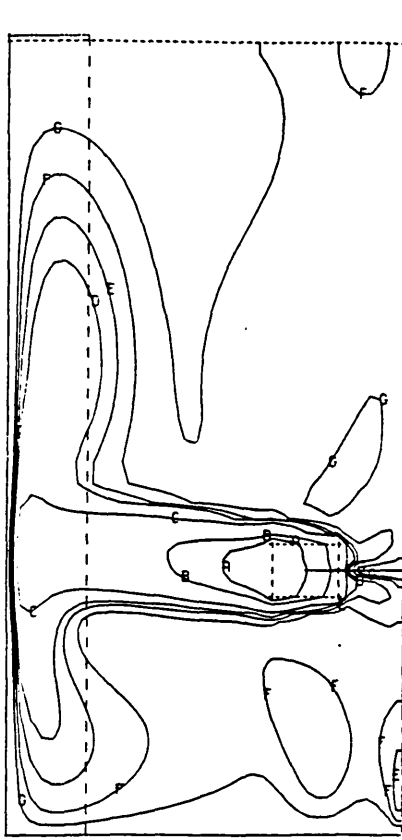
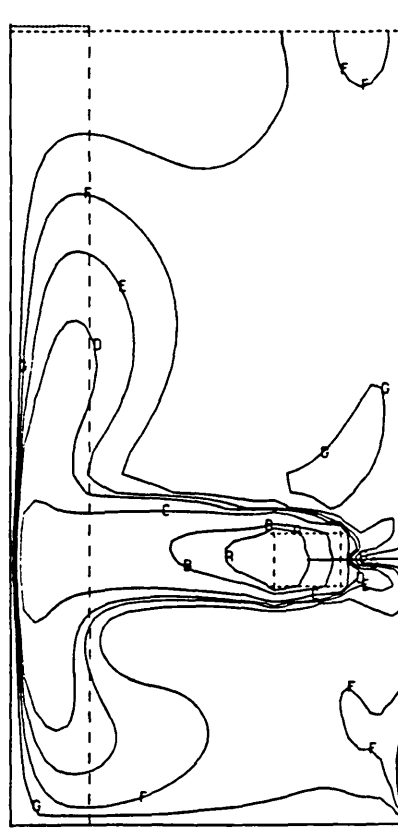


Figure 5.3.9 Normalised pressure in $r - \theta$ planes, finest grid, water in mixing vessel

1.5°



25.5°



Contour Values

A : 7.000

B : 4.000

C : 1.000

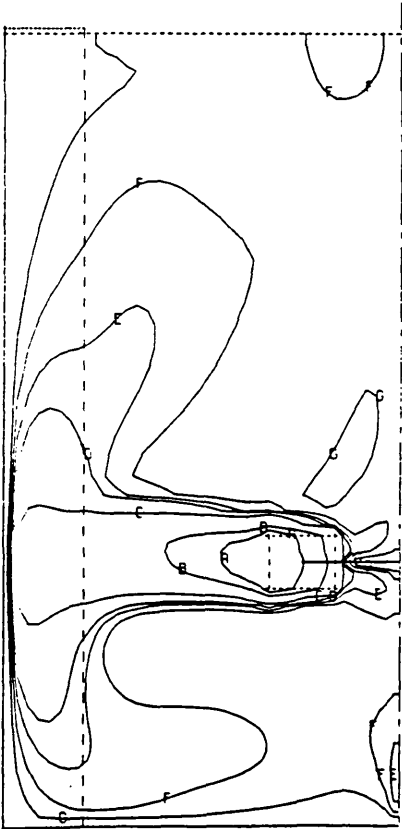
D : 0.500

E : 0.400

F : 0.300

G : 0.200

42.0°



44.0°

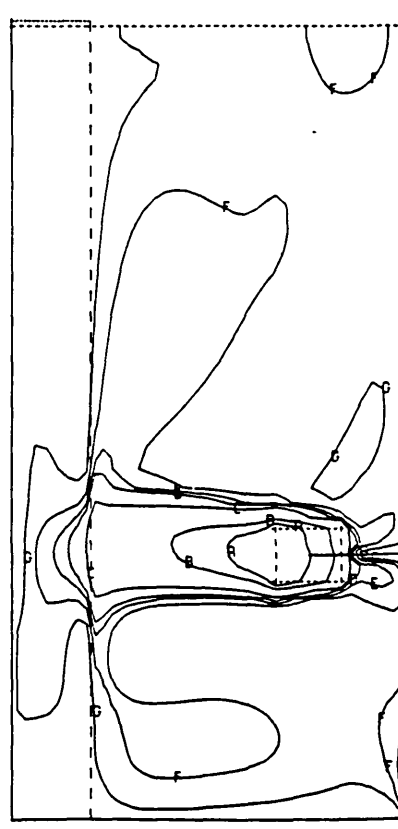


Figure 5.3.10 Normalised turbulence kinetic energy in $x - r$ planes,
finest grid, water in mixing vessel

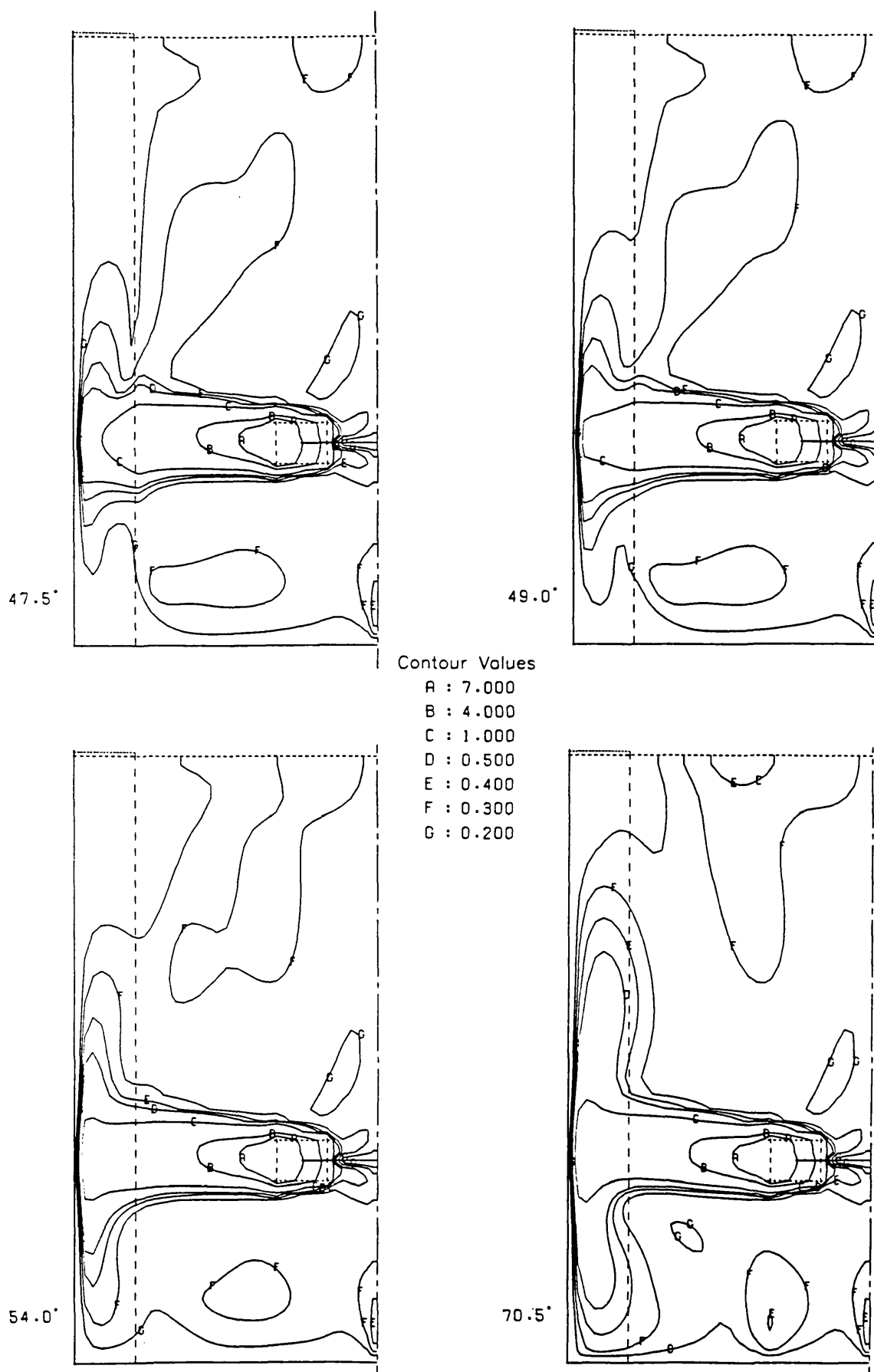


Figure 5.3.10 Normalised turbulence kinetic energy in $x - r$ planes, finest grid, water in mixing vessel

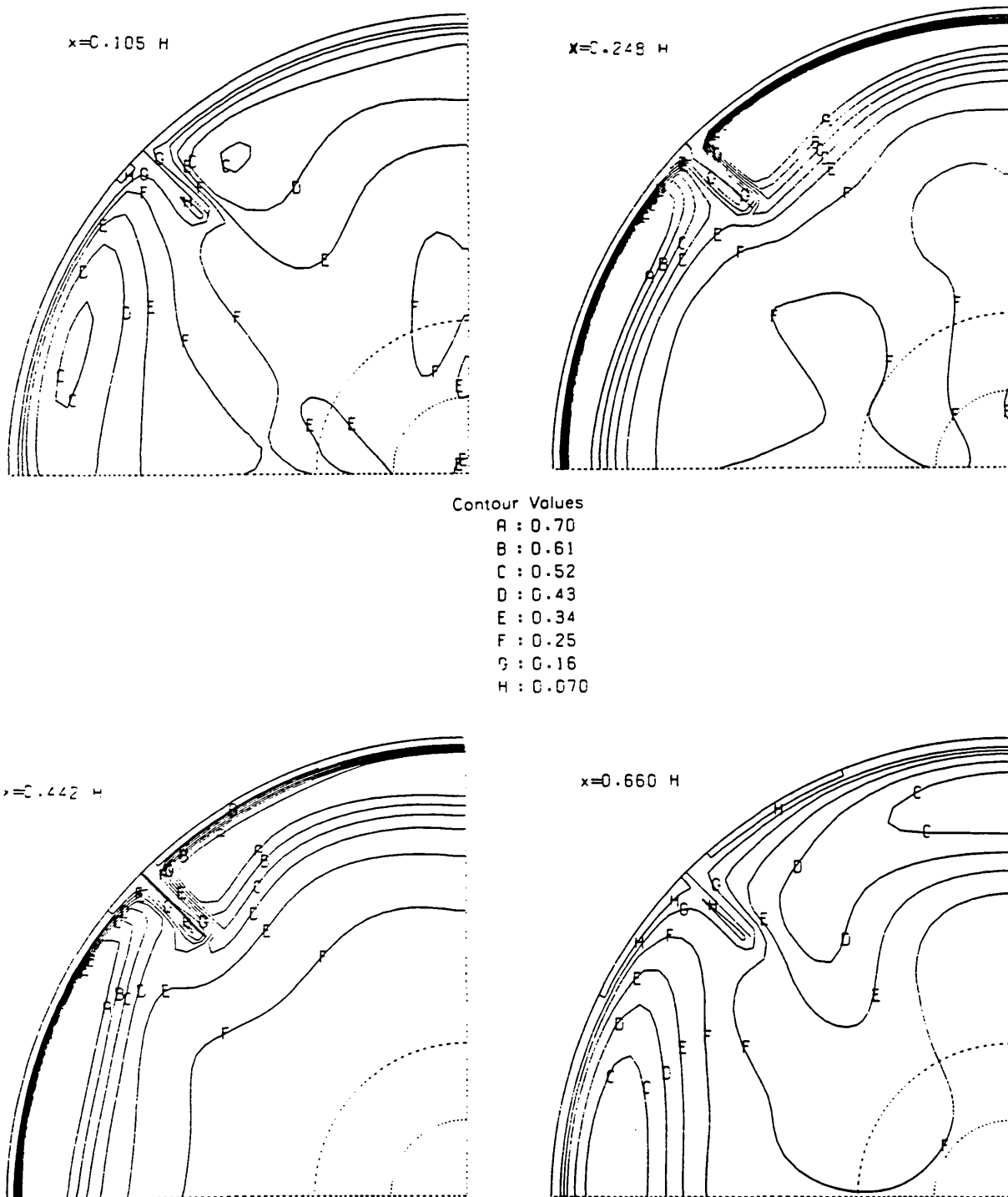


Figure 5.3.11 Normalised turbulence kinetic energy in $r - \theta$ planes,
finest grid, water in mixing vessel

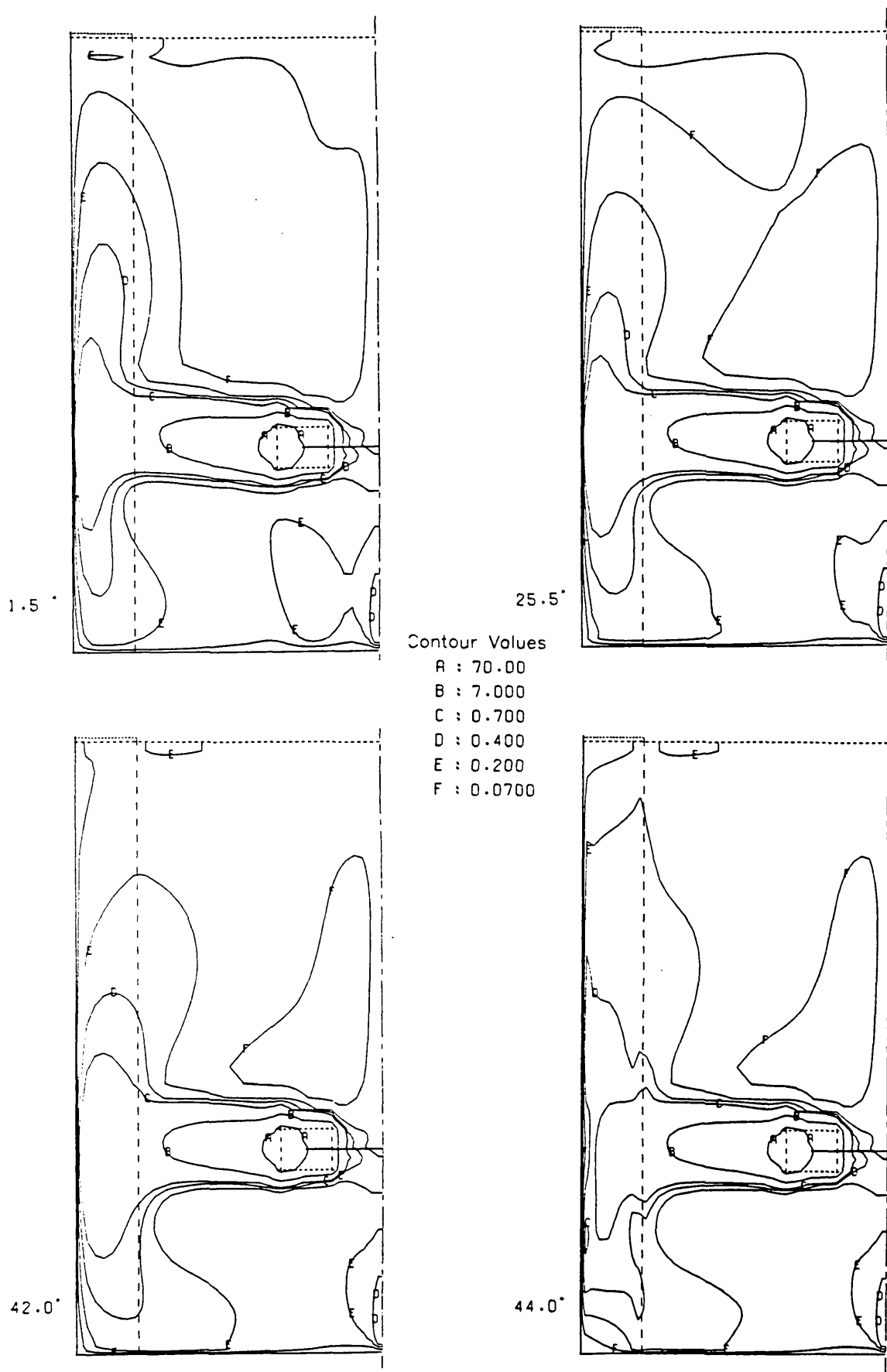


Figure 5.3.12 Normalised turbulence energy dissipation rate in $x - r$ planes, finest grid, water in mixing vessel

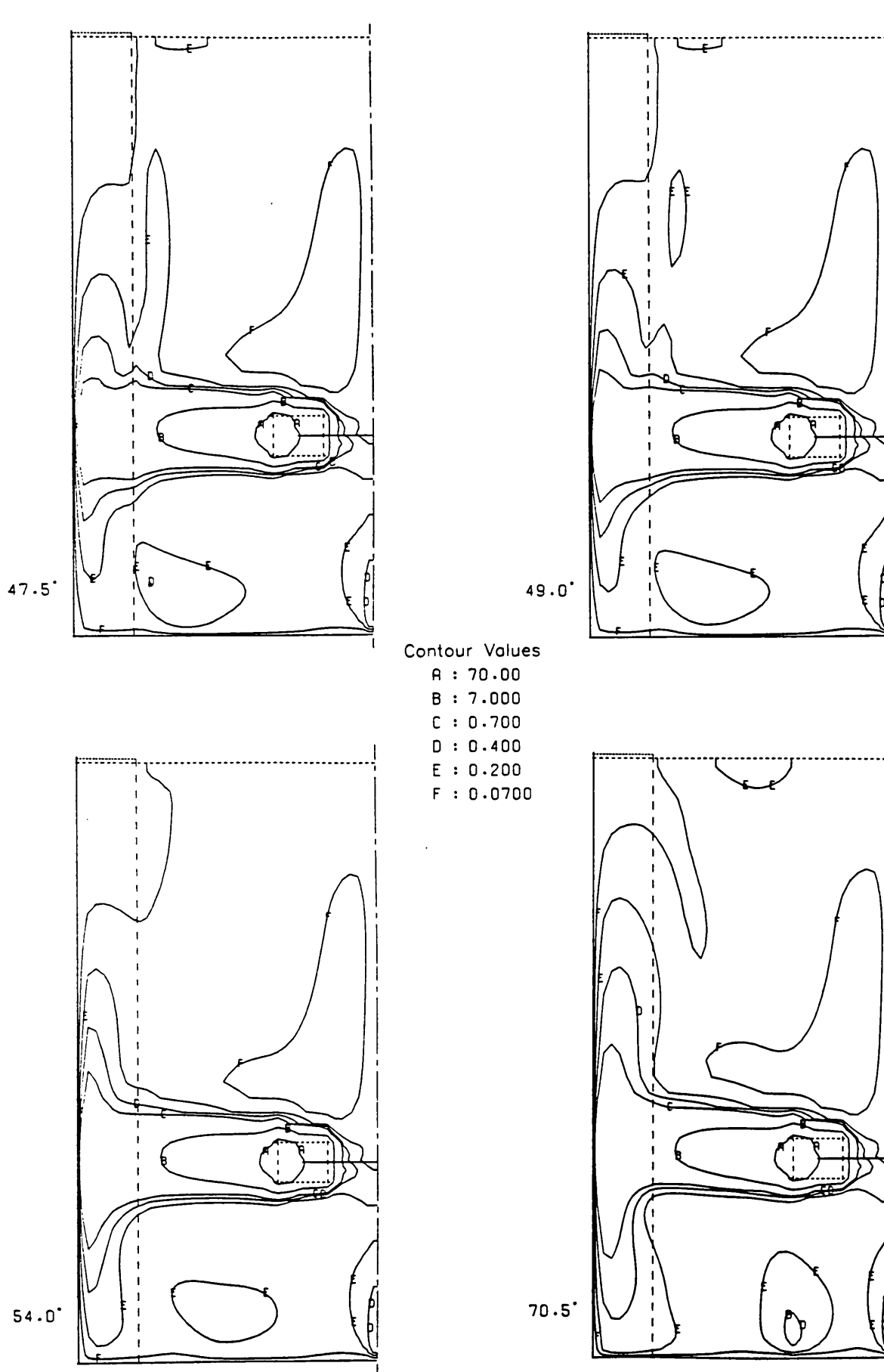


Figure 5.3.12 Normalised turbulence energy dissipation rate in $x - r$ planes, finest grid, water in mixing vessel

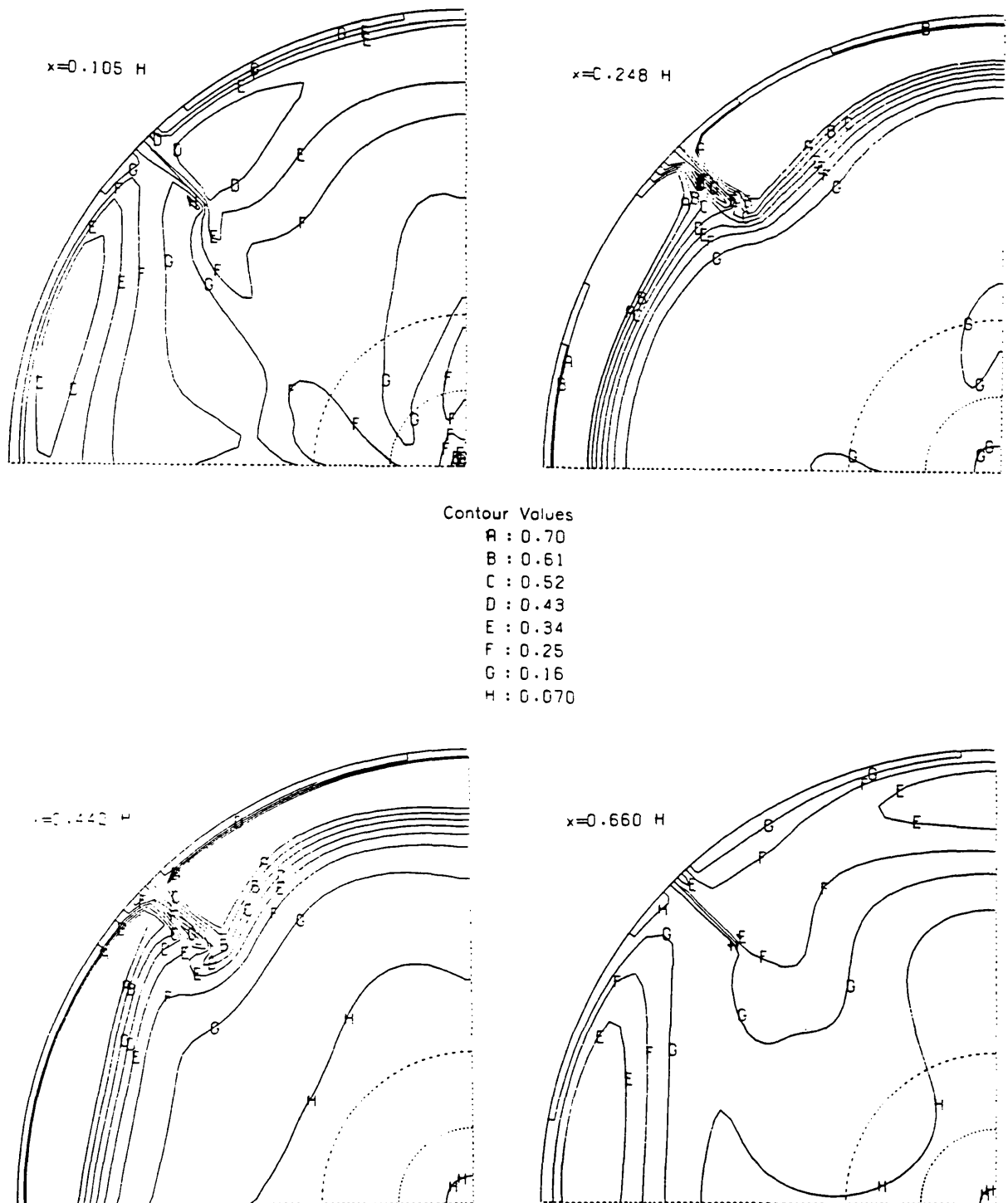


Figure 5.3.13 Normalised turbulence energy dissipation rate in $r - \theta$ planes, finest grid, water in mixing vessel

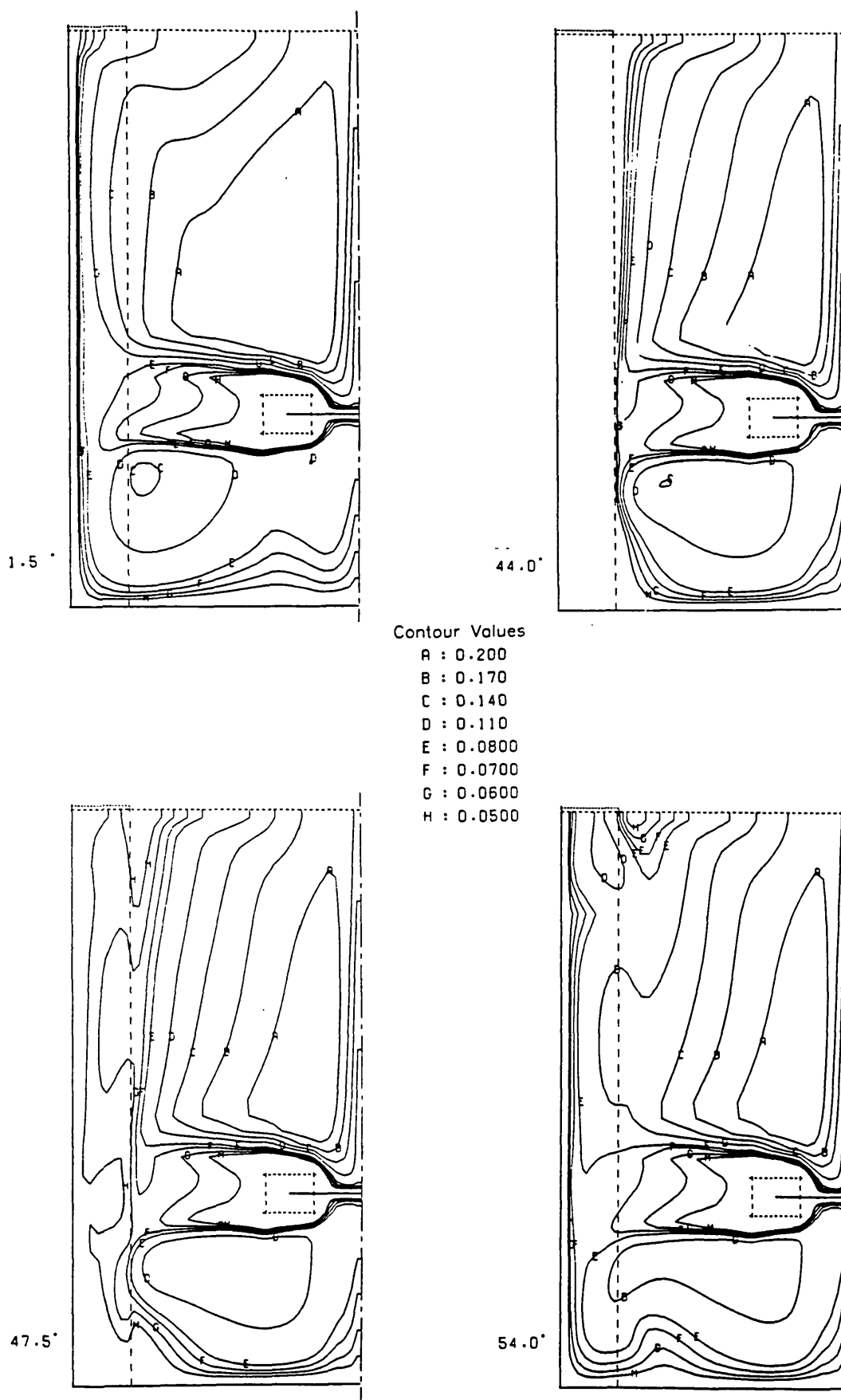


Figure 5.3.14 Normalised turbulence length scales in $x - r$ planes, finest grid, water in mixing vessel

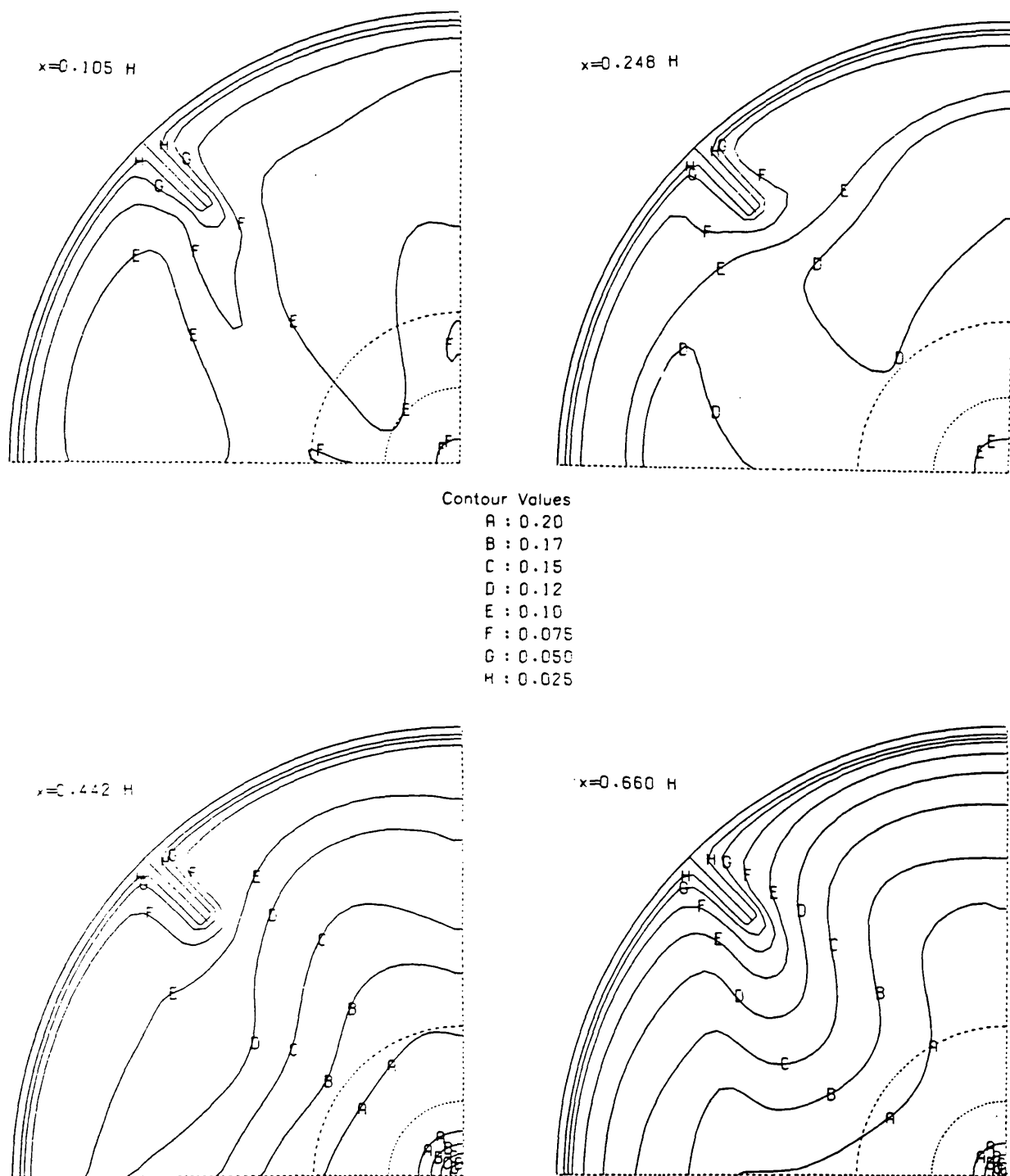


Figure 5.3.15 Normalised turbulence length scales in $r - \theta$ planes,
finest grid, water in mixing vessel

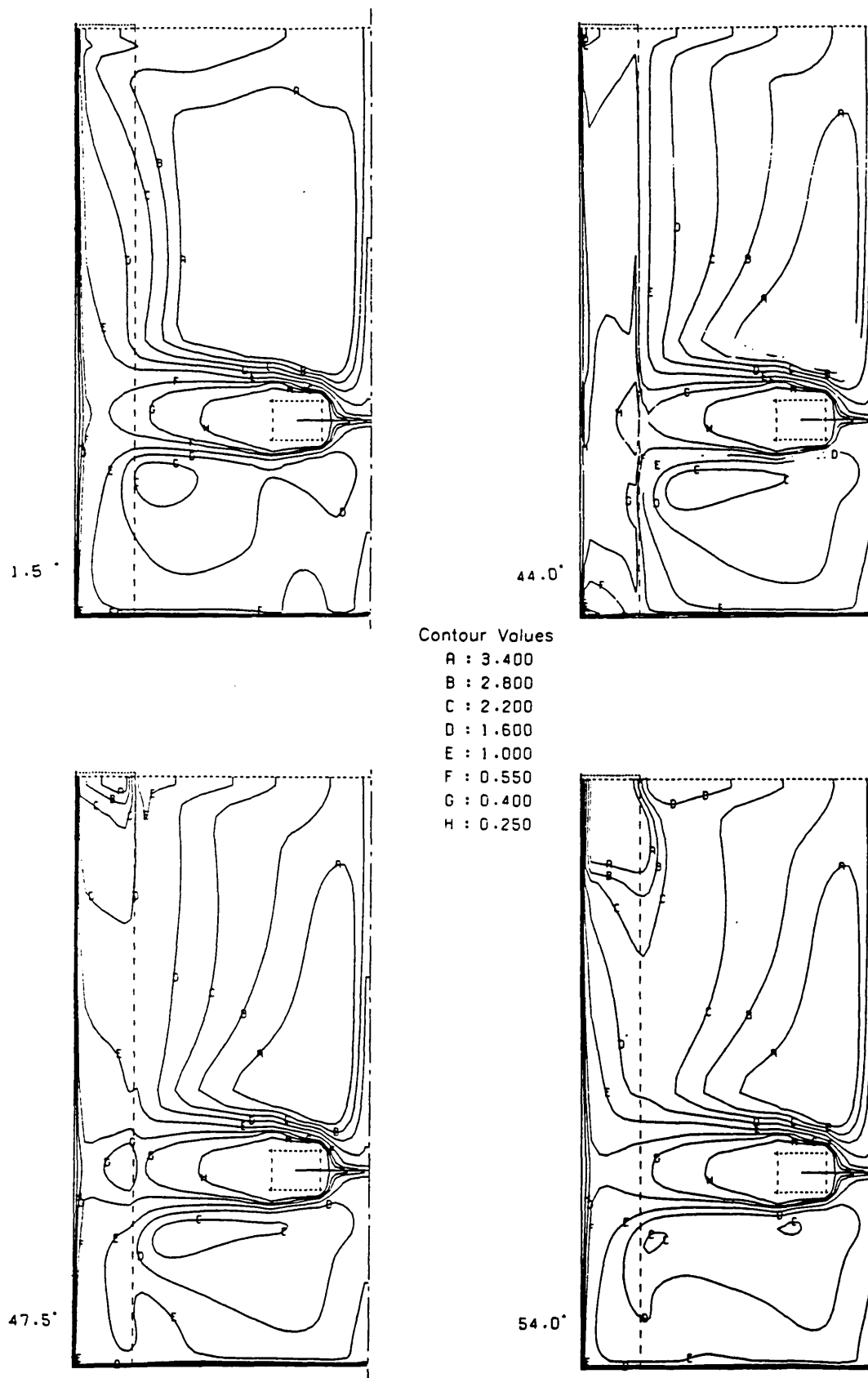


Figure 5.3.16 Normalised turbulence time scales in $x - r$ planes, finest grid, water in mixing vessel

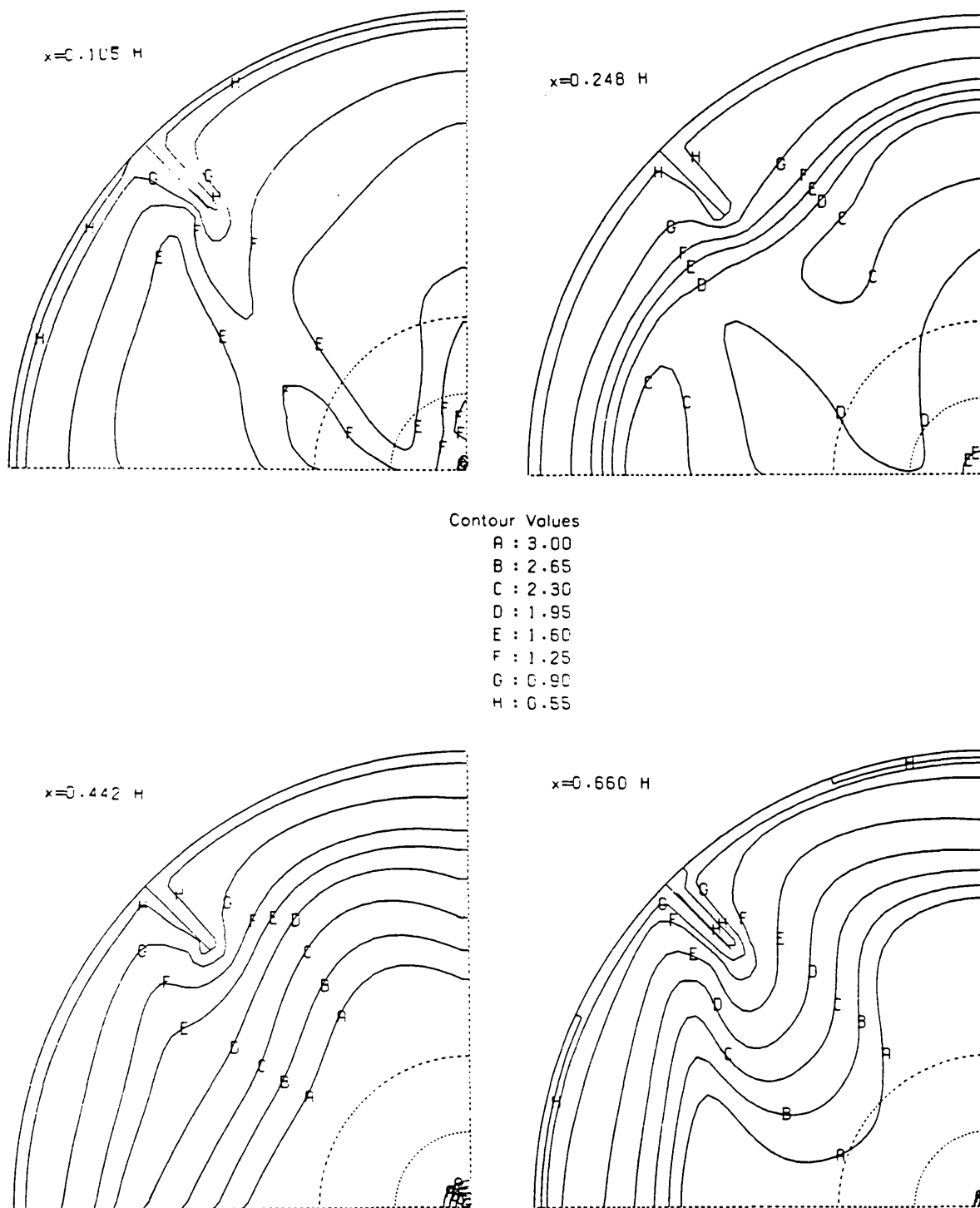


Figure 5.3.17 Normalised turbulence time scales in $r - \theta$ planes, finest grid, water in mixing vessel

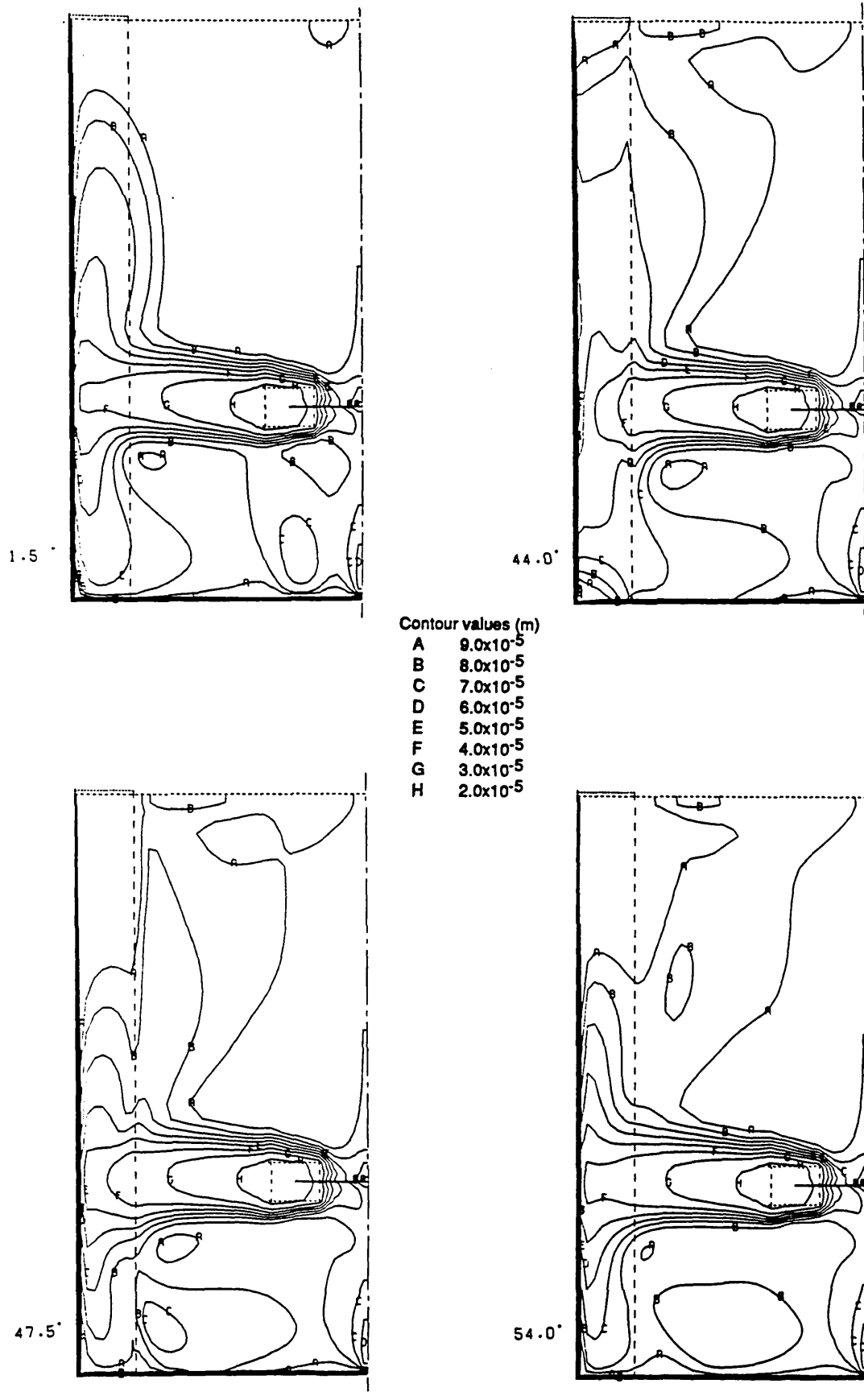


Figure 5.3.18 Kolmogorov length scales (m) in $x - r$ planes,
finest grid, water in mixing vessel

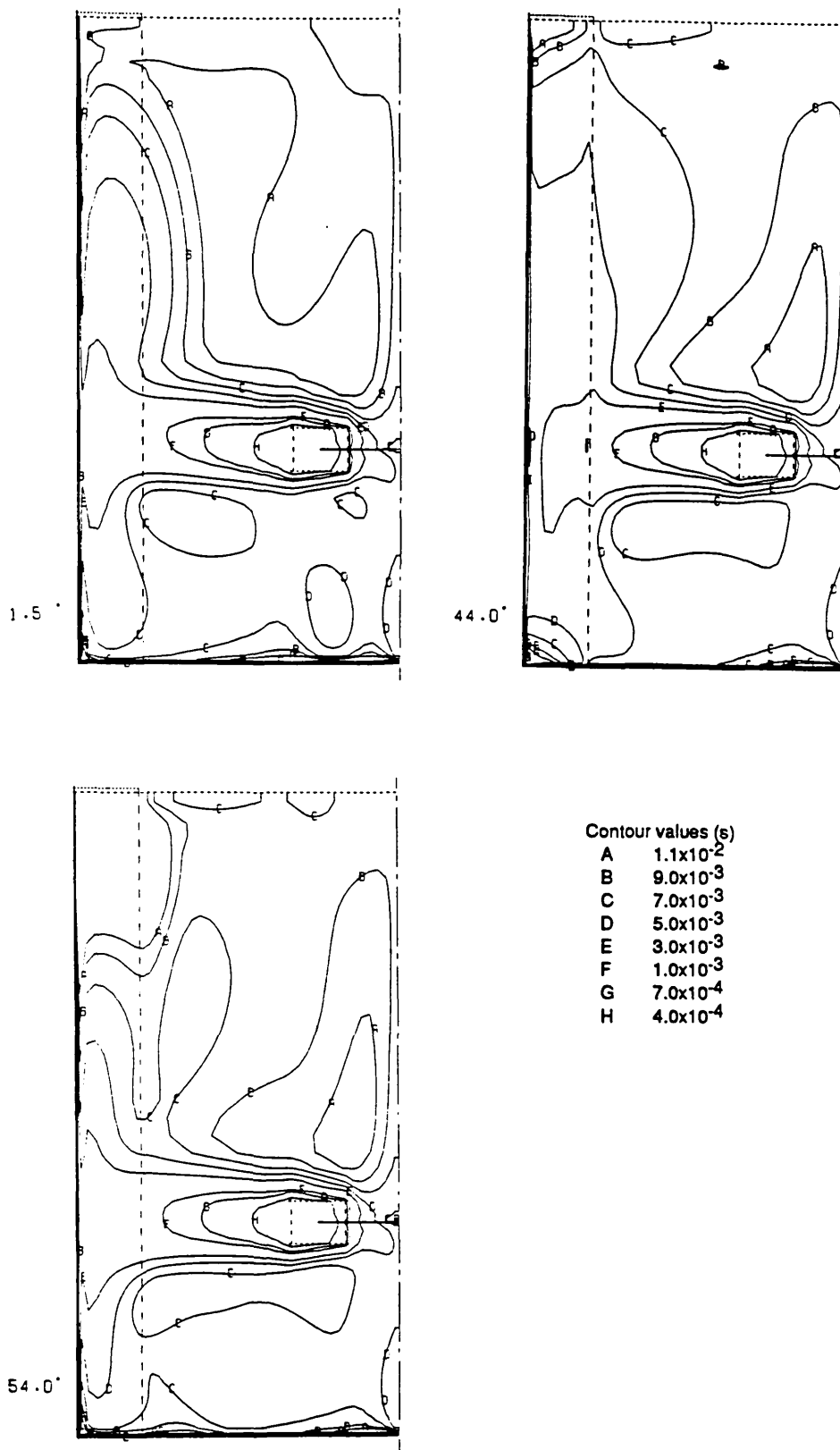


Figure 5.3.19 Kolmogorov time scales (s) in $x - r$ planes, finest grid, water in mixing vessel

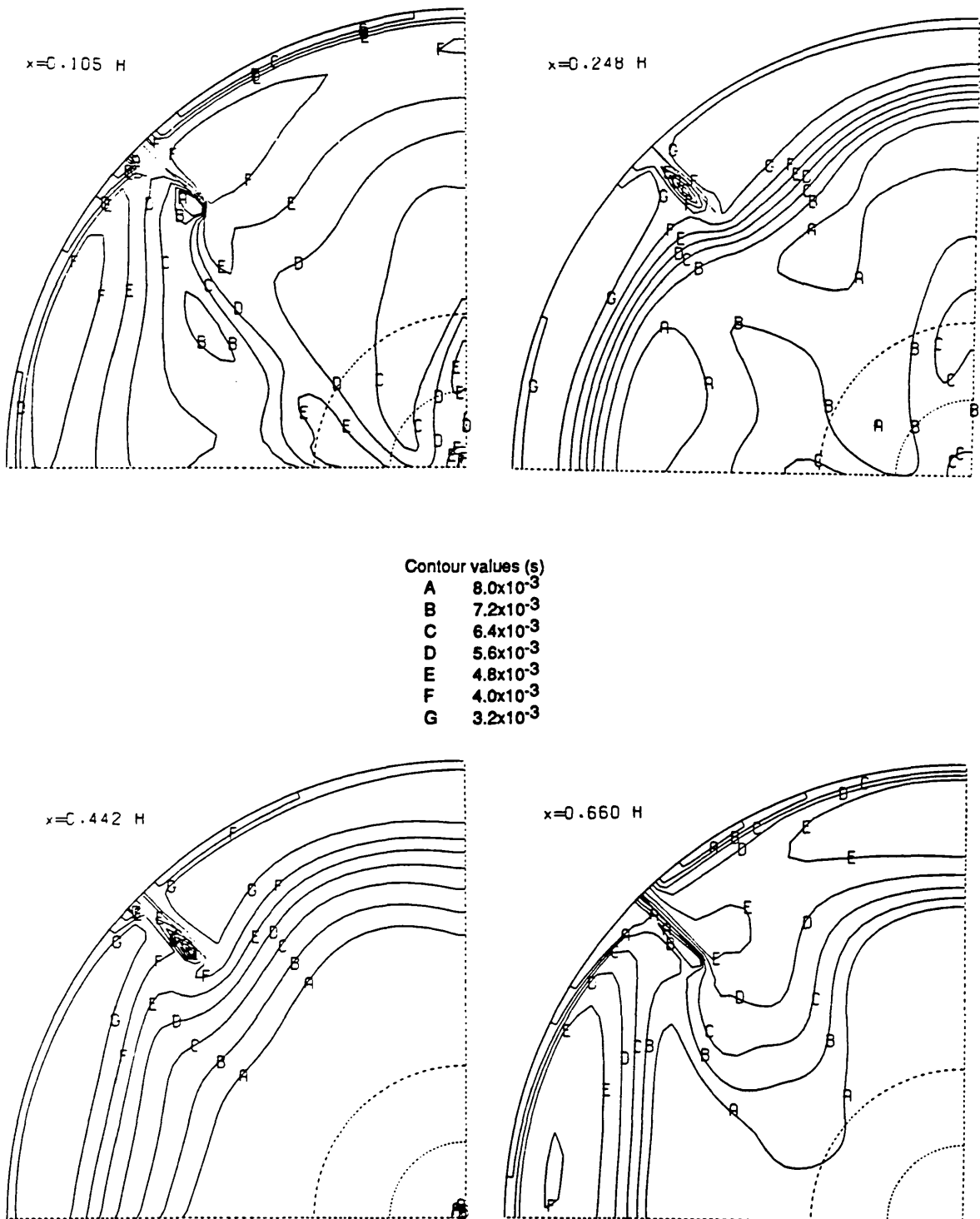


Figure 5.3.20 Kolmogorov time scales (s) in $r - \theta$ planes, finest grid, water in mixing vessel

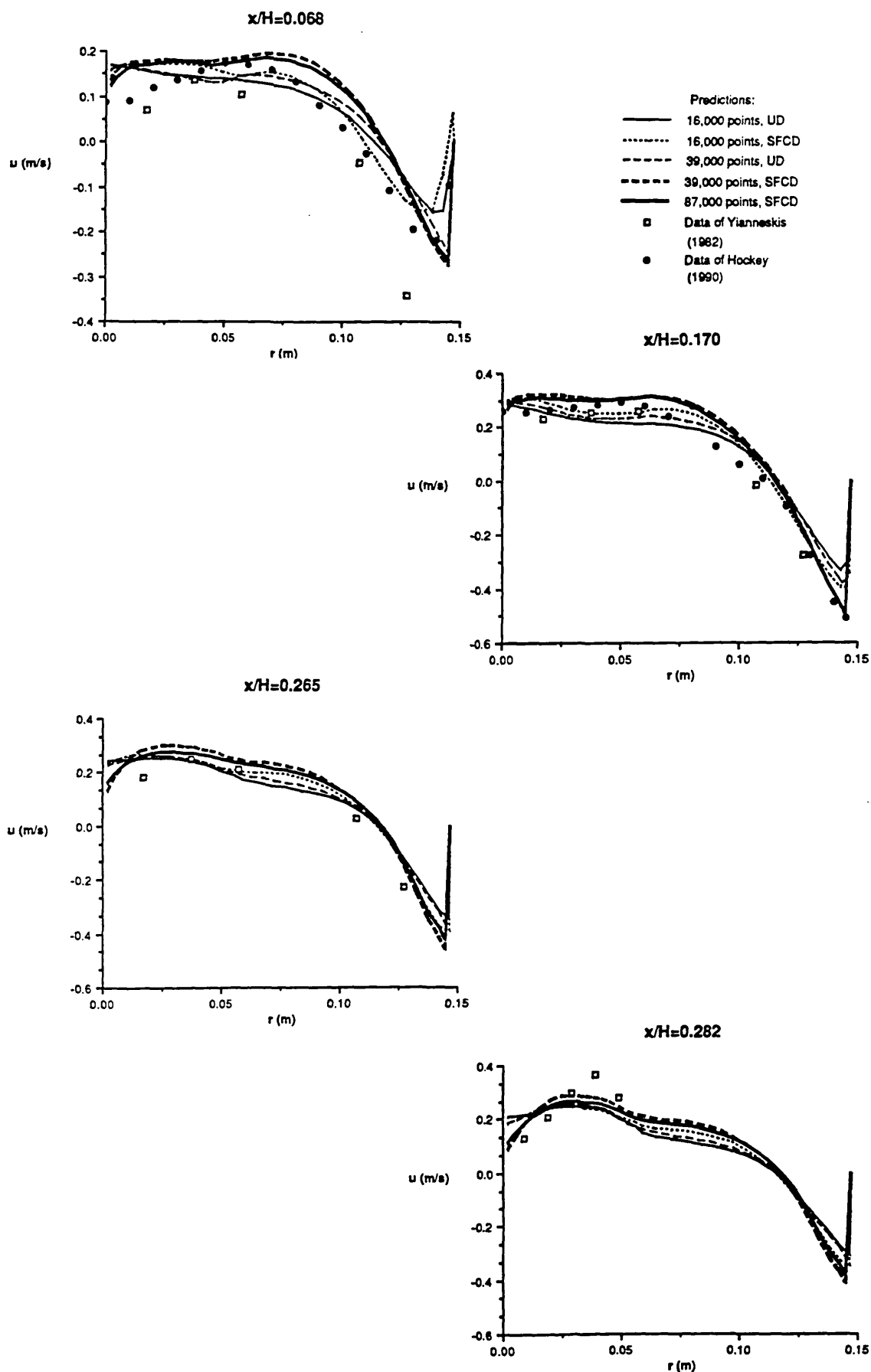


Figure 5.4.1 Below-impeller axial velocity comparisons, 0° plane, water in mixing vessel

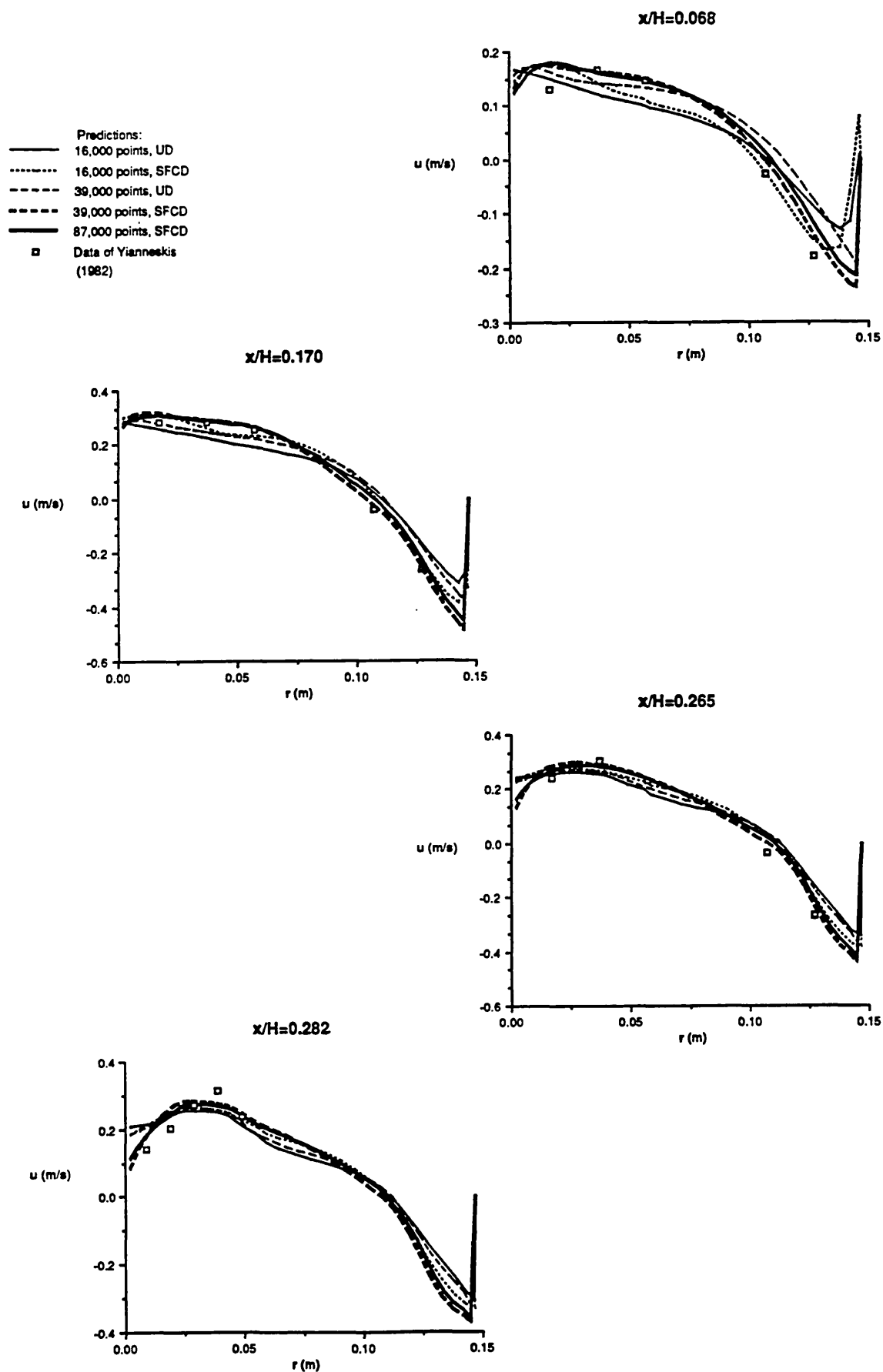


Figure 5.4.2 Below-impeller axial velocity comparisons, 22.5° plane, water in mixing vessel

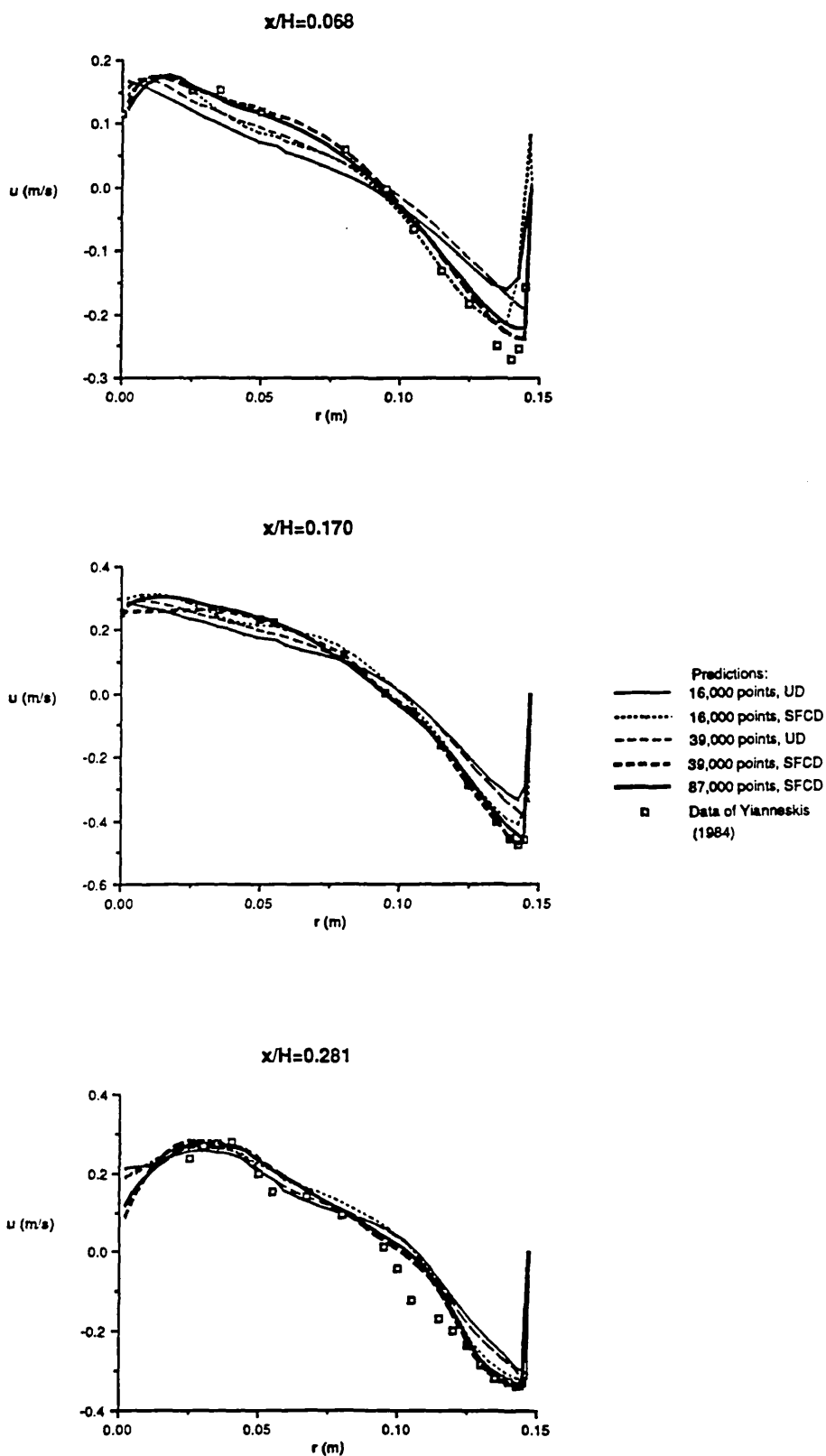


Figure 5.4.3 Below-impeller axial velocity comparisons, 33.75° plane, water in mixing vessel

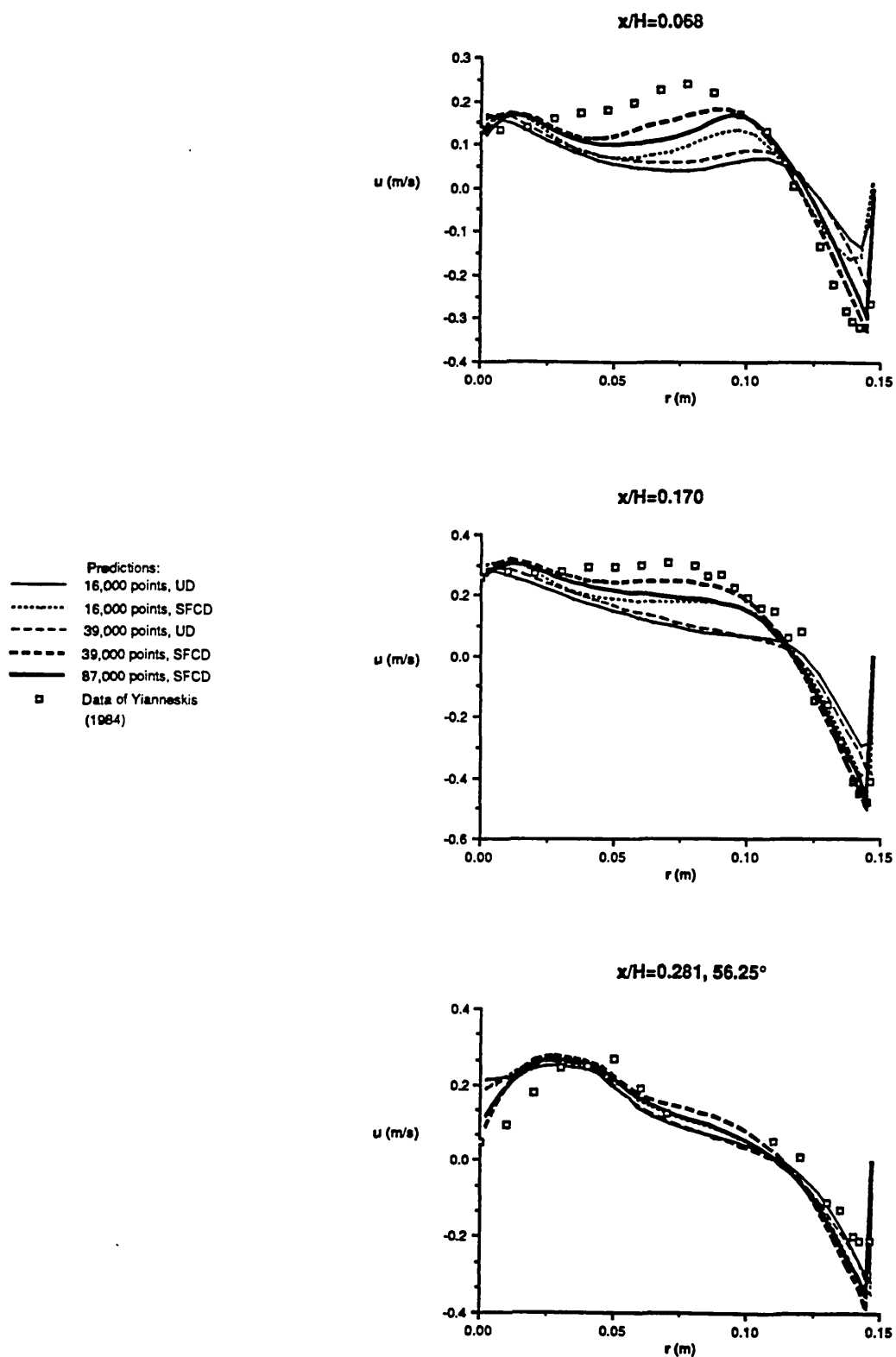


Figure 5.4.4 Below-impeller axial velocity comparisons, 56.25° plane, water in mixing vessel

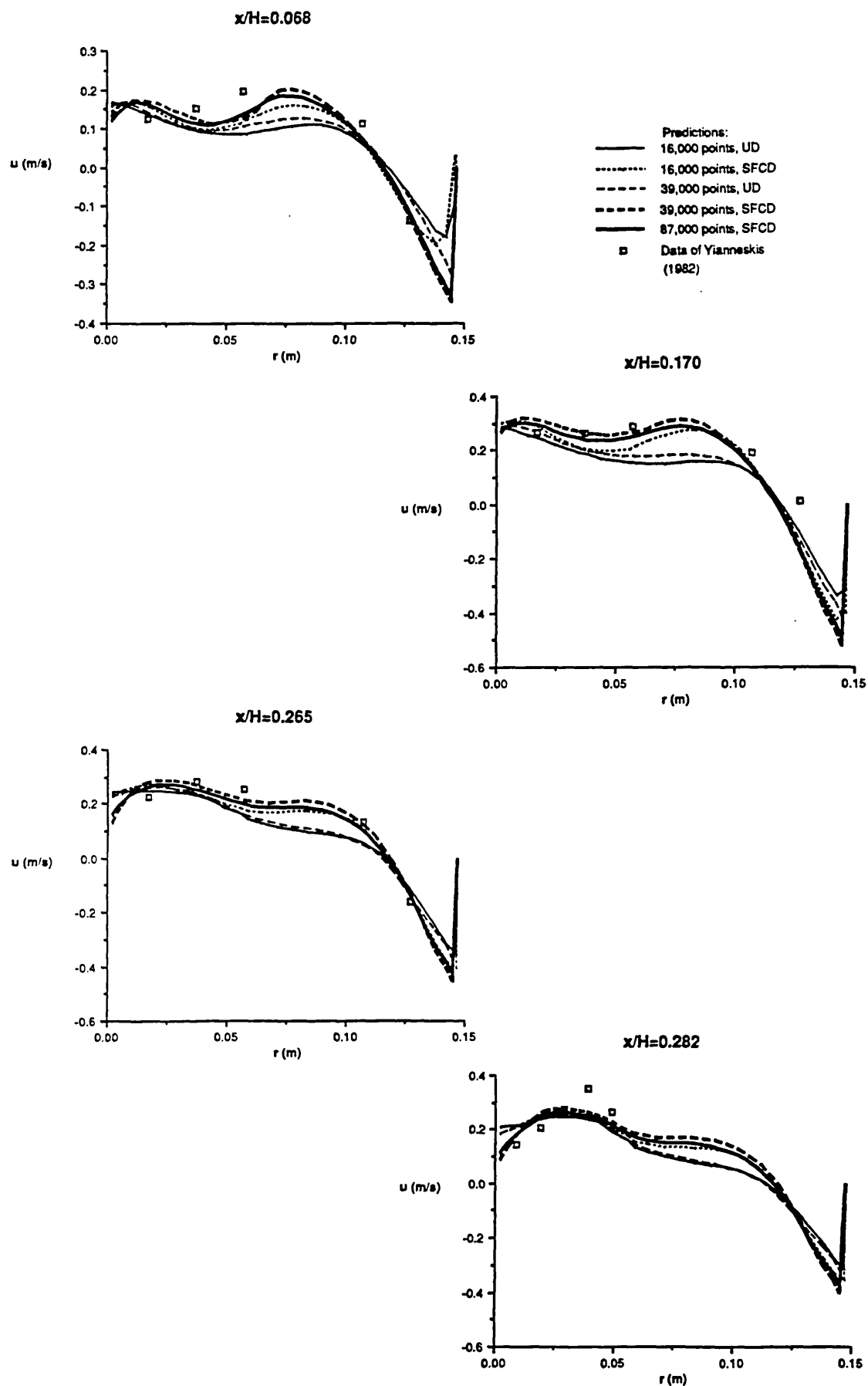


Figure 5.4.5 Below-impeller axial velocity comparisons, 67.5° plane, water in mixing vessel

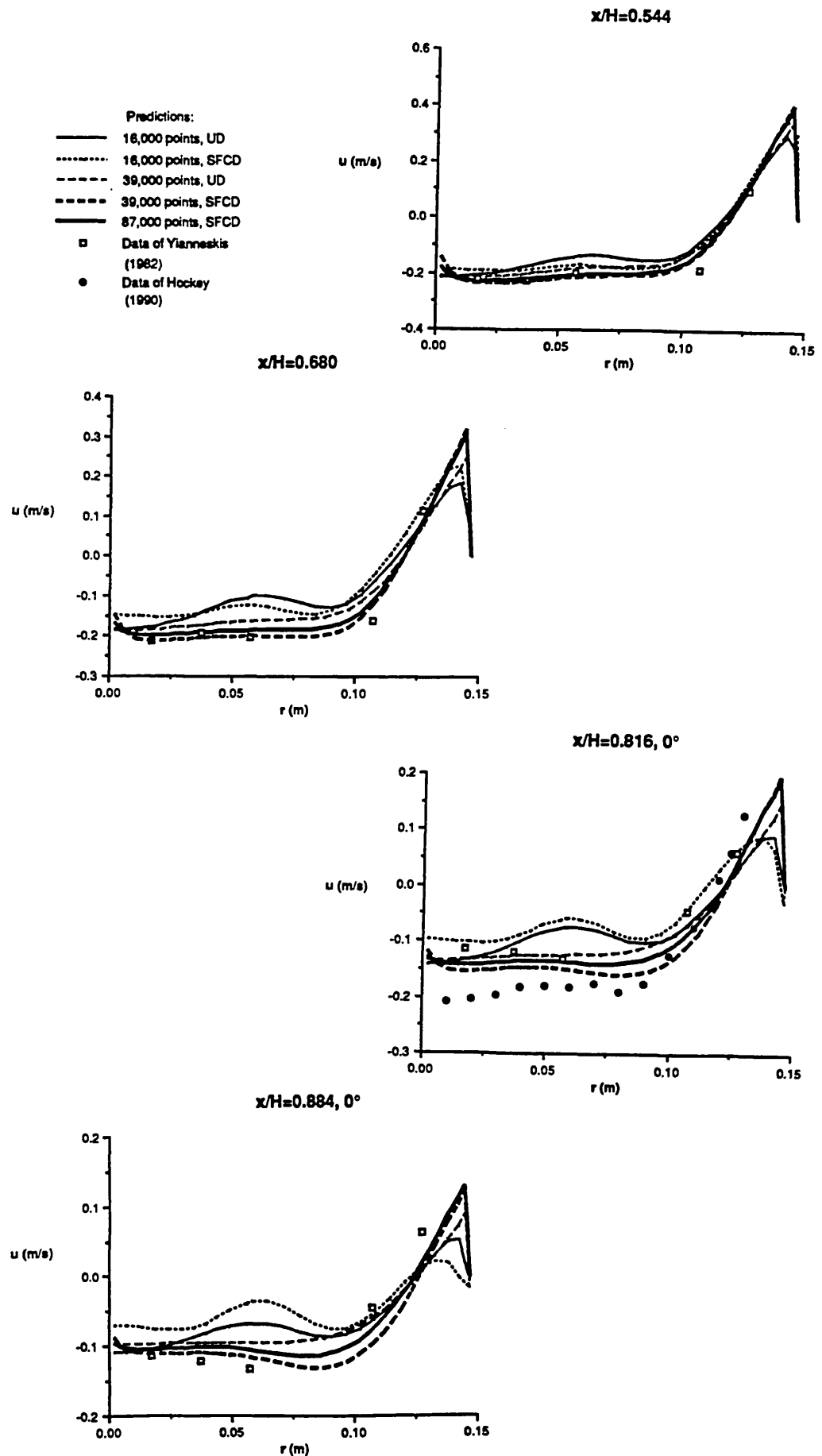


Figure 5.4.6 Above-impeller axial velocity comparisons, 0° plane, water in mixing vessel

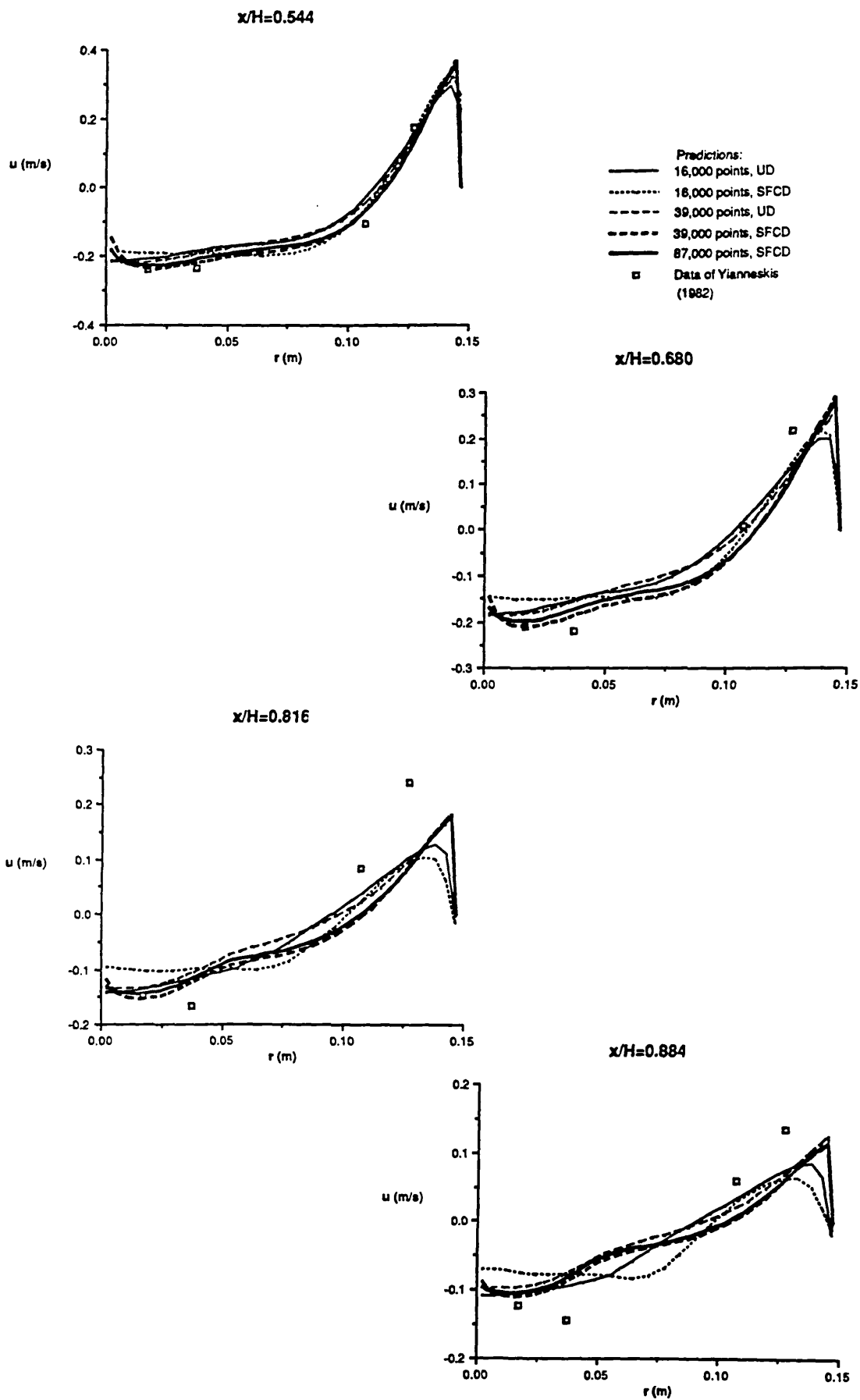


Figure 5.4.7 Above-impeller axial velocity comparisons, 22.5° plane, water in mixing vessel

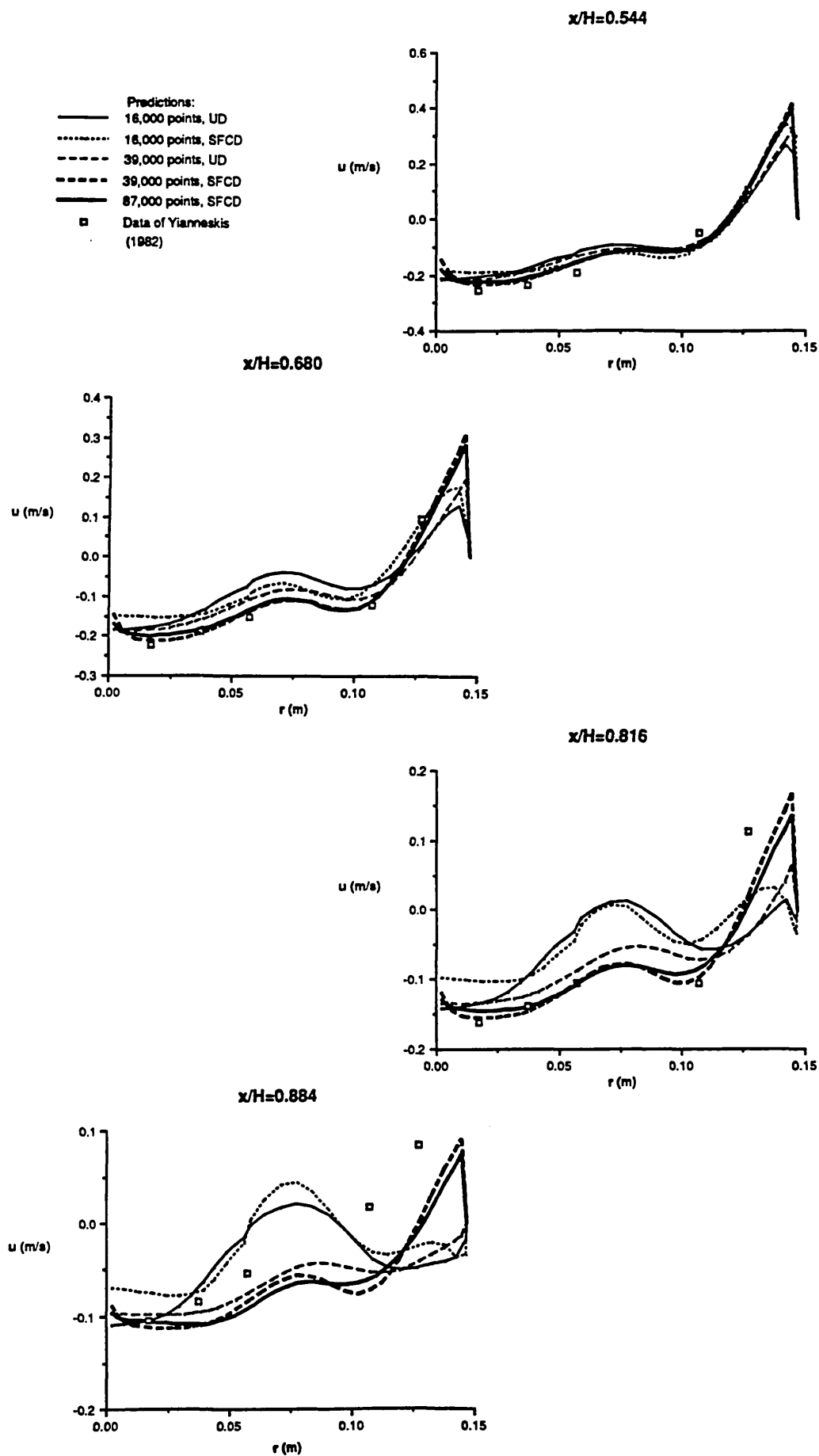


Figure 5.4.8 Above-impeller axial velocity comparisons, 67.5° plane, water in mixing vessel

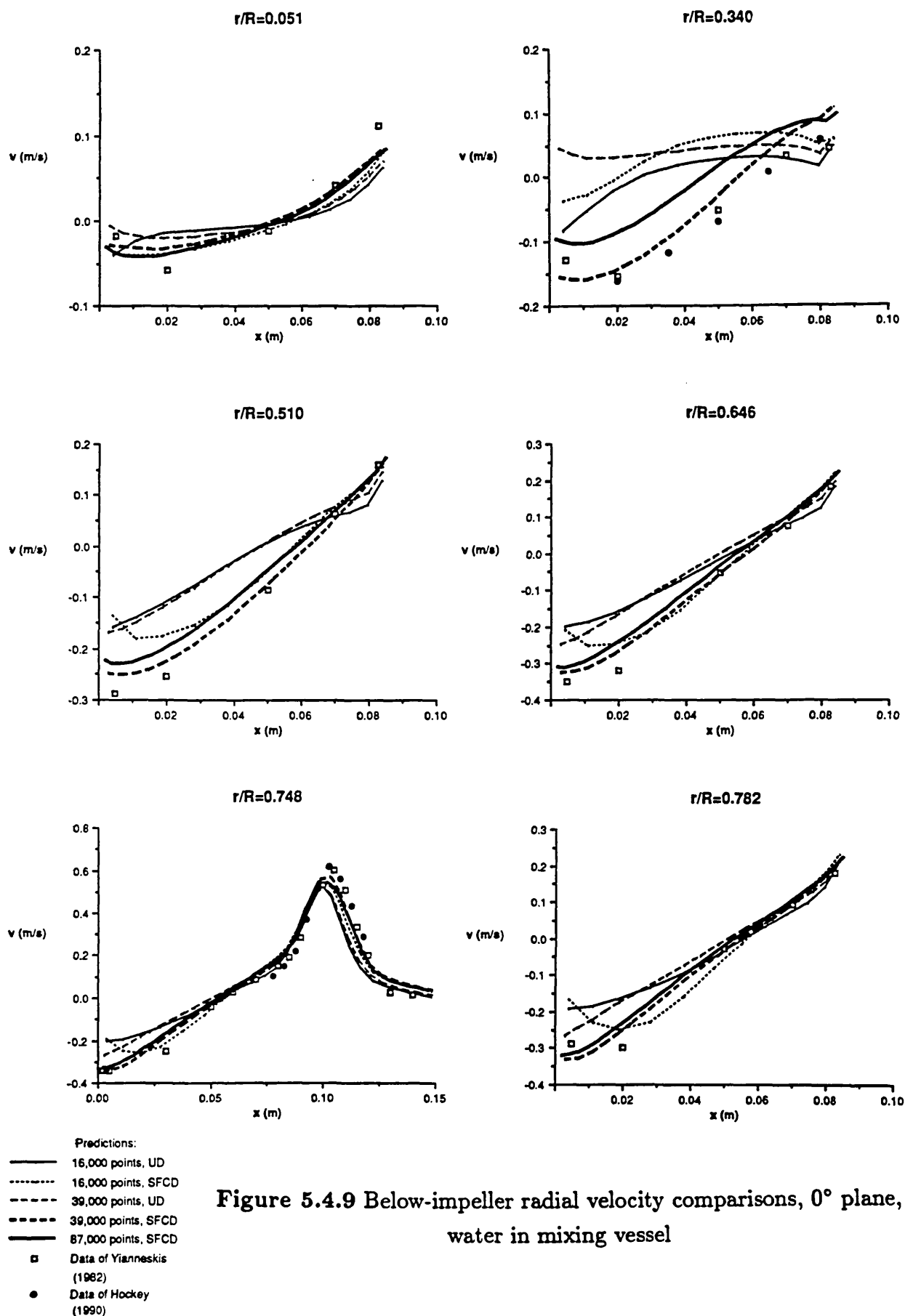


Figure 5.4.9 Below-impeller radial velocity comparisons, 0° plane, water in mixing vessel

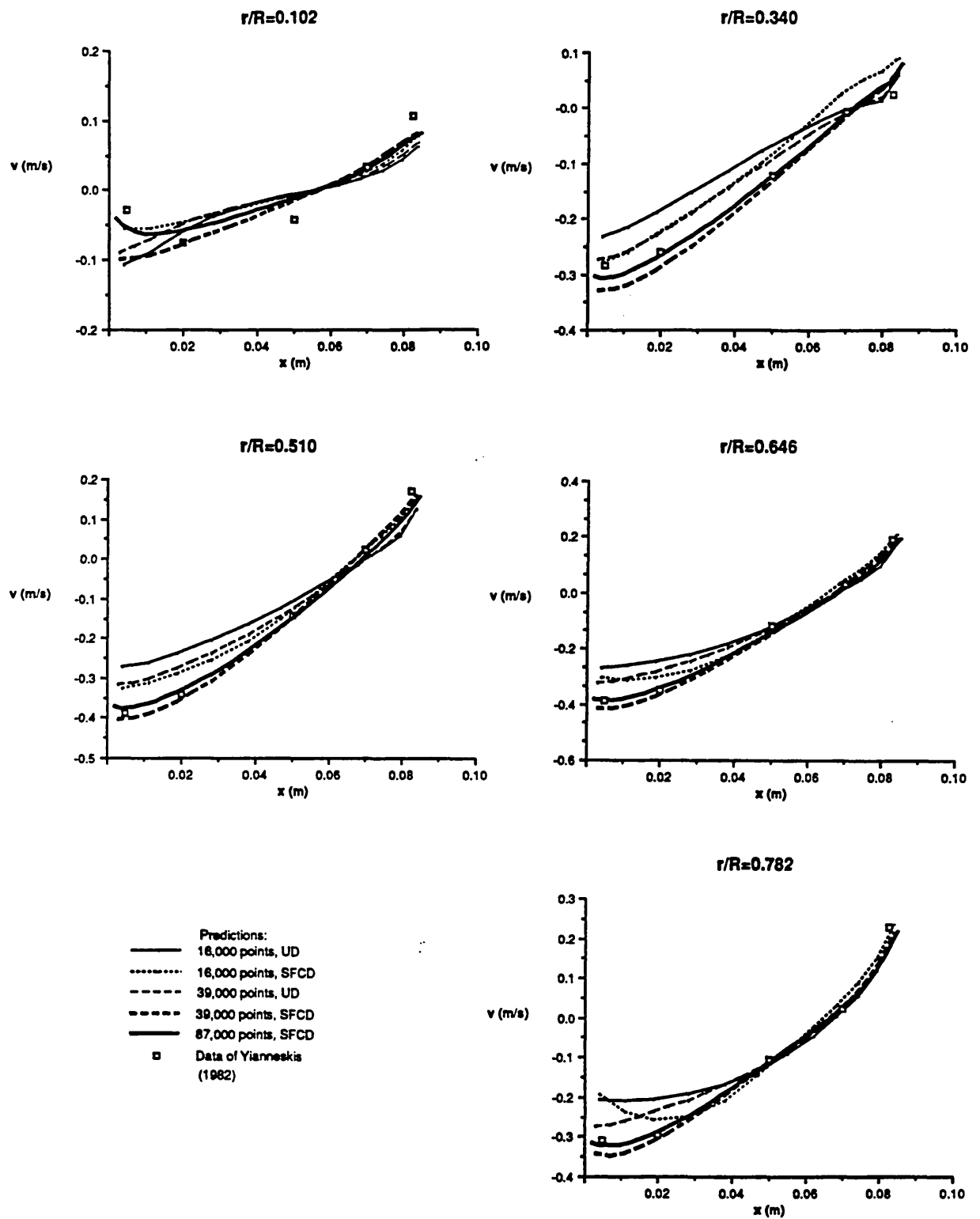


Figure 5.4.10 Below-impeller radial velocity comparisons, 22.5° plane, water in mixing vessel

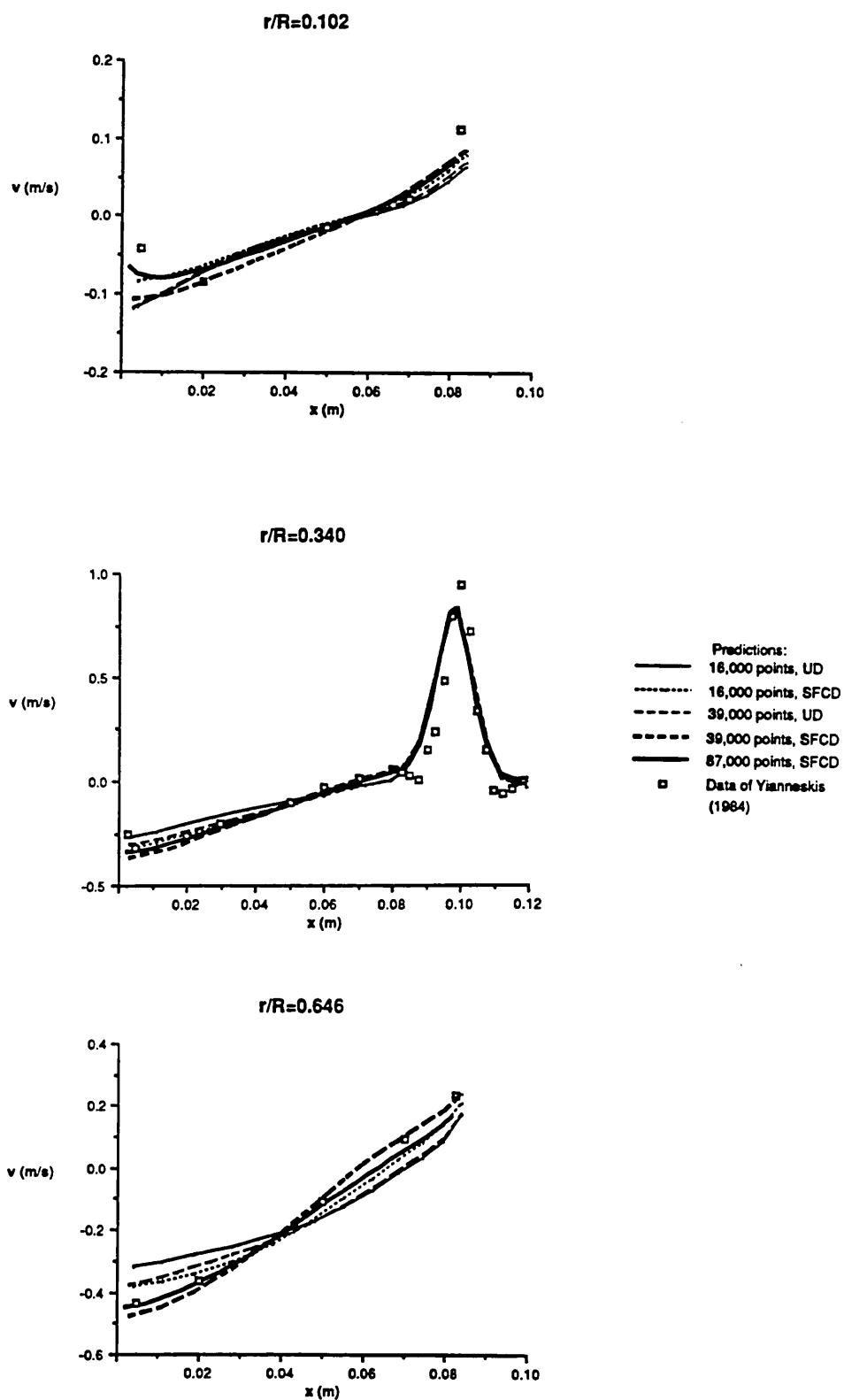


Figure 5.4.11 Below-impeller radial velocity comparisons, 33.75° plane, water in mixing vessel

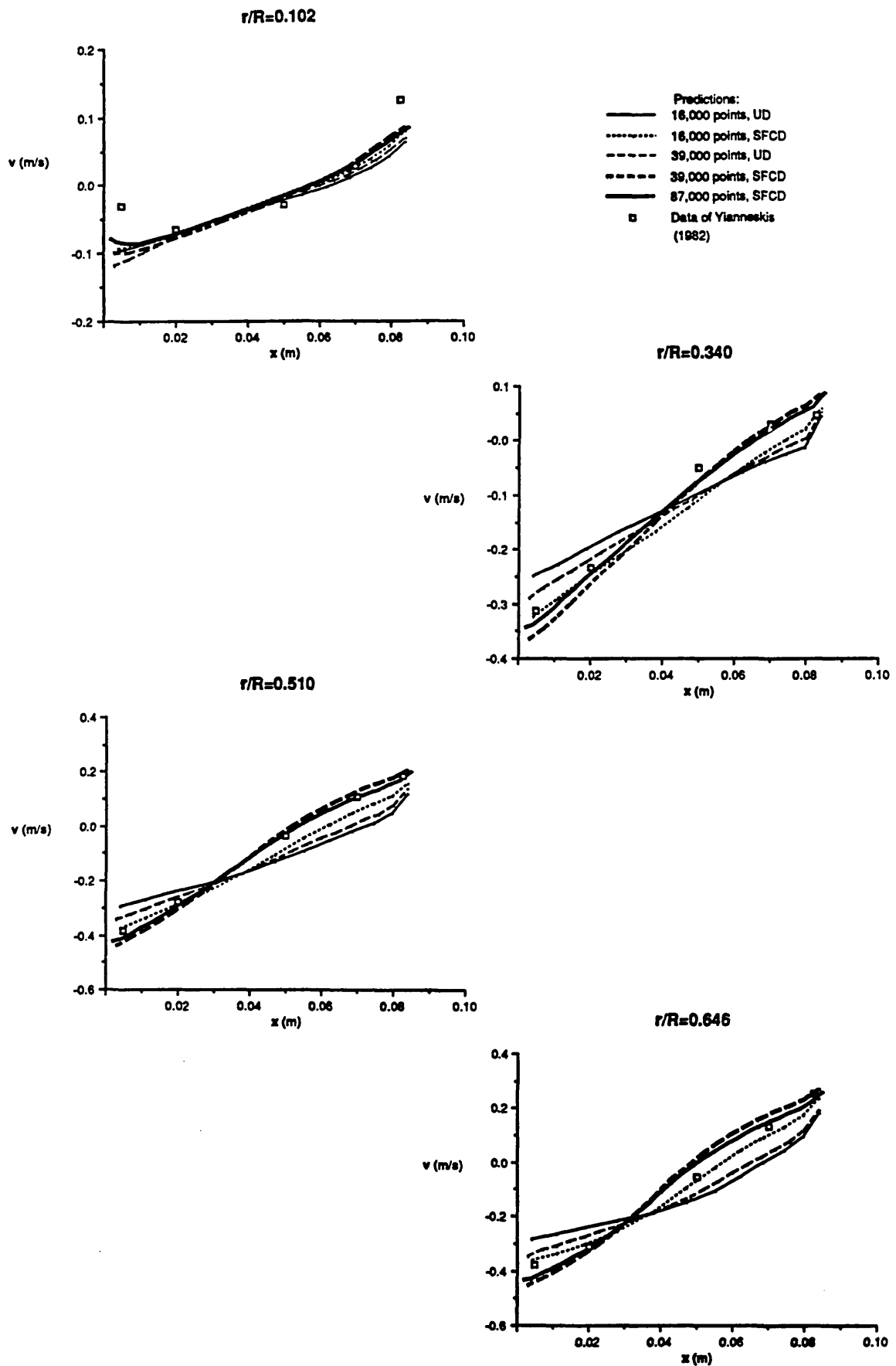


Figure 5.4.12 Below-impeller radial velocity comparisons, 45° plane, water in mixing vessel

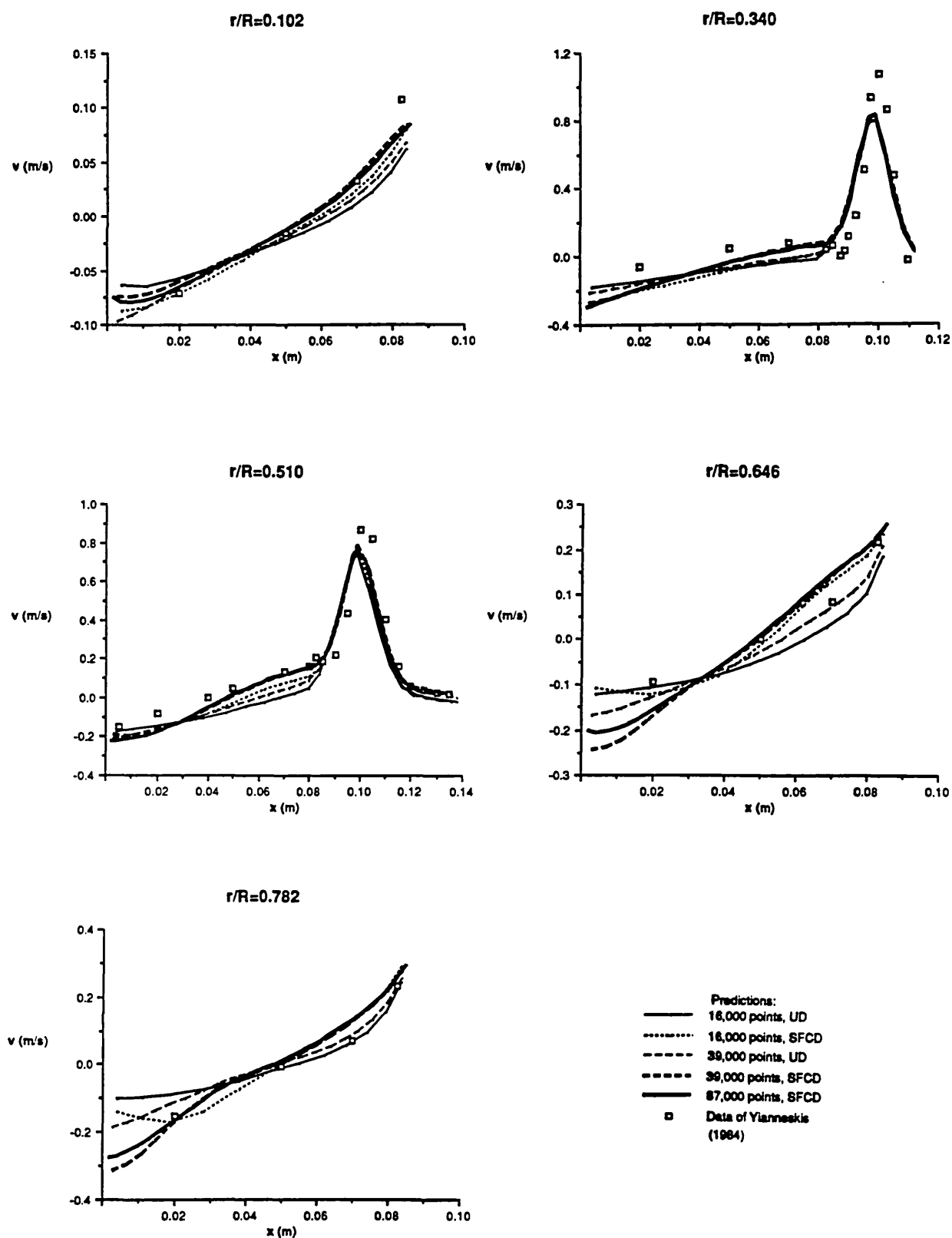


Figure 5.4.13 Below-impeller radial velocity comparisons, 56.25° plane, water in mixing vessel

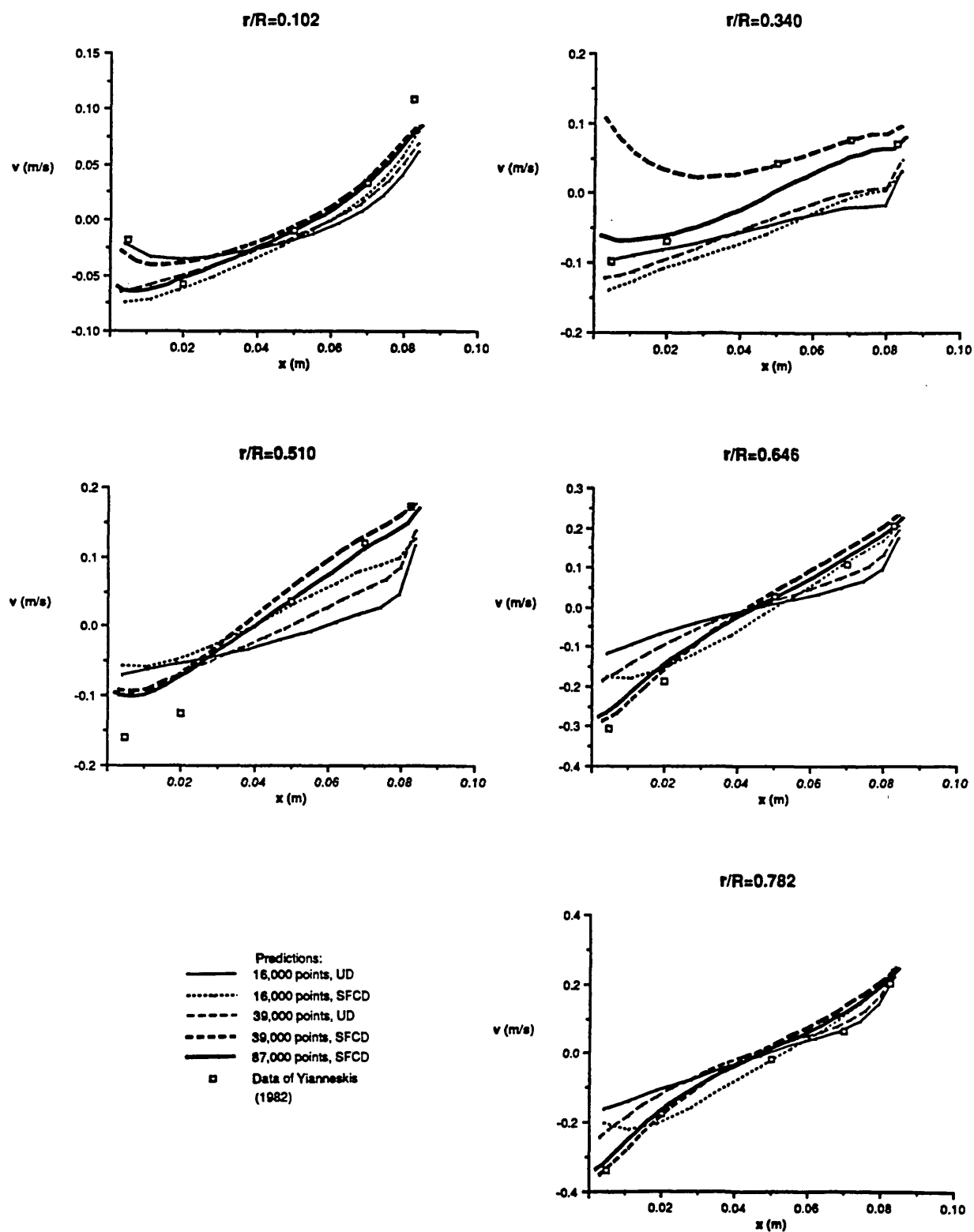


Figure 5.4.14 Below-impeller radial velocity comparisons, 67.5° plane, water in mixing vessel

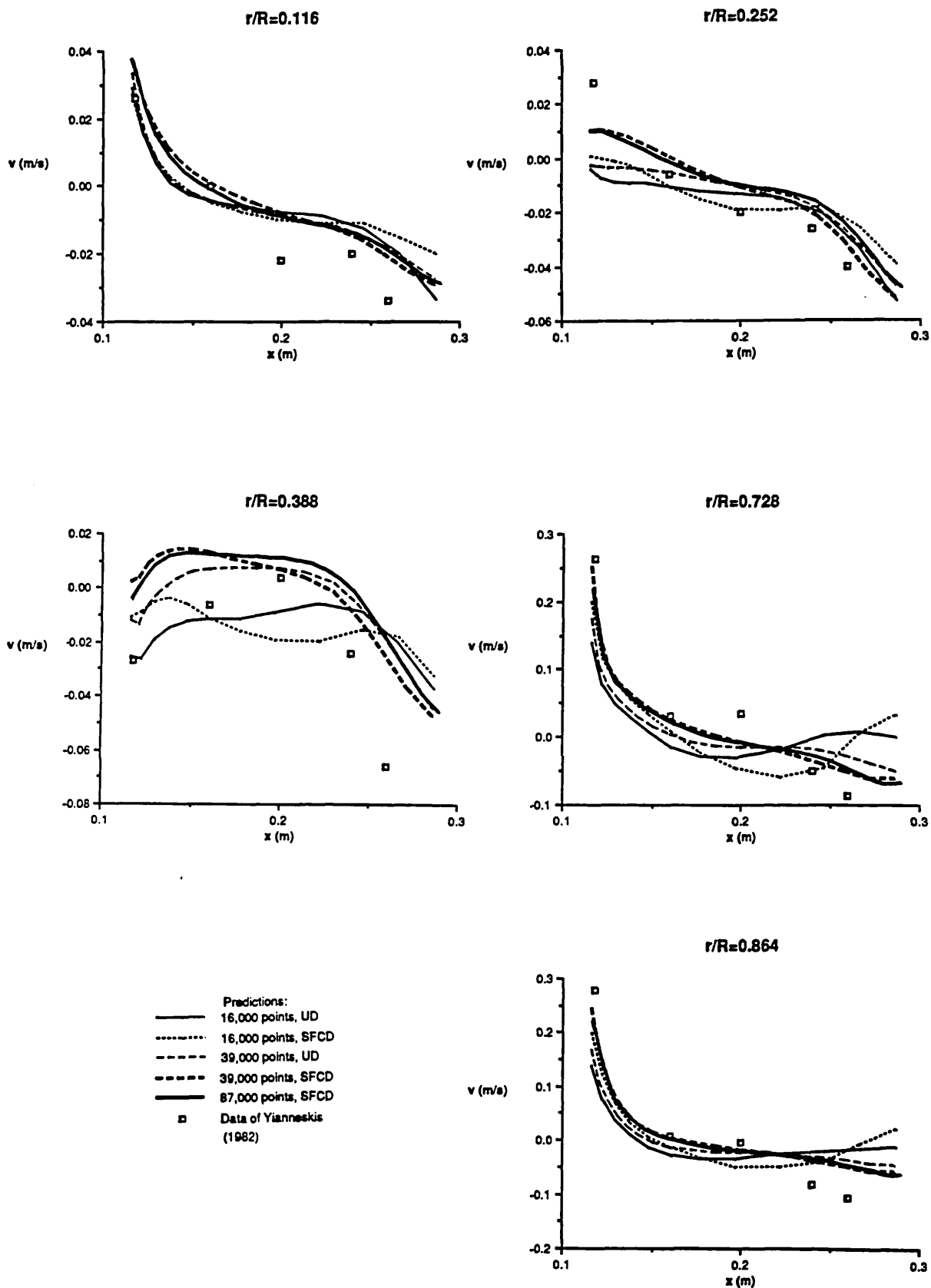


Figure 5.4.15 Above-impeller radial velocity comparisons, 0° plane, water in mixing vessel

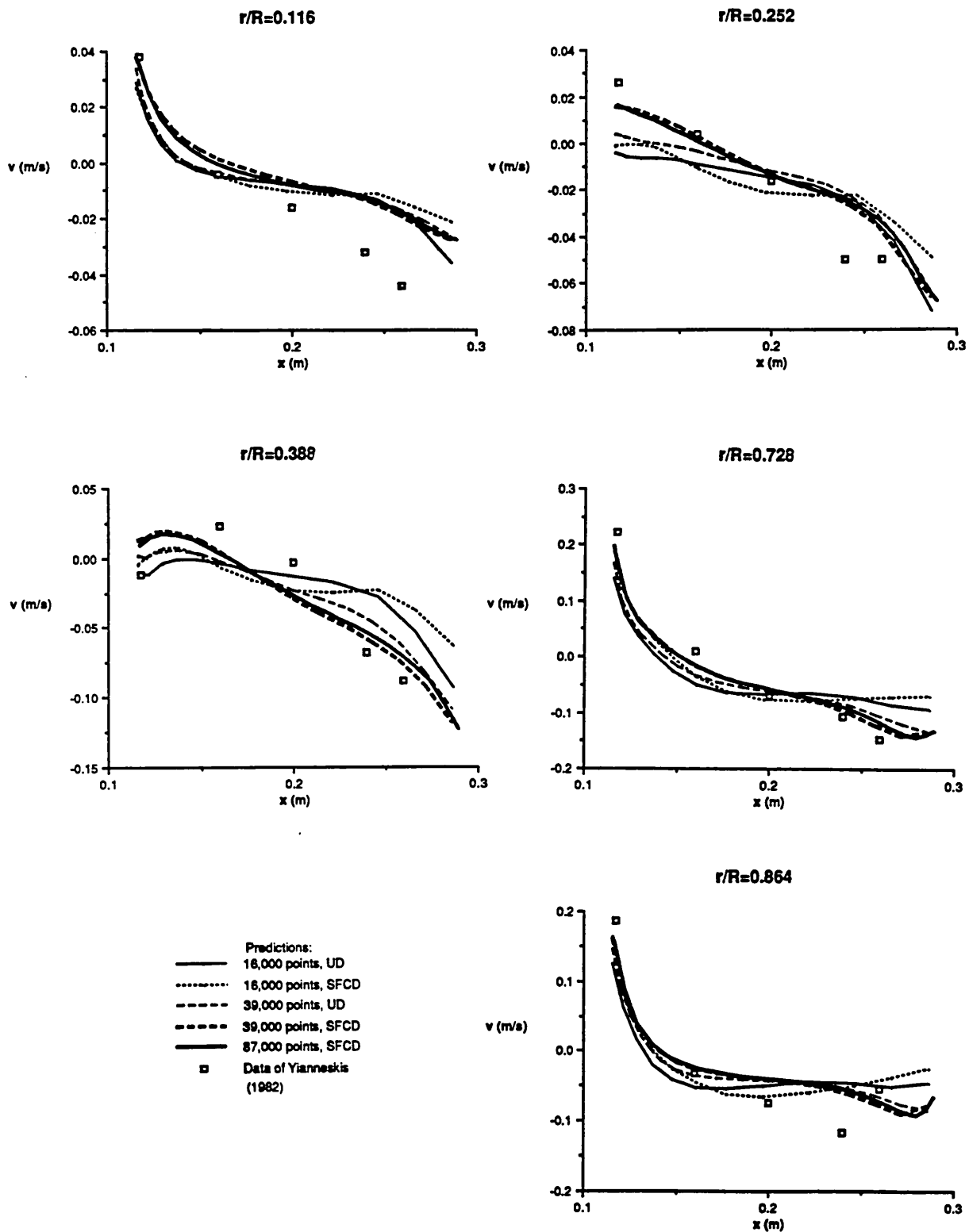


Figure 5.4.16 Above-impeller radial velocity comparisons, 22.5° plane, water in mixing vessel

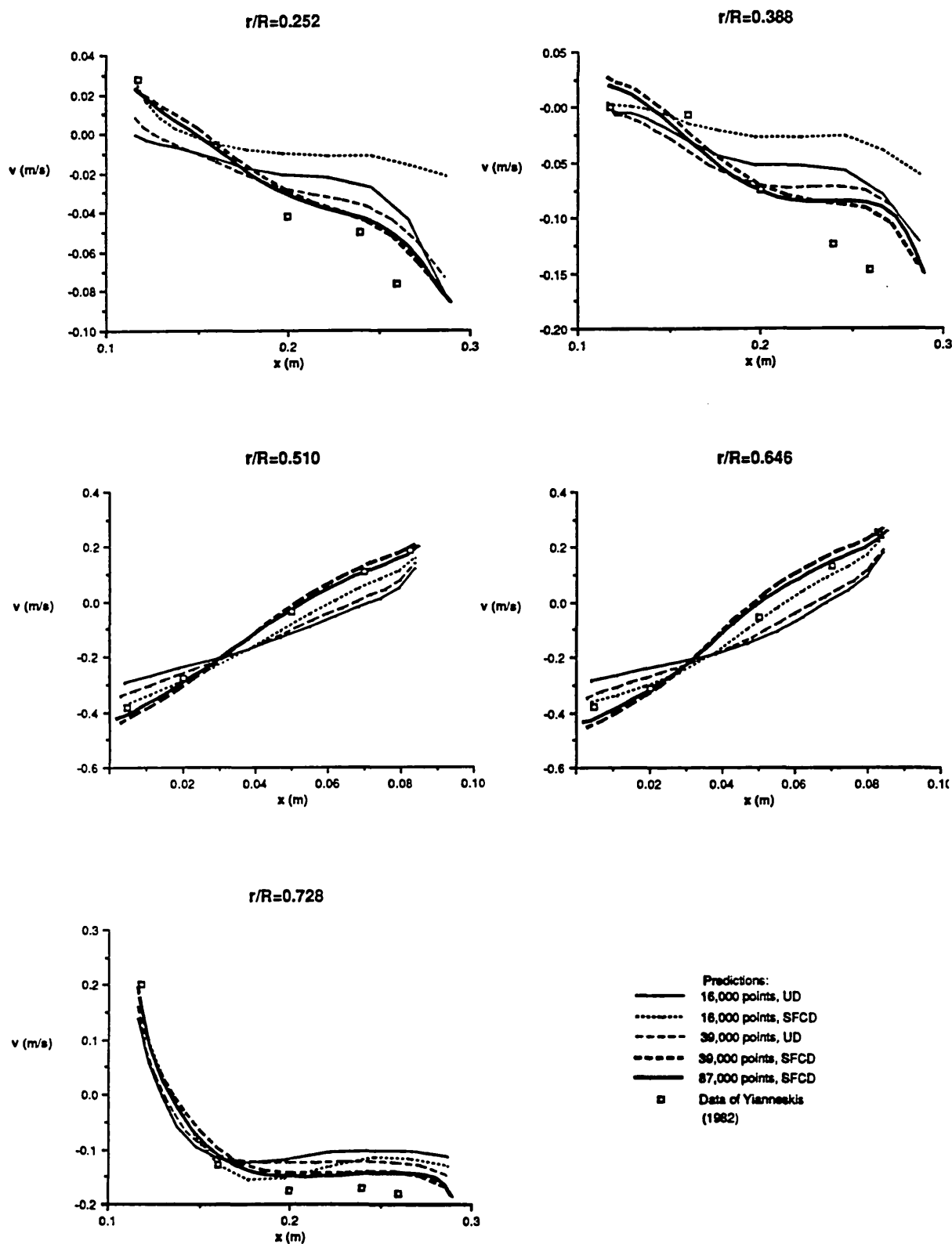


Figure 5.4.17 Above-impeller radial velocity comparisons, 45° plane, water in mixing vessel

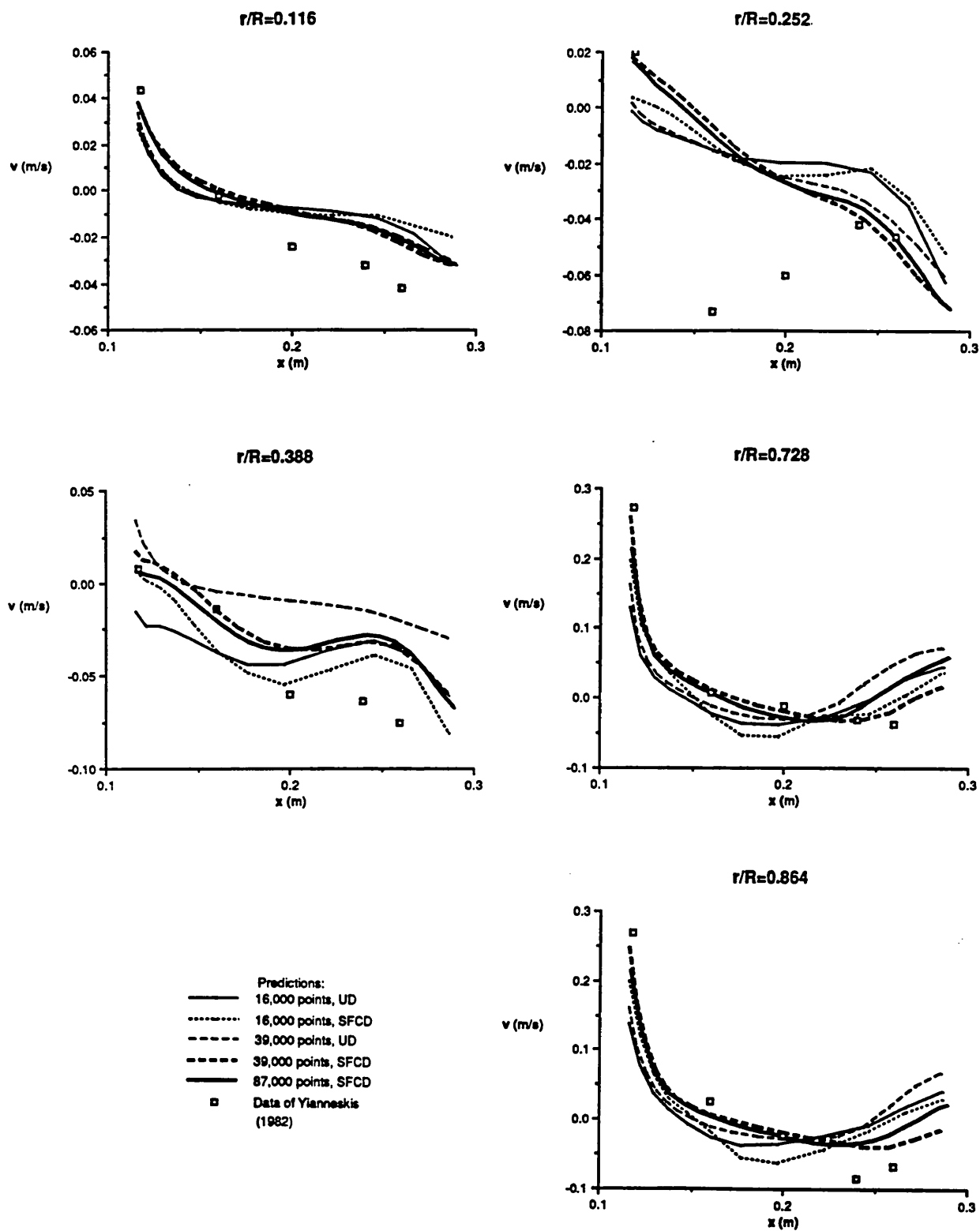


Figure 5.4.18 Above-impeller radial velocity comparisons, 67.5° plane, water in mixing vessel

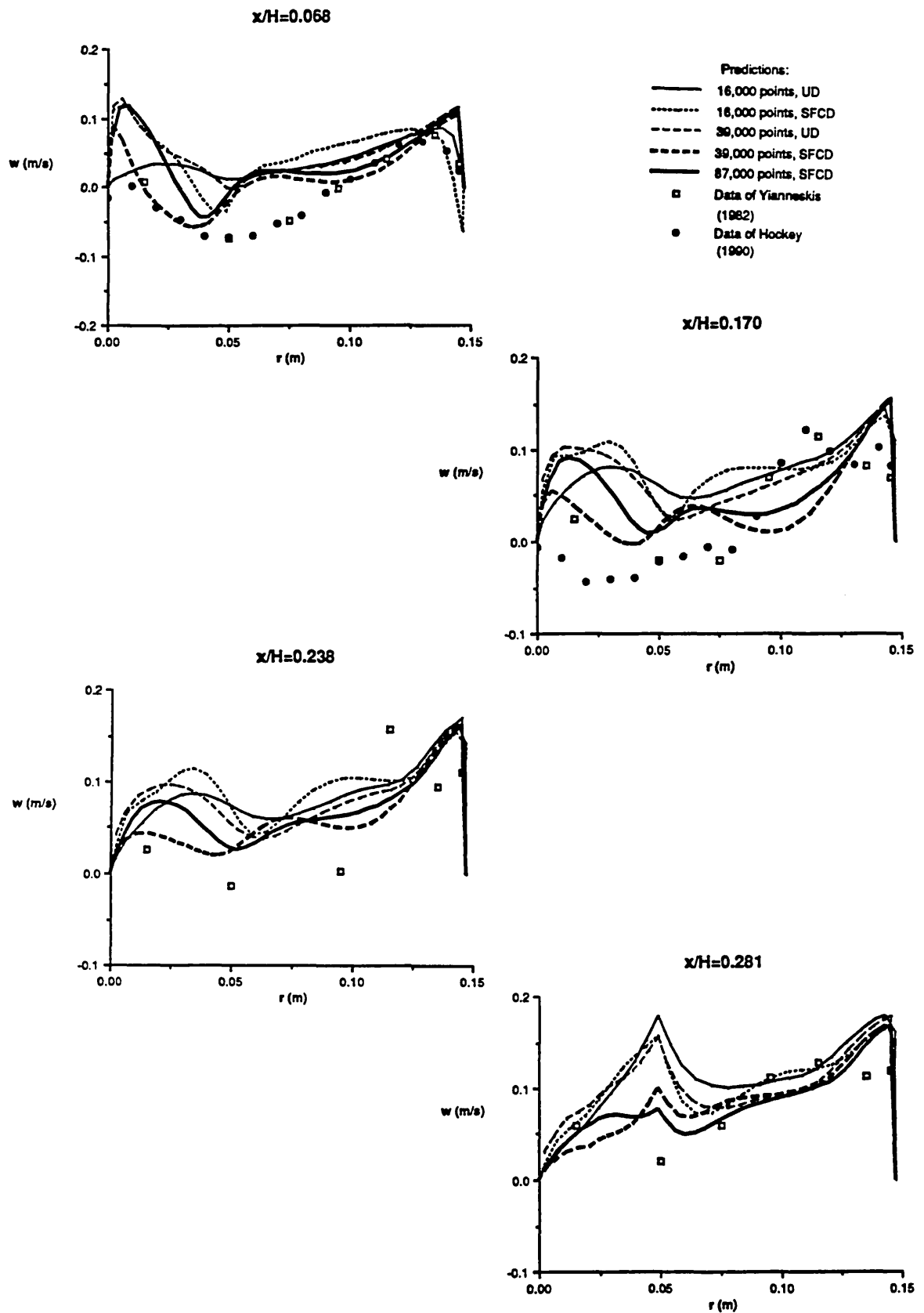


Figure 5.4.19 Below-impeller swirl velocity comparisons, 0° plane, water in mixing vessel

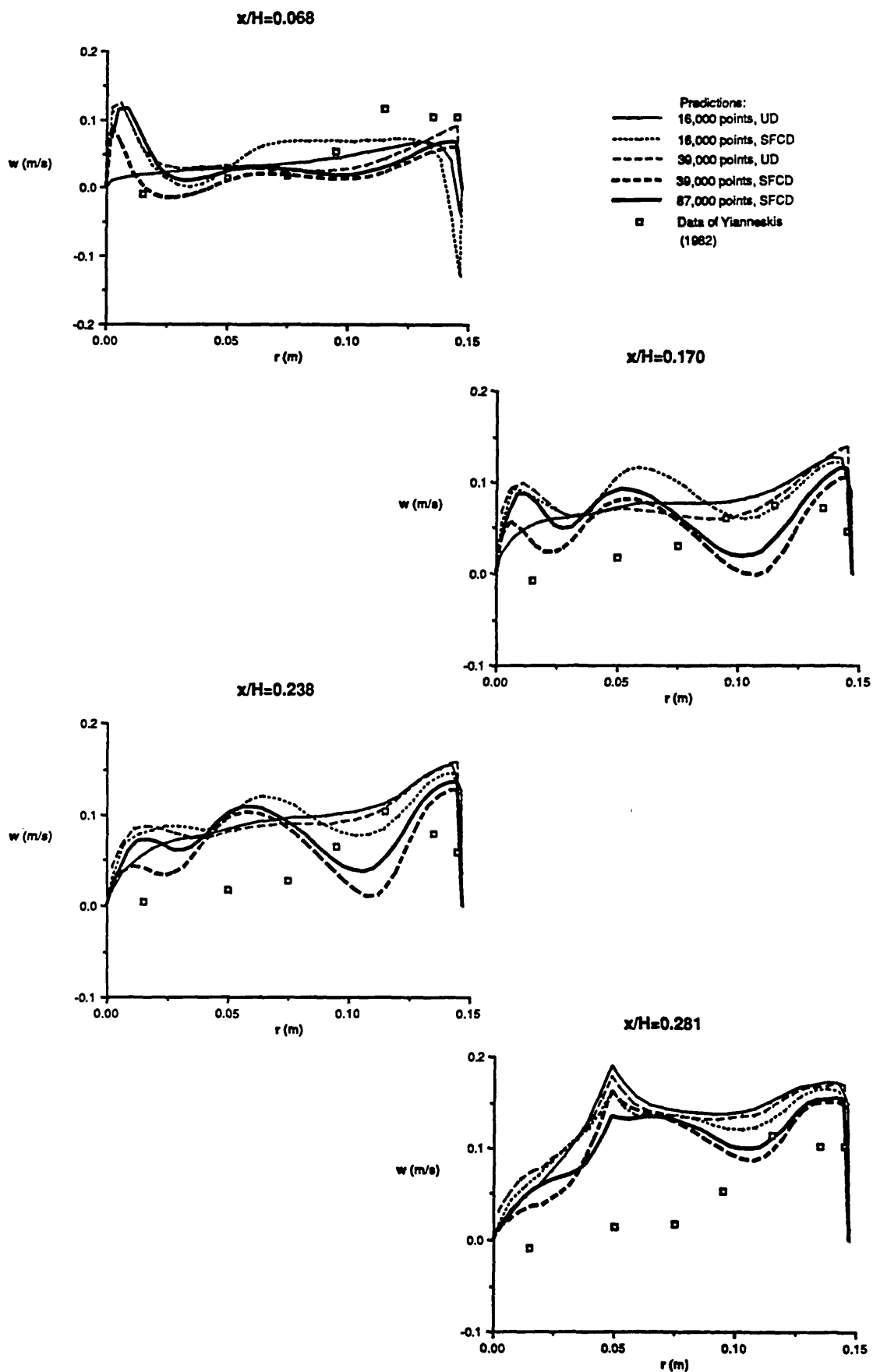


Figure 5.4.20 Below-impeller swirl velocity comparisons, 22.5° plane, water in mixing vessel

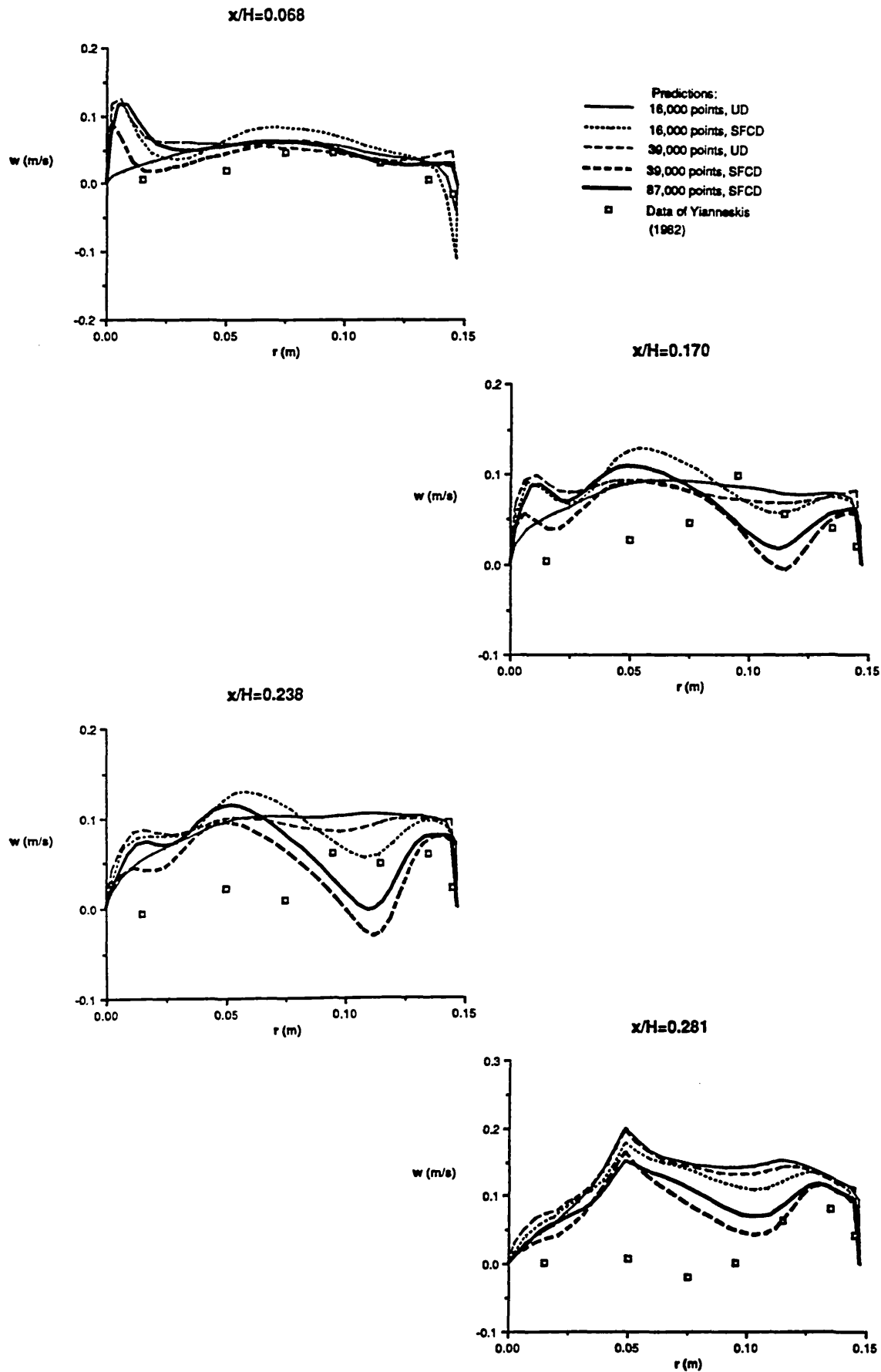


Figure 5.4.21 Below-impeller swirl velocity comparisons, 33.75° plane, water in mixing vessel

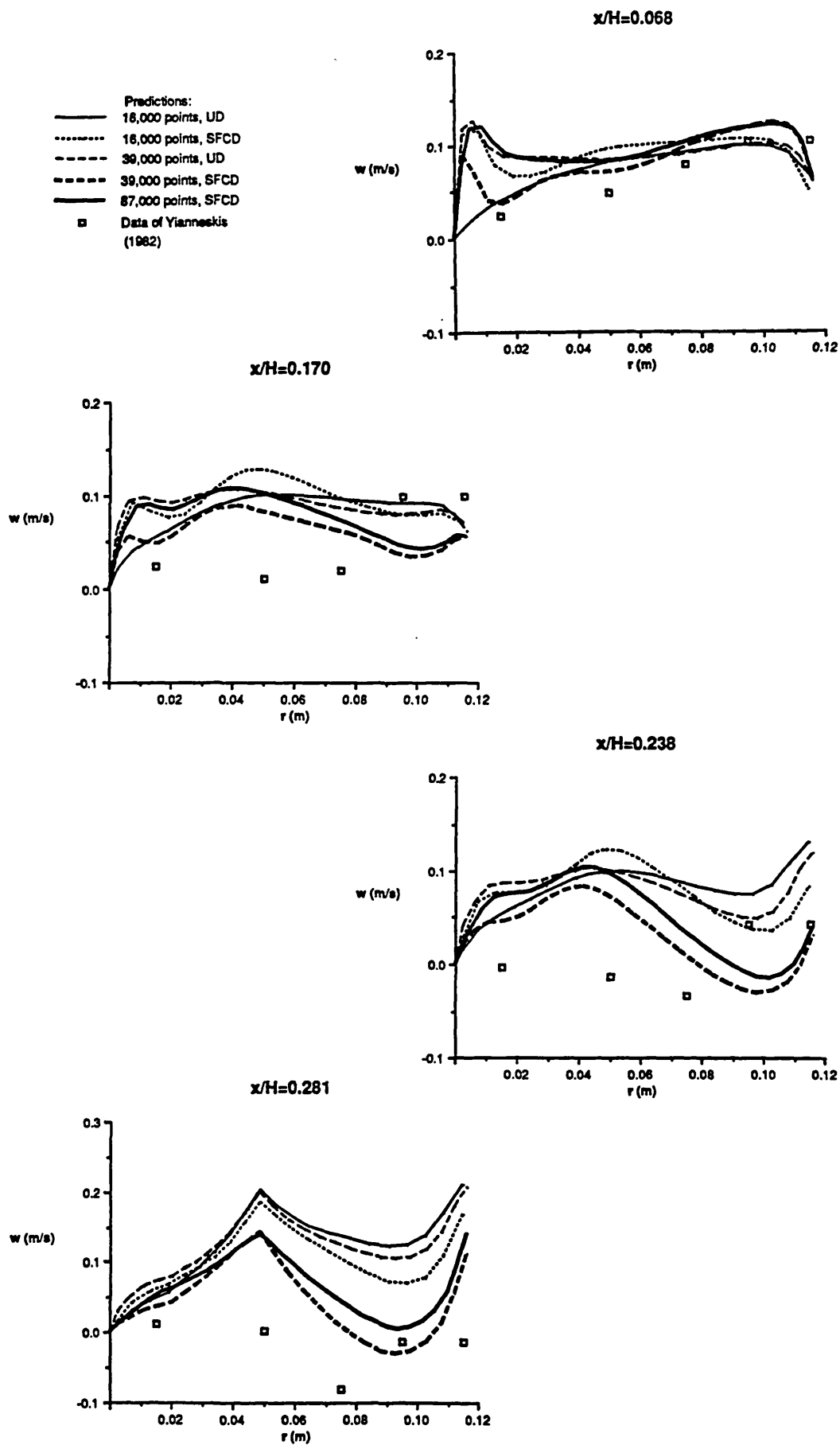


Figure 5.4.22 Below-impeller swirl velocity comparisons, 45° plane, water in mixing vessel

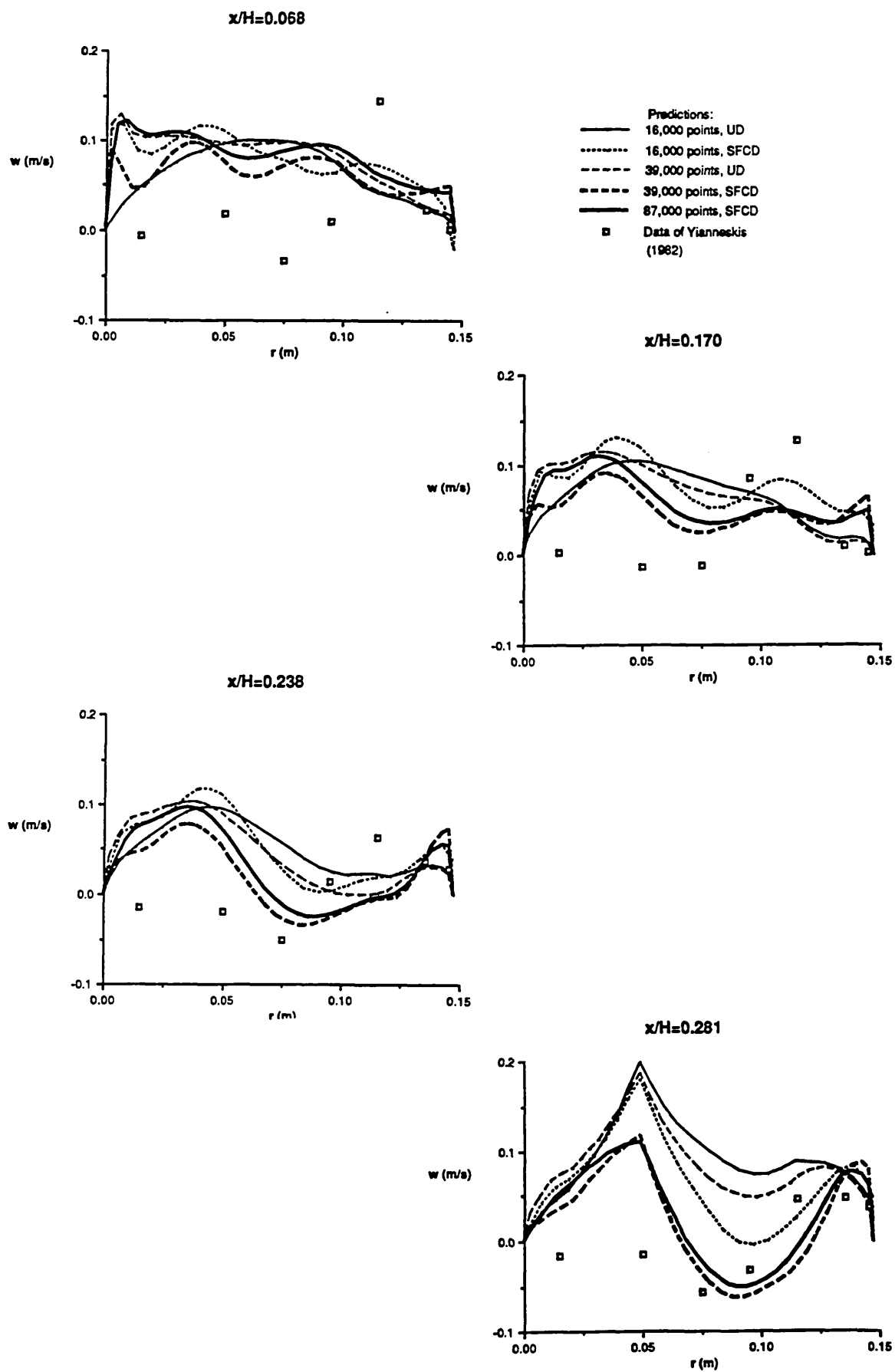


Figure 5.4.23 Below-impeller swirl velocity comparisons, 56.25° plane, water in mixing vessel

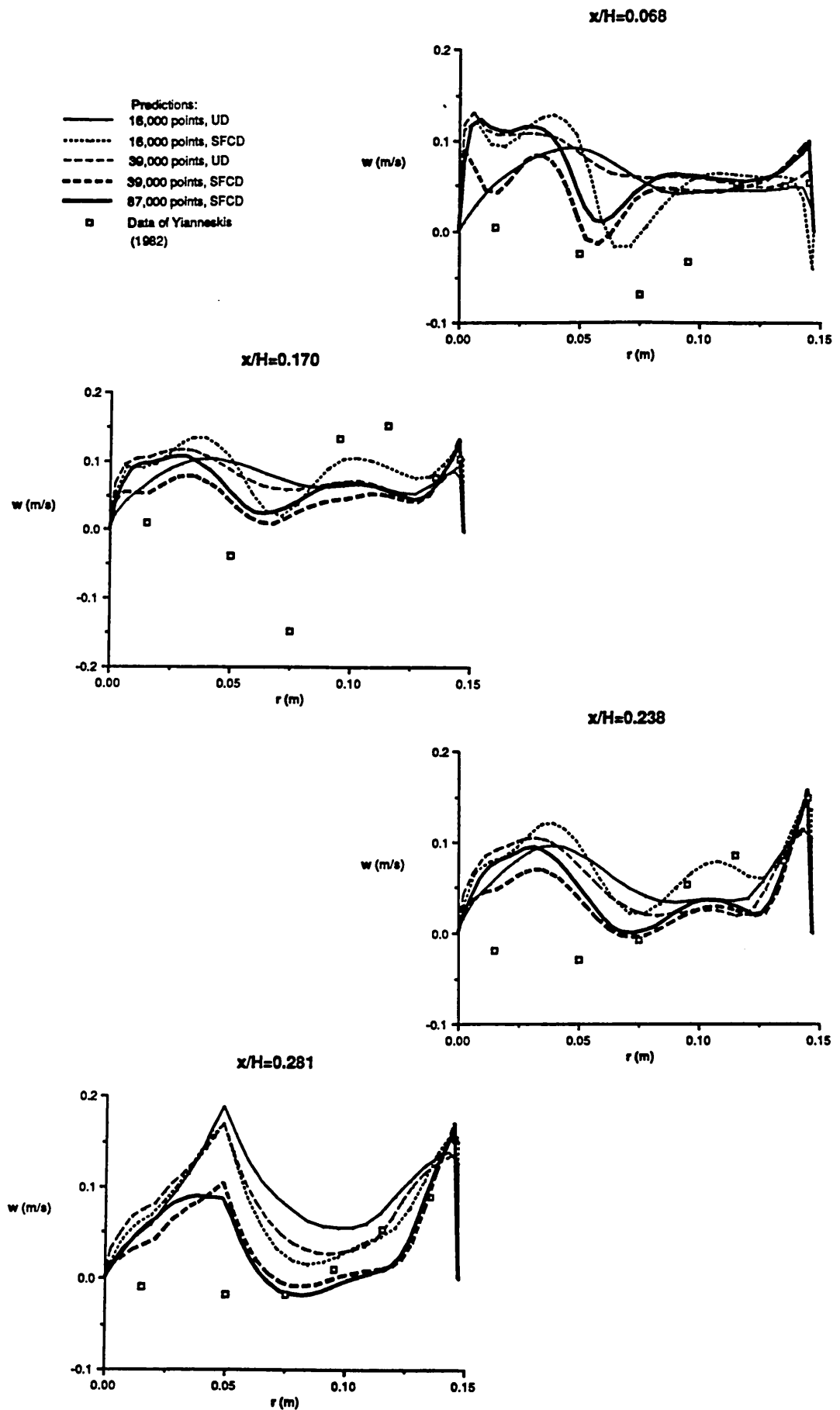


Figure 5.4.24 Below-impeller swirl velocity comparisons, 67.5° plane, water in mixing vessel

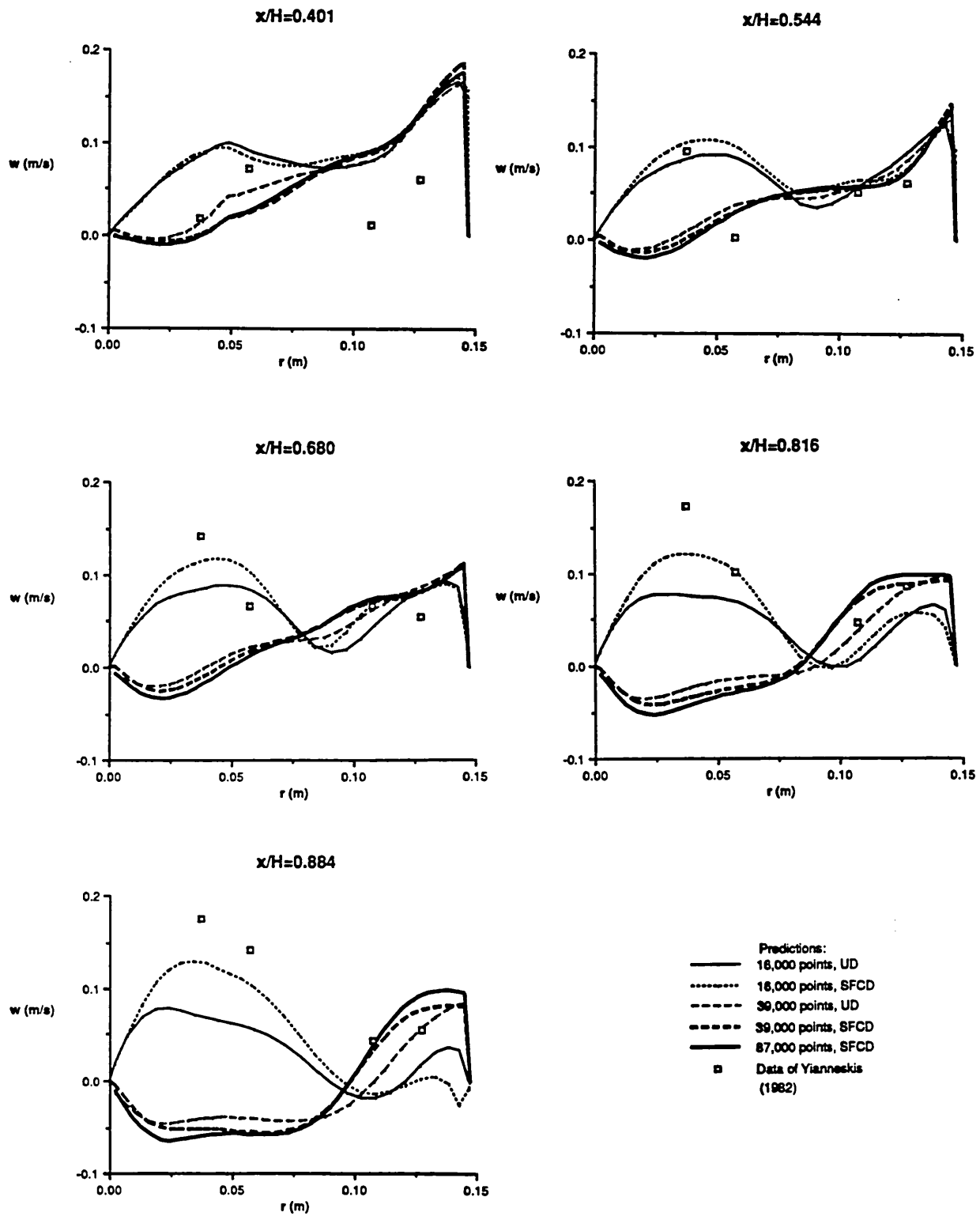


Figure 5.4.25 Above-impeller swirl velocity comparisons, 0° plane, water in mixing vessel

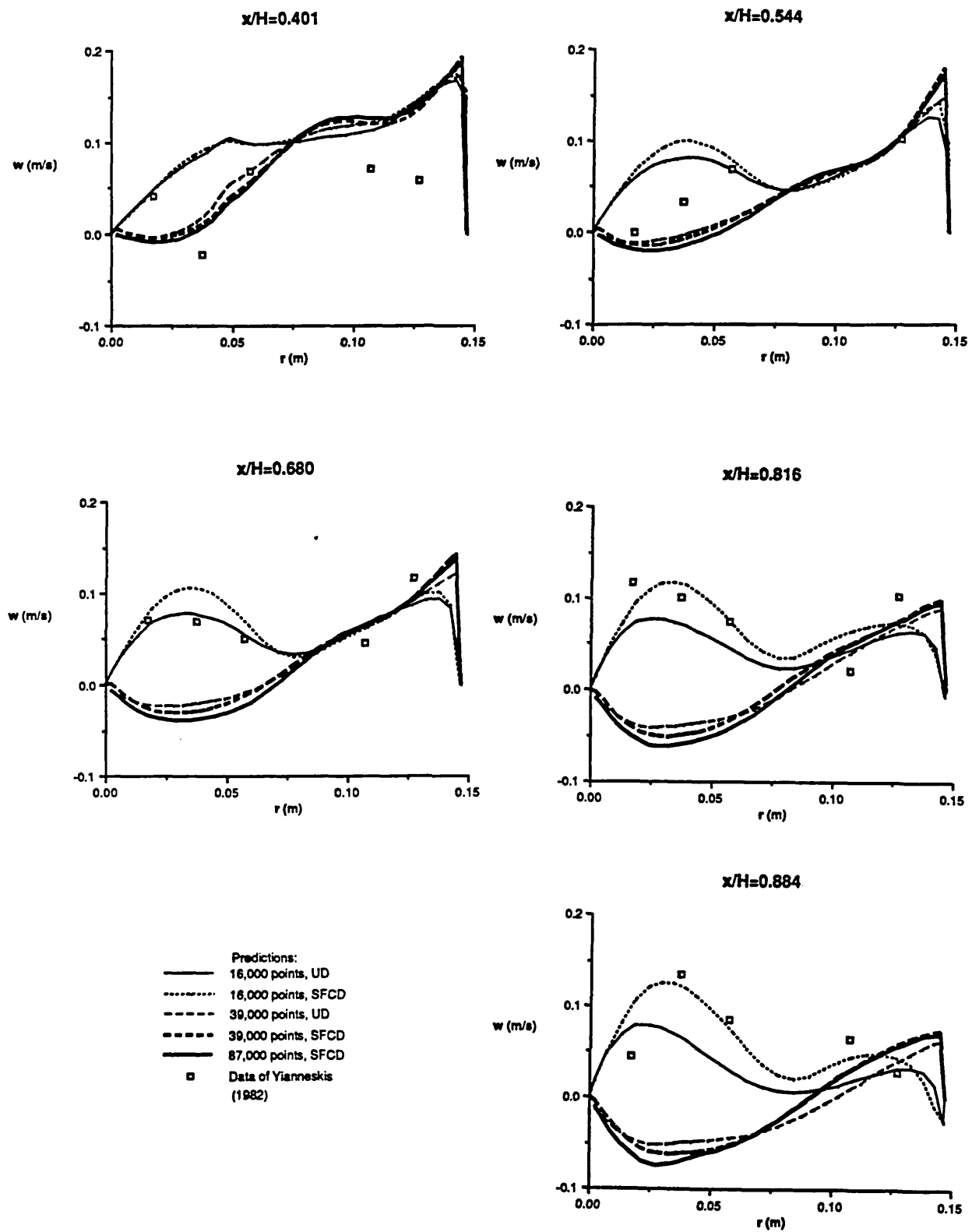


Figure 5.4.26 Above-impeller swirl velocity comparisons, 22.5° plane, water in mixing vessel

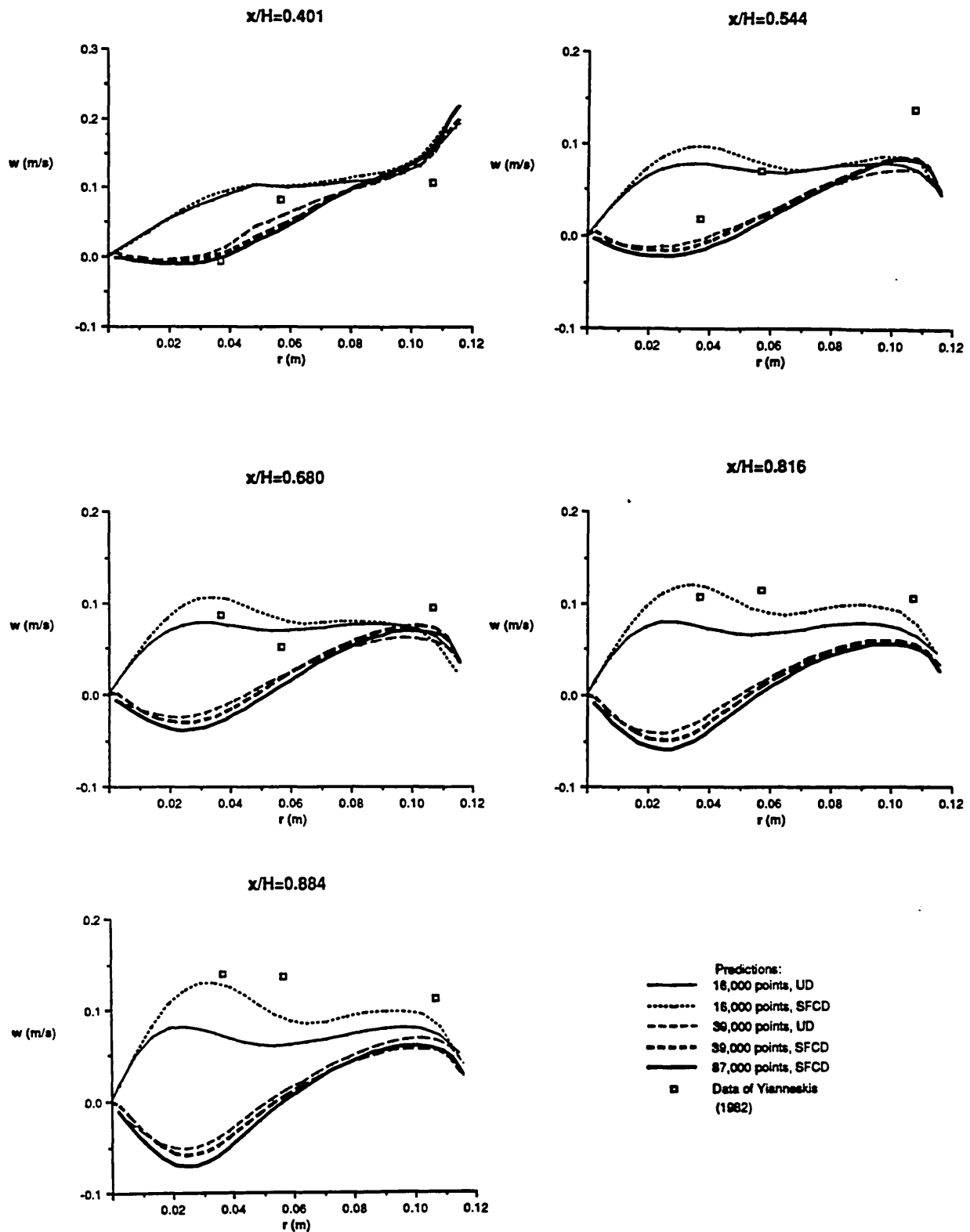


Figure 5.4.27 Above-impeller swirl velocity comparisons, 45° plane, water in mixing vessel

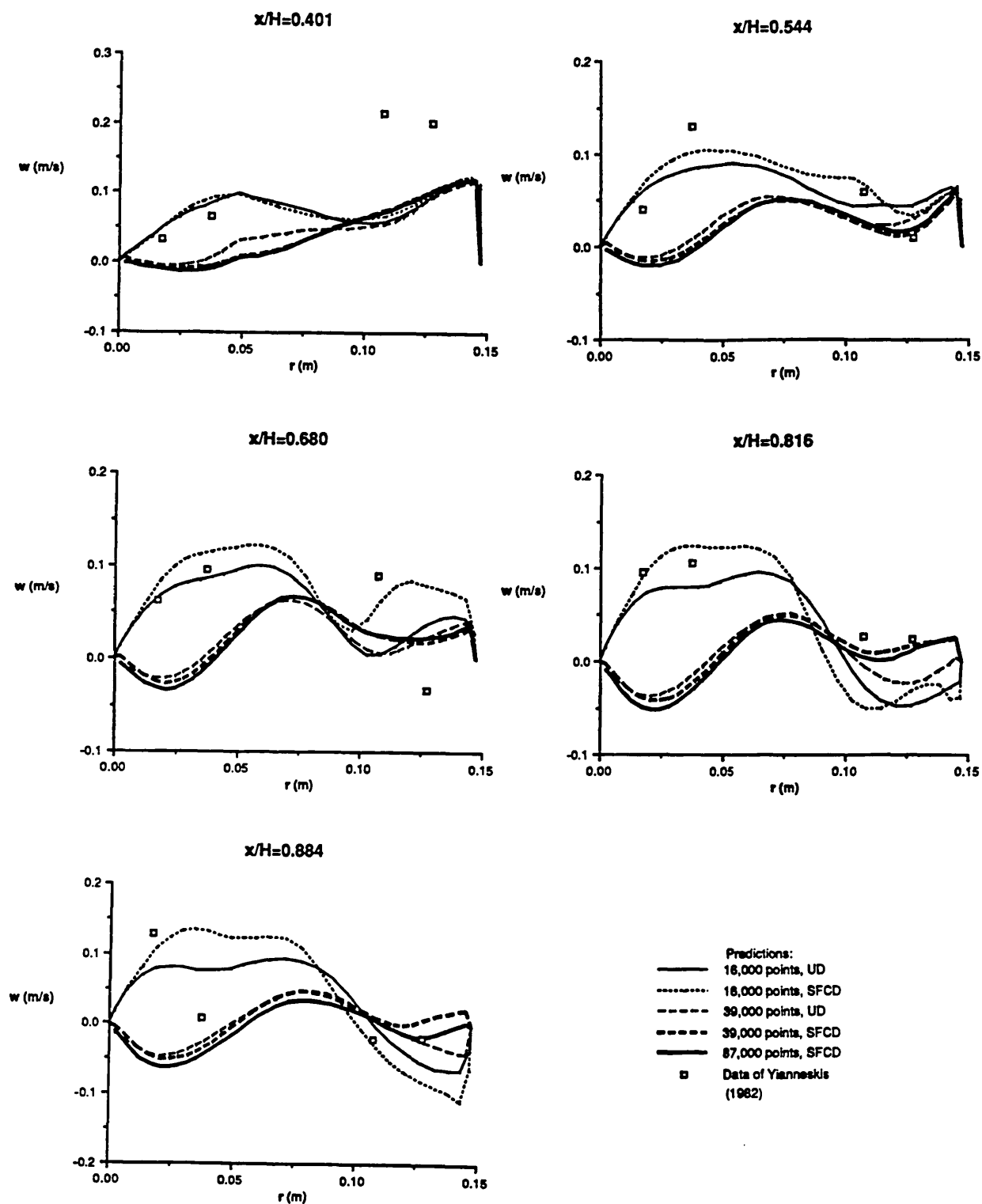


Figure 5.4.28 Above-impeller swirl velocity comparisons, 67.5° plane, water in mixing vessel

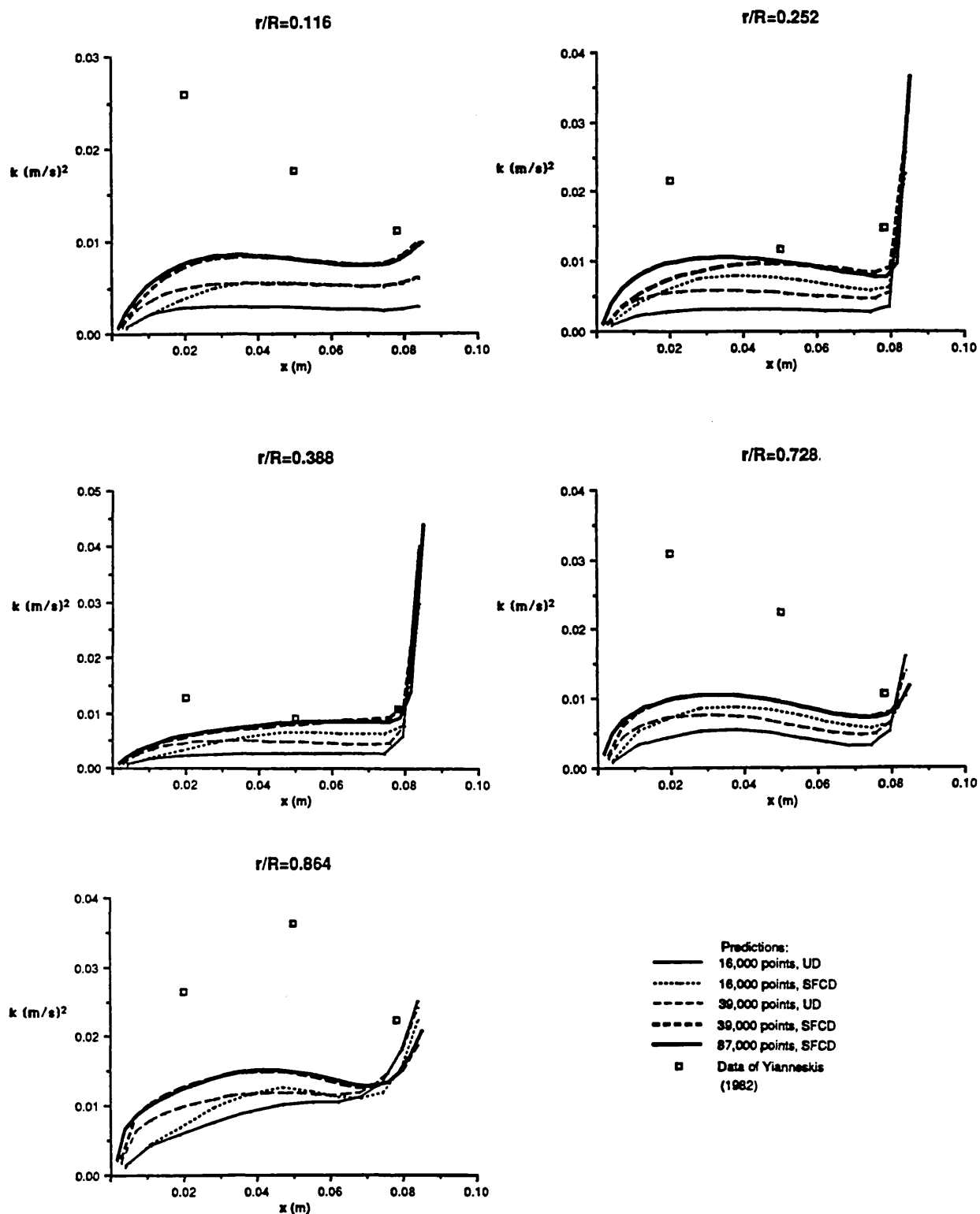


Figure 5.4.29 Below-impeller turbulence kinetic energy comparisons, 0° plane, water in mixing vessel

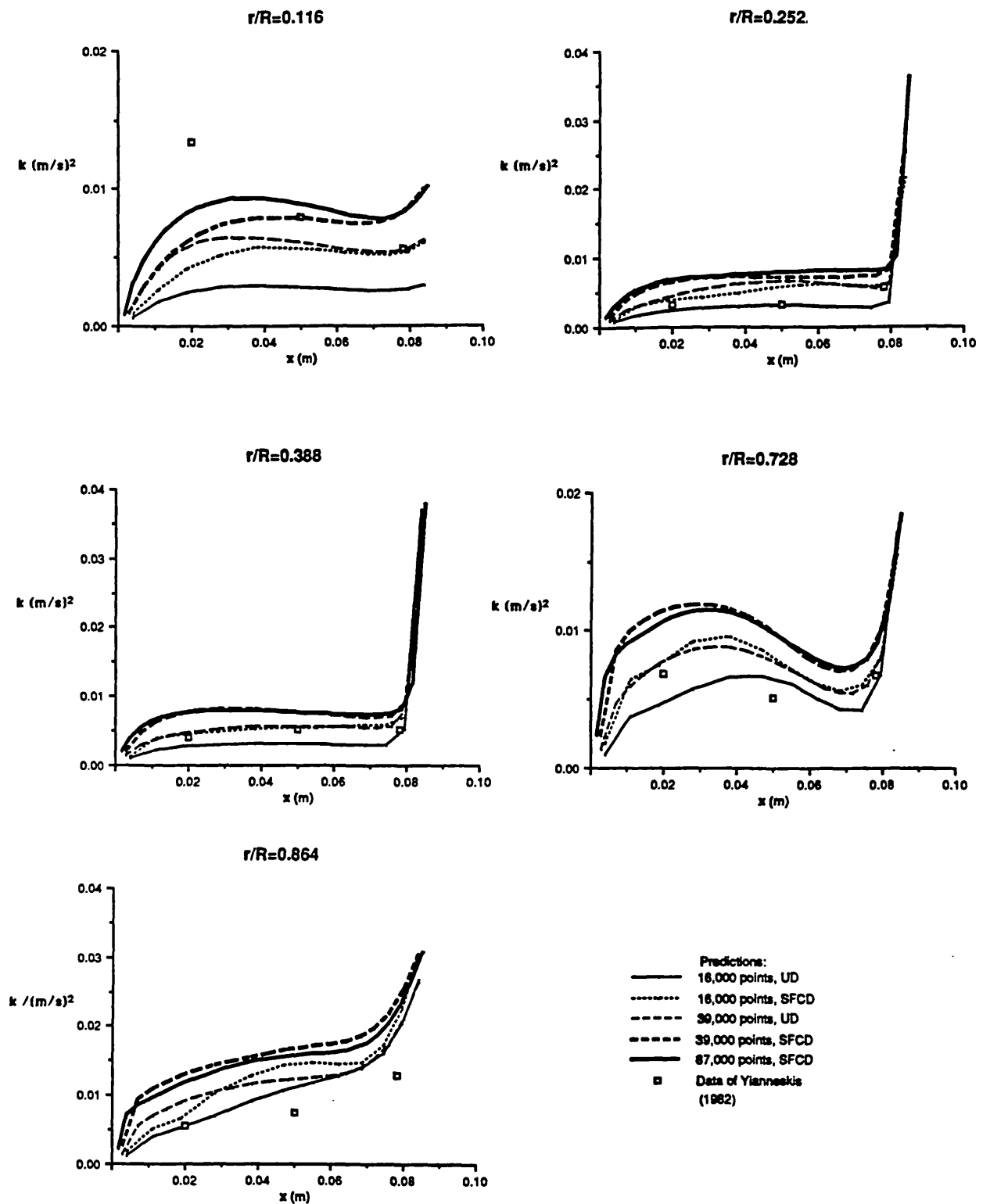


Figure 5.4.30 Below-impeller turbulence kinetic energy comparisons, 22.5° plane, water in mixing vessel

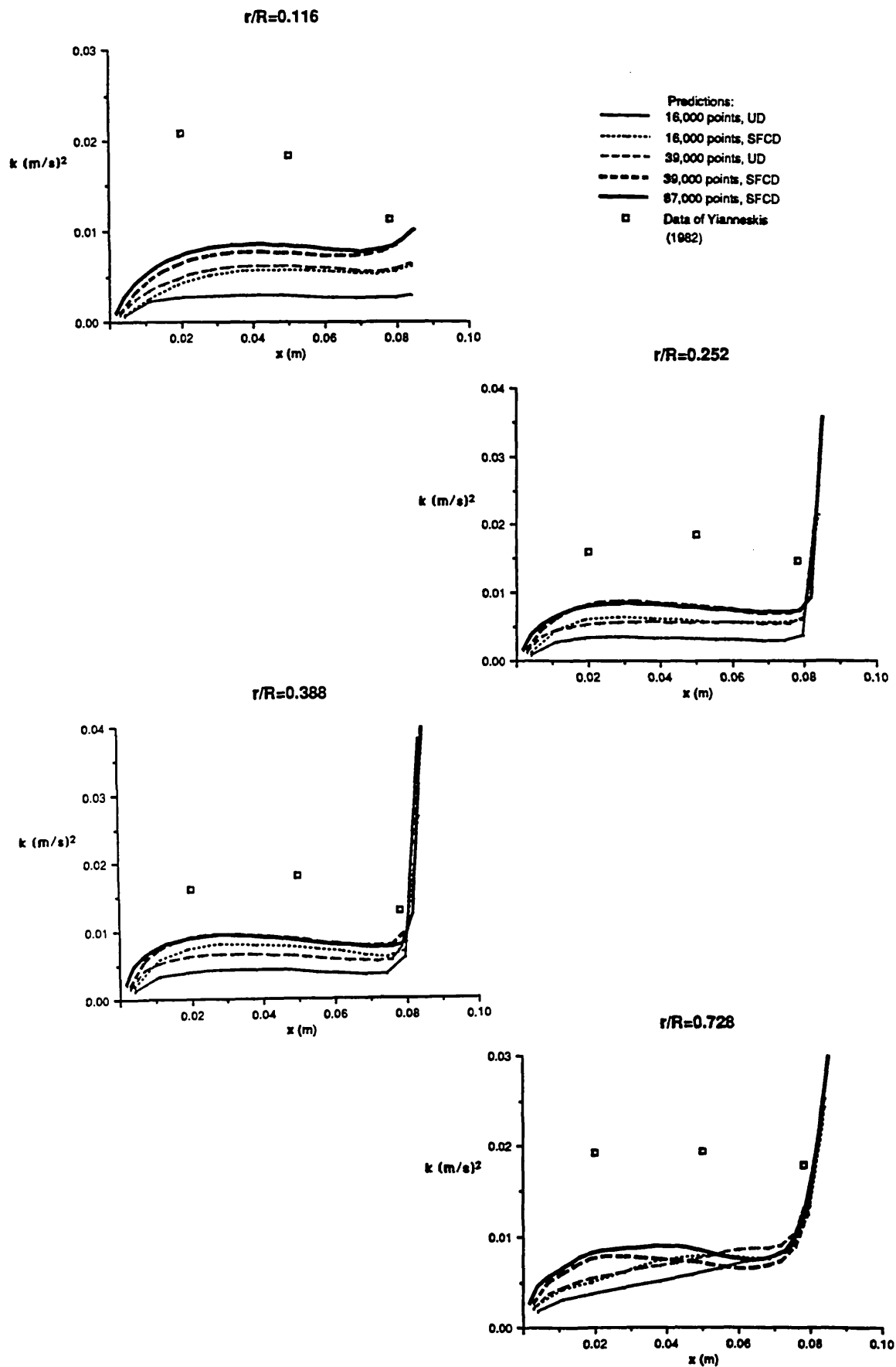


Figure 5.4.31 Below-impeller turbulence kinetic energy comparisons, 45° plane, water in mixing vessel

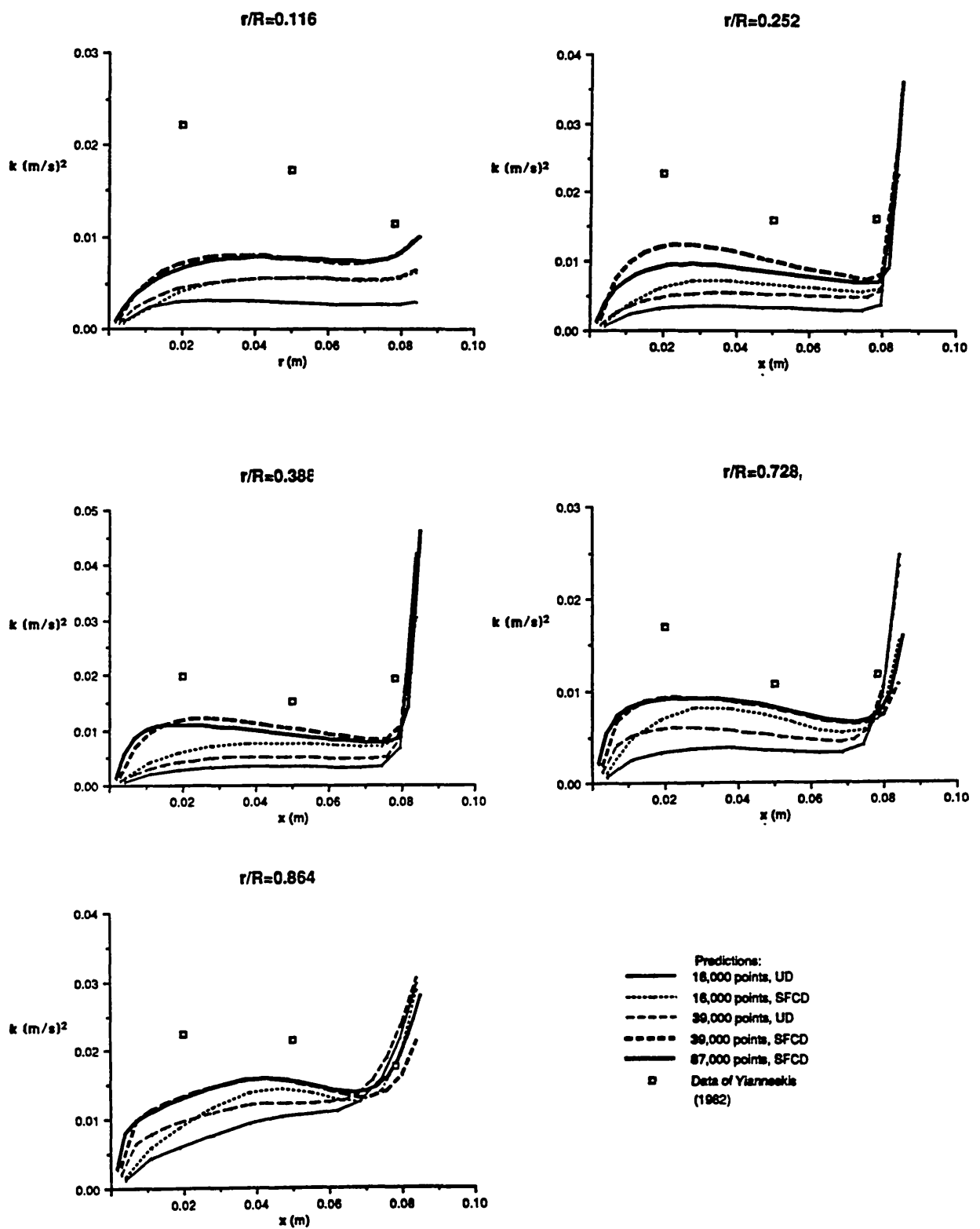


Figure 5.4.32 Below-impeller turbulence kinetic energy comparisons, 67.5° plane, water in mixing vessel

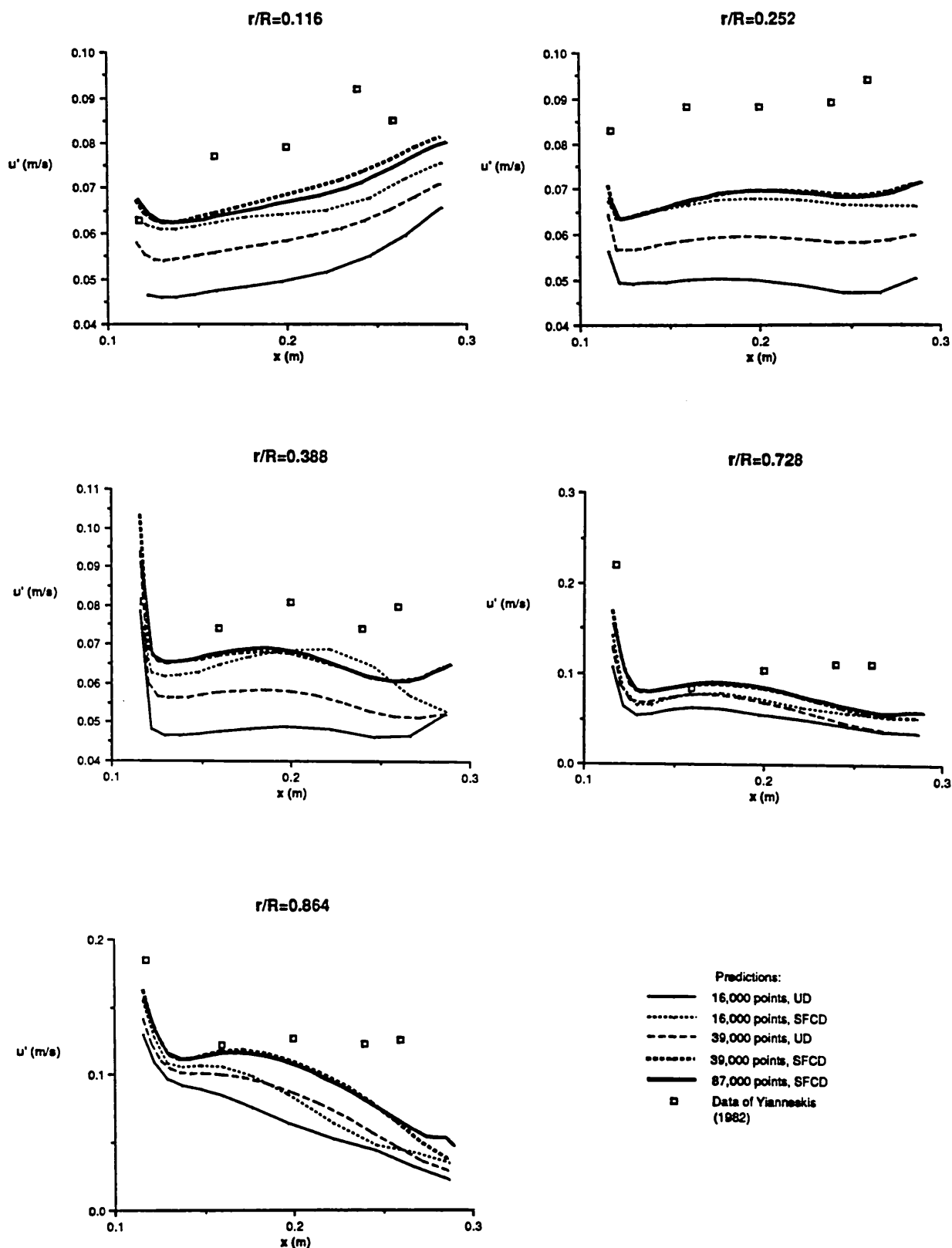


Figure 5.4.33 Above-impeller turbulence kinetic energy comparisons, 0° plane, water in mixing vessel

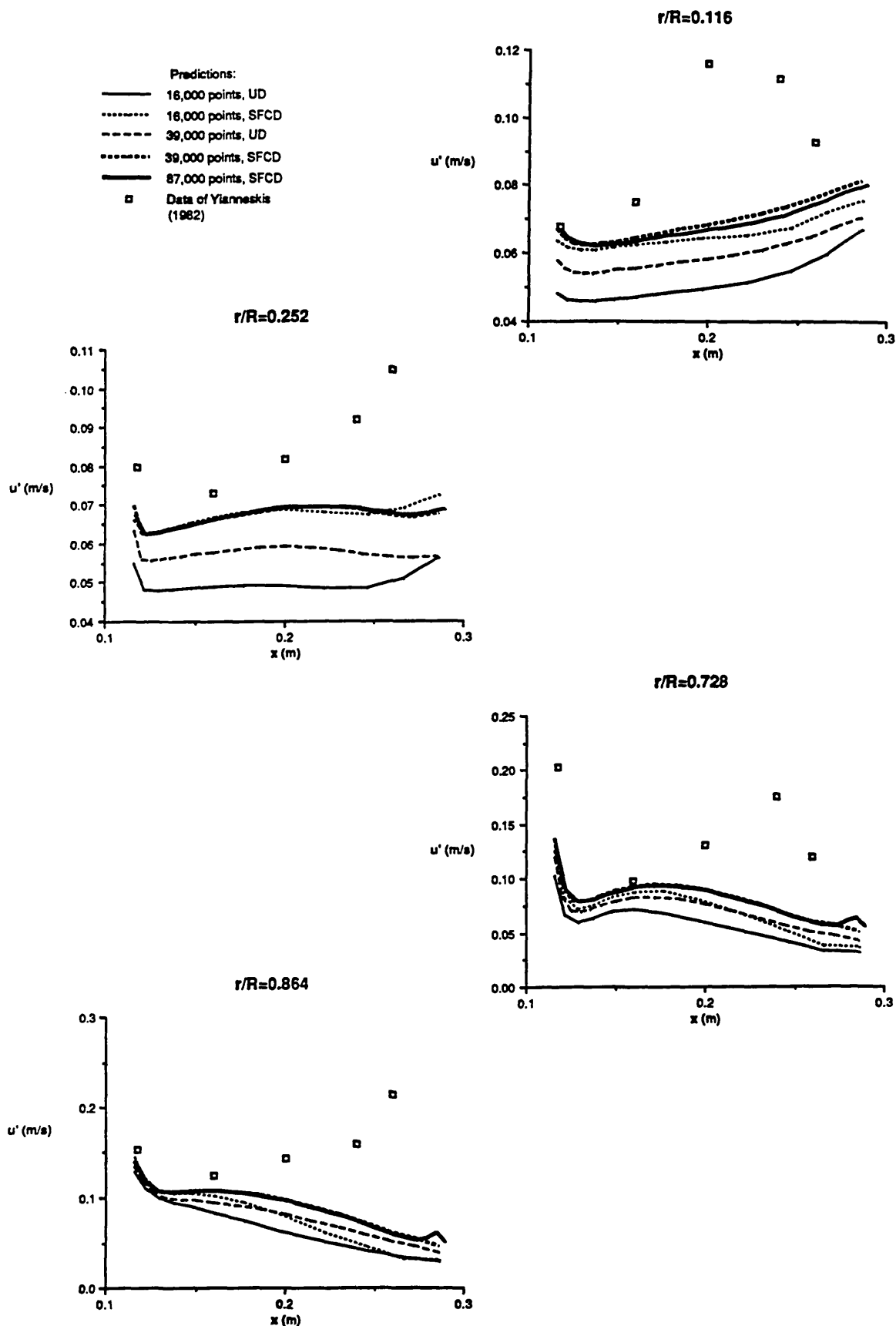


Figure 5.4.34 Above-impeller turbulence kinetic energy comparisons, 22.5° plane, water in mixing vessel

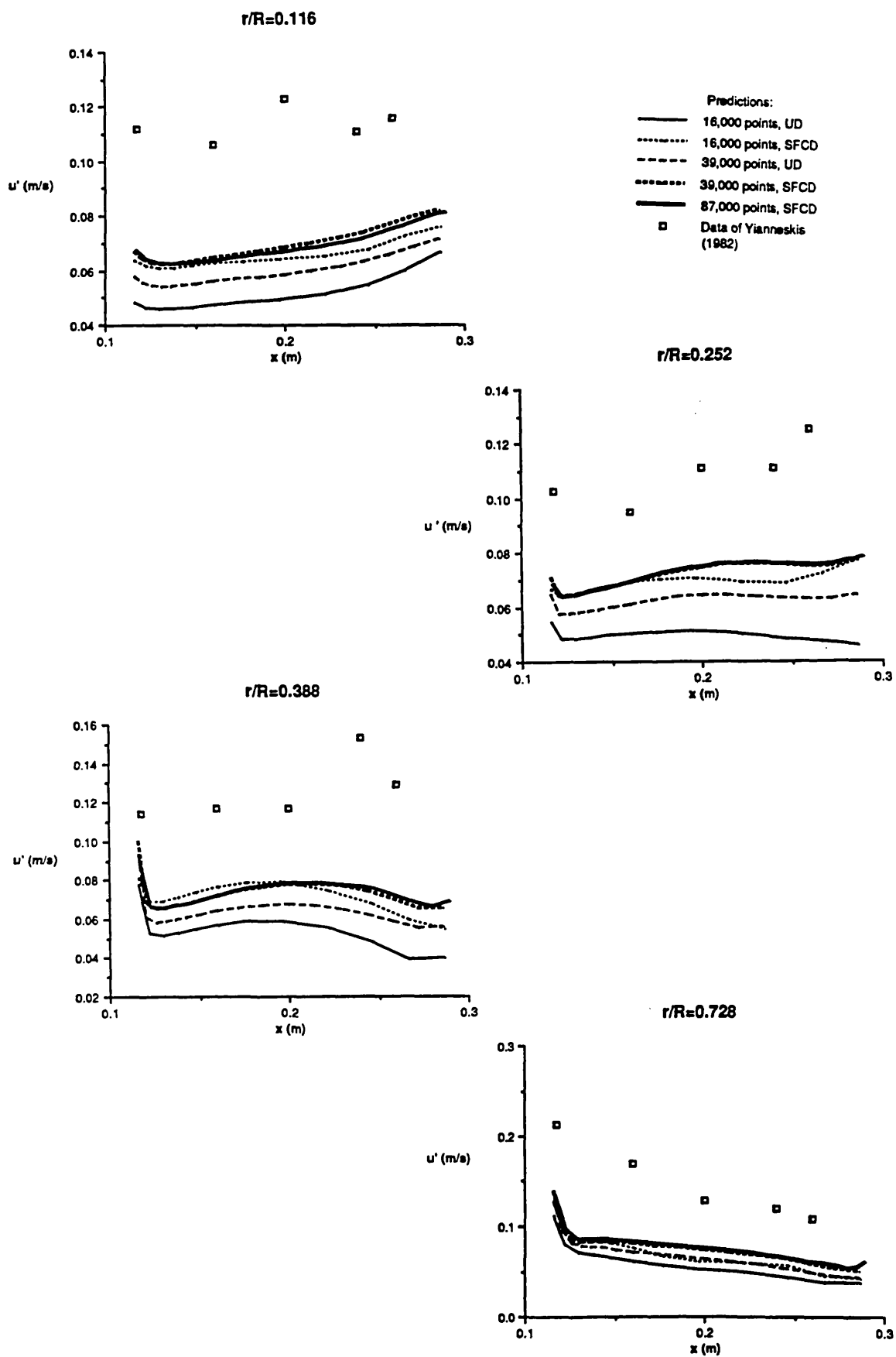


Figure 5.4.35 Above-impeller turbulence kinetic energy comparisons, 45° plane, water in mixing vessel

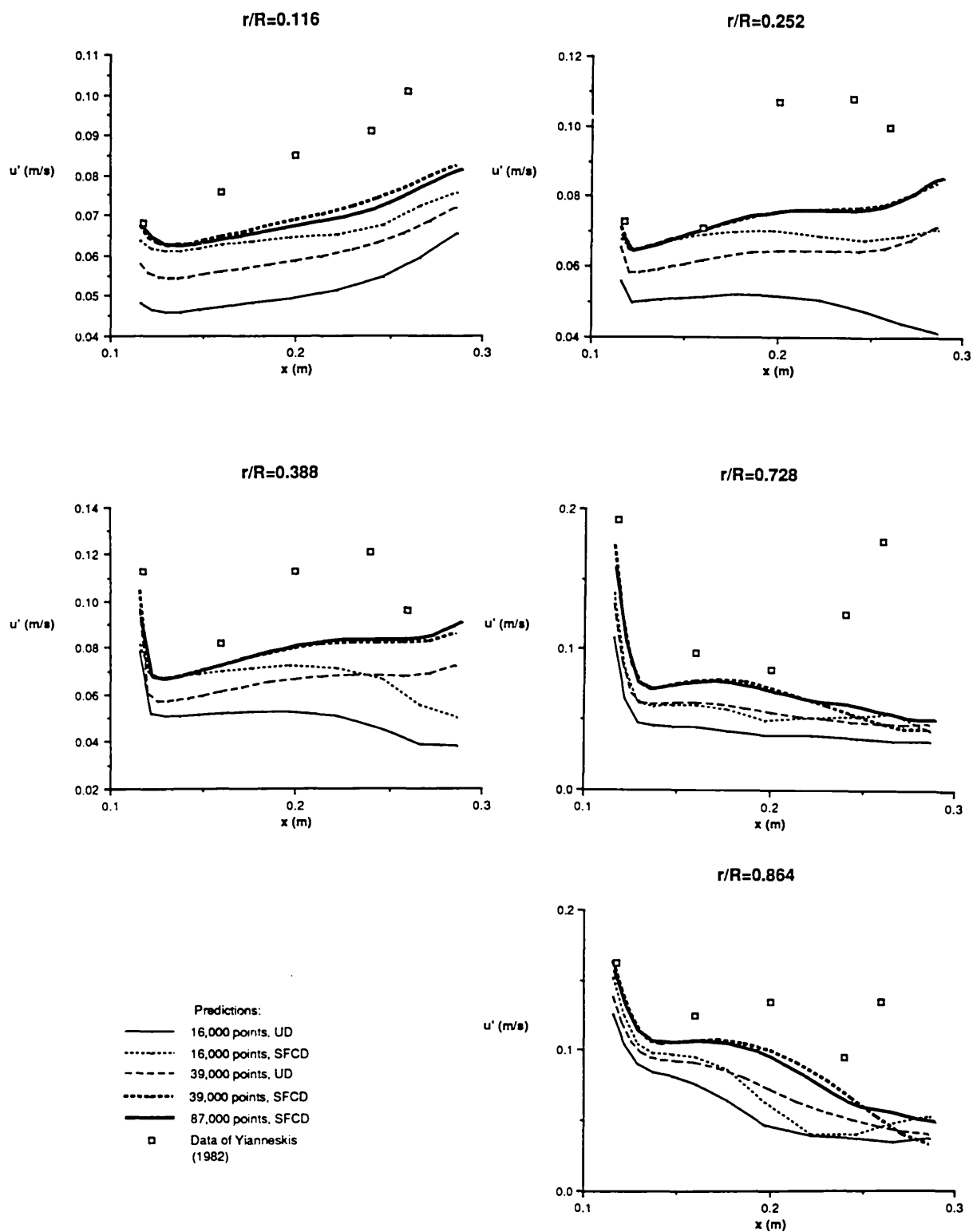


Figure 5.4.38 Above-impeller turbulence kinetic energy comparisons, 67.5° plane, water in mixing vessel

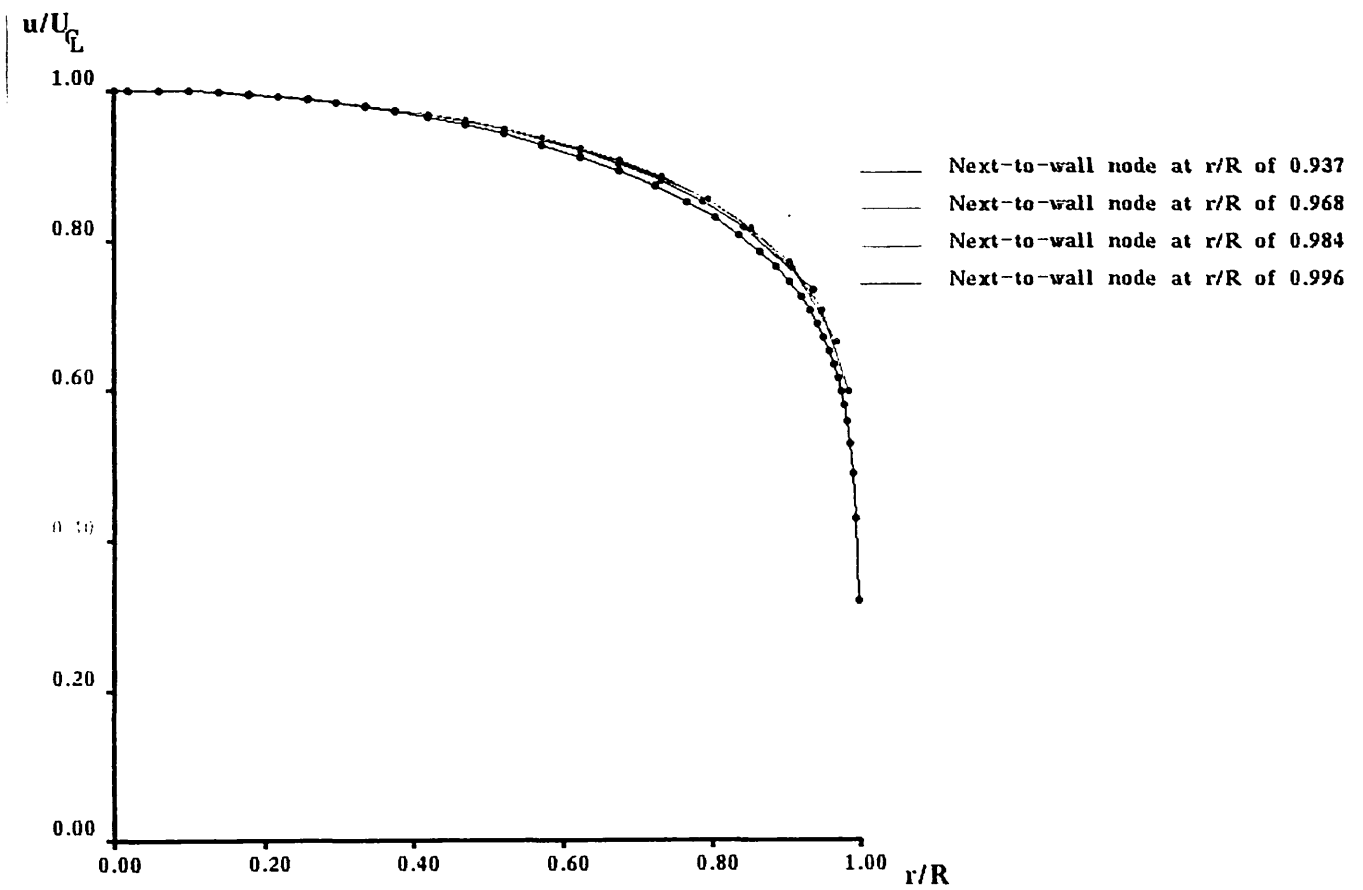
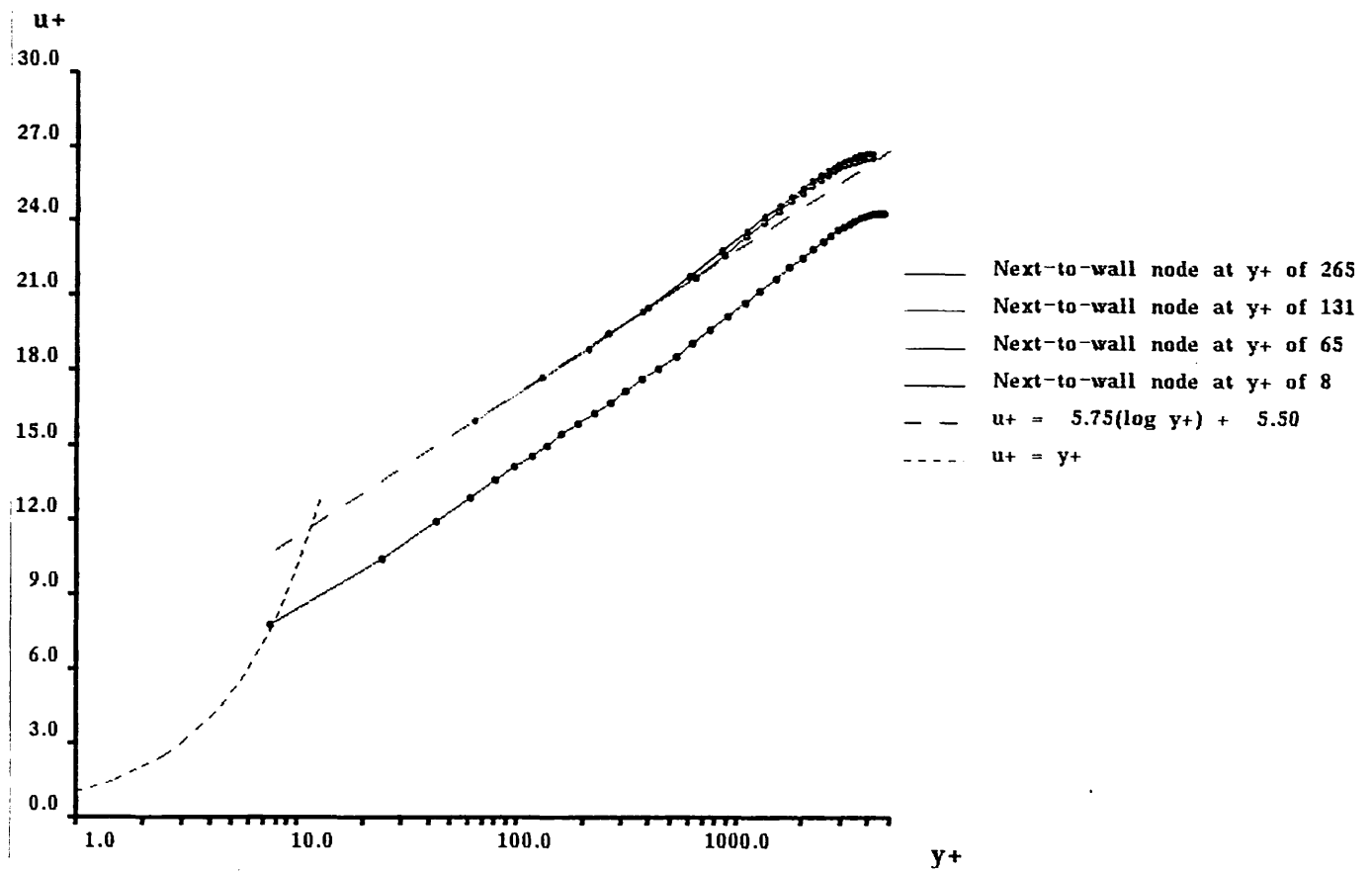


Figure 6.2.1 Axial velocity predictions for various next-to-wall locations, fully developed pipe flow of a Newtonian fluid

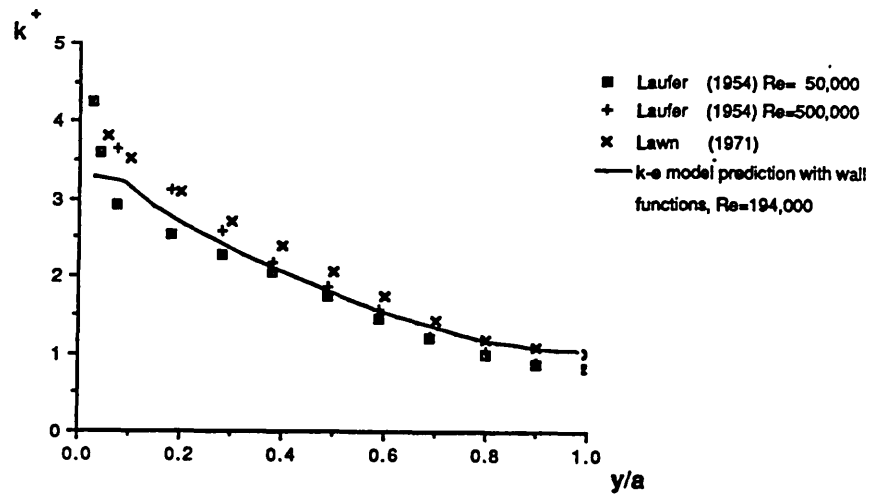


Figure 6.2.2 Comparison of k - ϵ model/wall function prediction of wall-to-axis turbulence energy distribution with experimental data

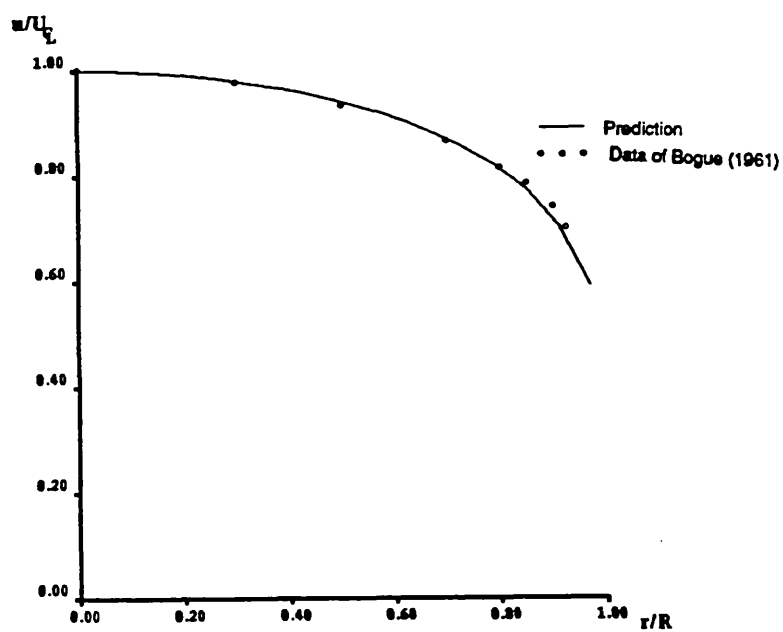
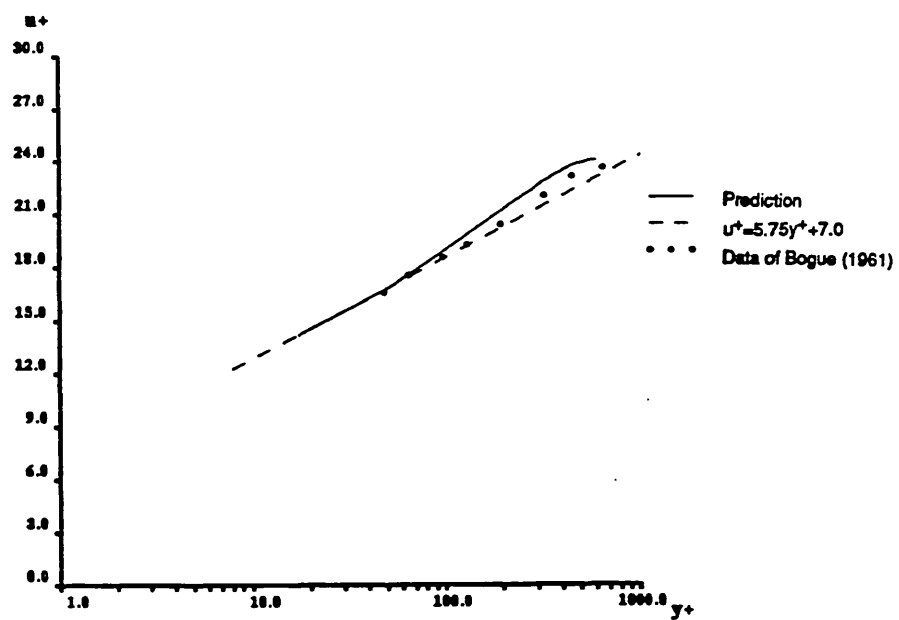


Figure 6.2.3 Comparison of predicted and measured mean axial velocity, fully developed pipe flow of shear-thinning 0.3% Carbopol solution ($n=0.70$)

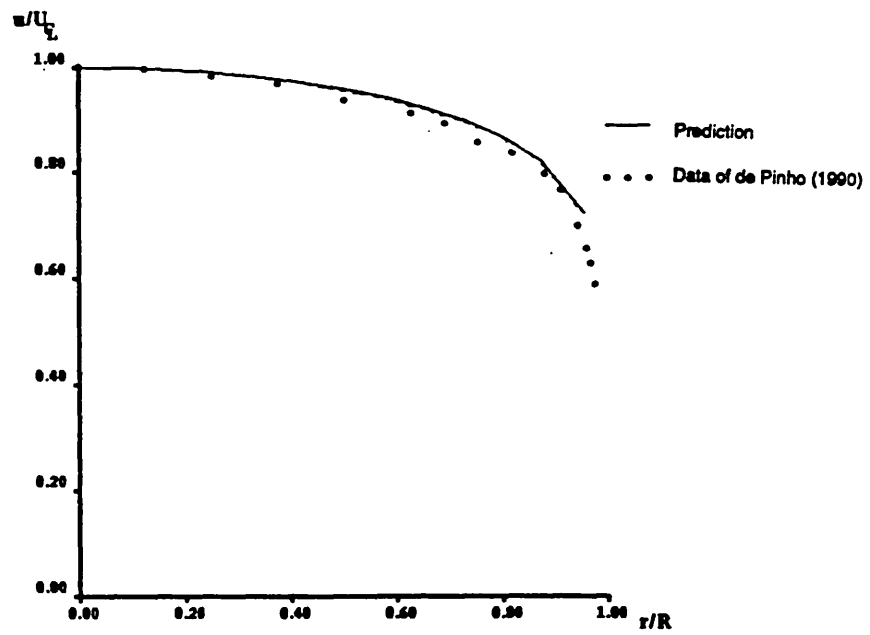
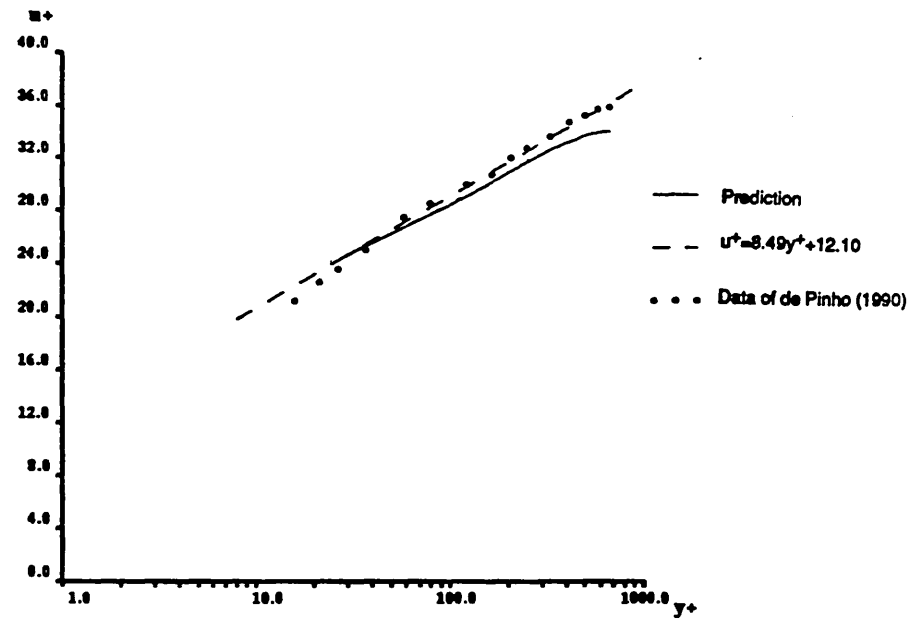


Figure 6.2.4 Comparison of predicted and measured mean axial velocity, fully developed pipe flow of shear-thinning 0.1% CMC solution ($n=0.905$)

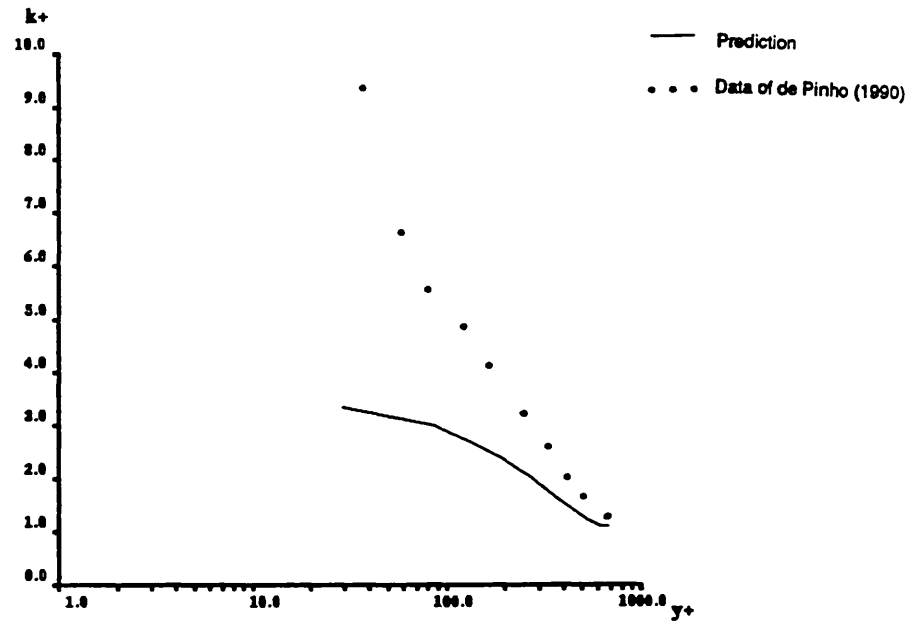


Figure 6.2.5 Comparison of predicted and measured turbulence kinetic energy, fully developed pipe flow of shear-thinning 0.1% CMC solution ($n=0.905$)

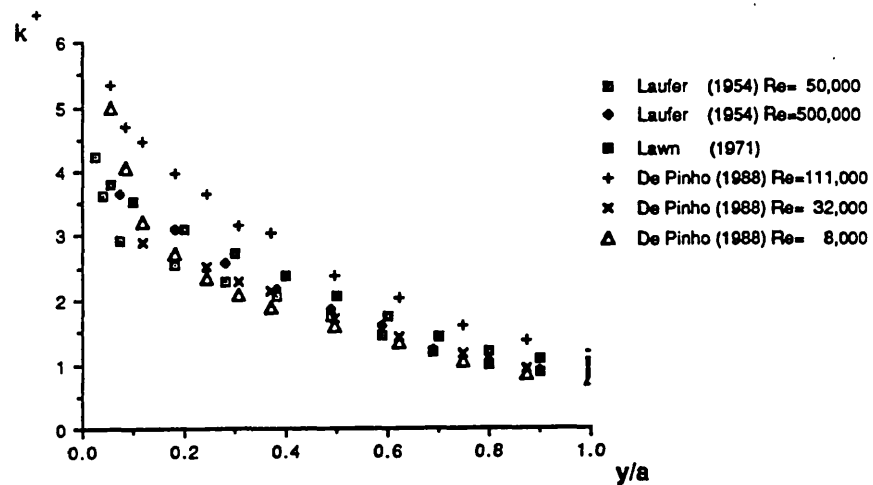


Figure 6.2.6 Comparison of turbulence kinetic energy data of de Pinho (1990) with that of earlier investigators

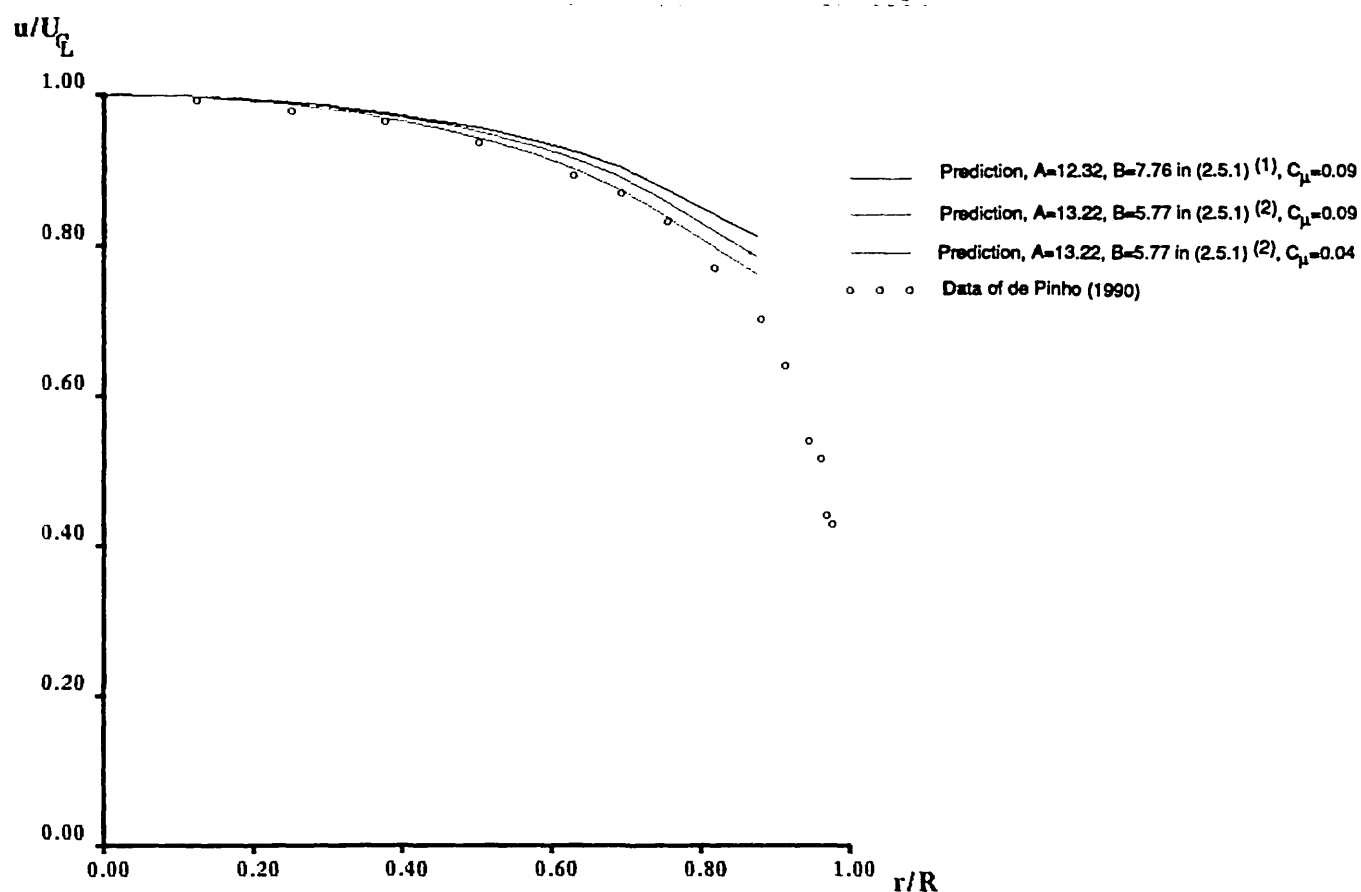
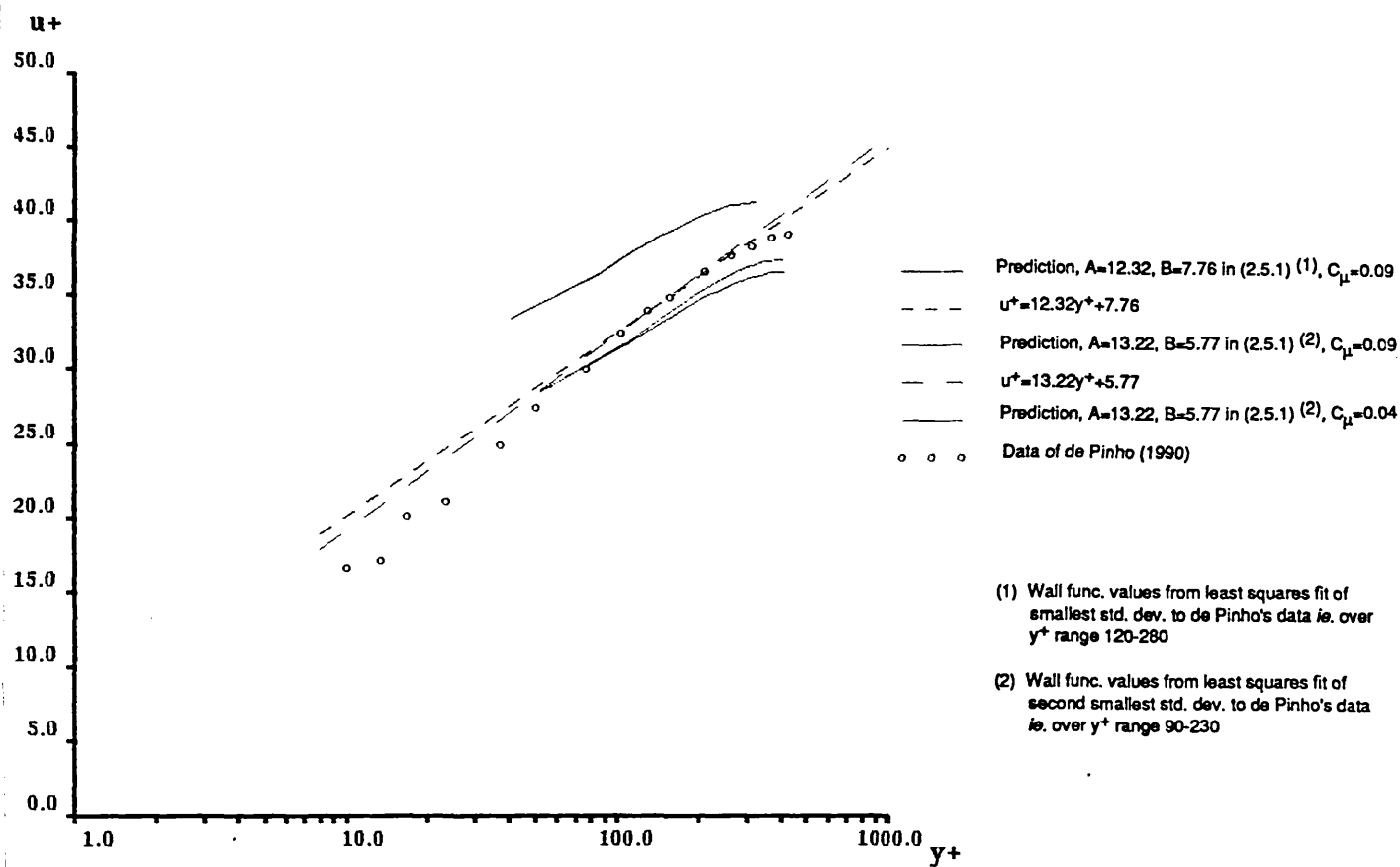


Figure 6.2.7 Comparison of predicted and measured mean axial velocity, fully developed pipe flow of shear-thinning 0.2% CMC solution ($n=0.73$)

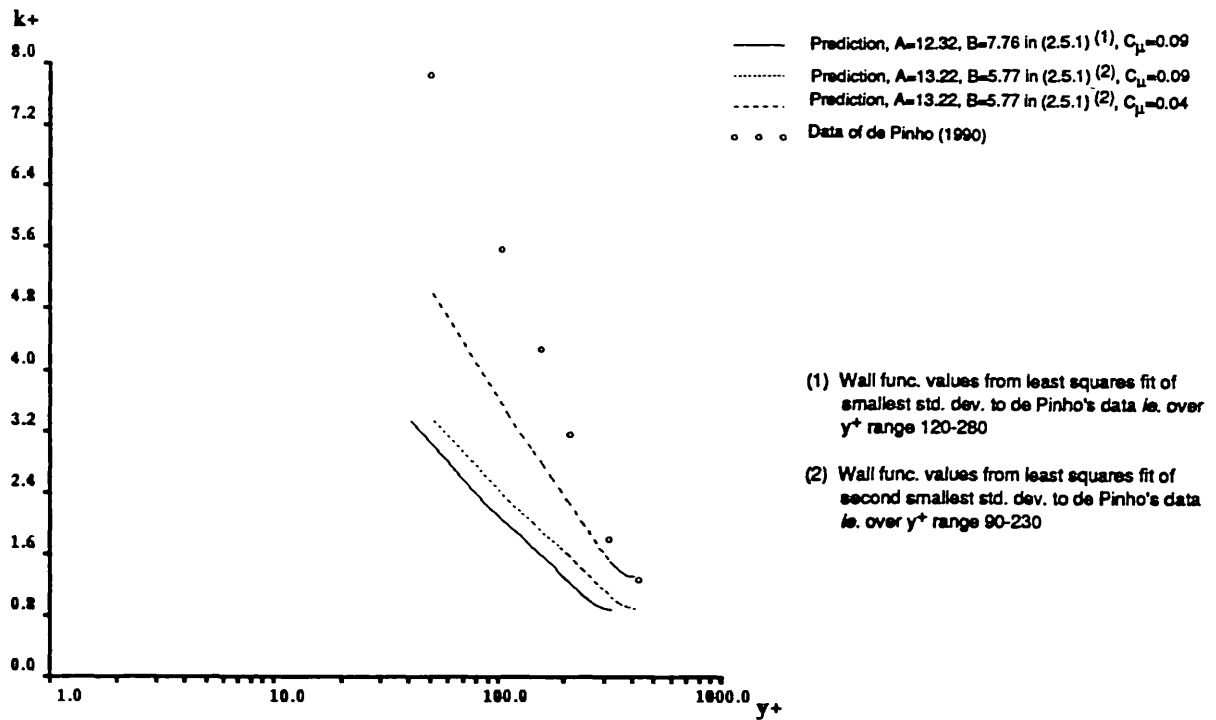


Figure 6.2.8 Comparison of predicted and measured turbulence kinetic energy, fully developed pipe flow of shear-thinning 0.2% CMC solution ($n=0.73$)

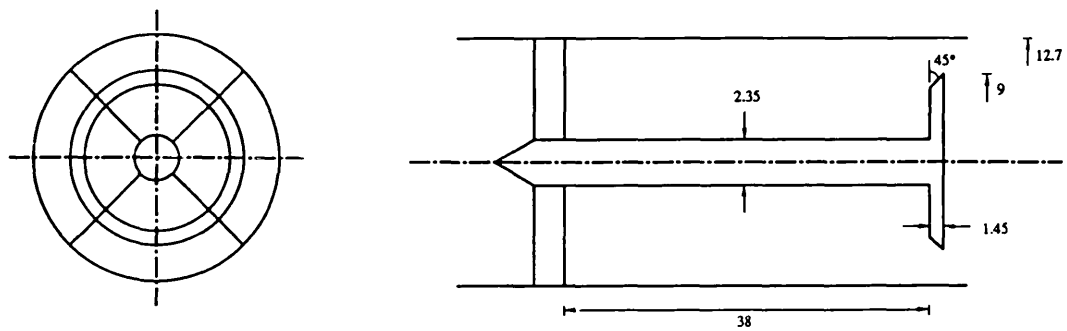
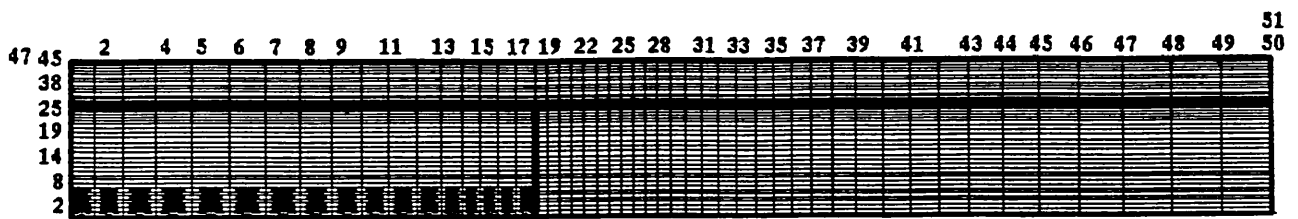
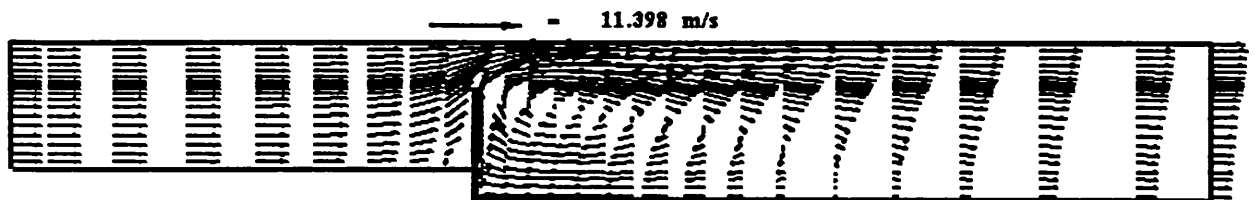


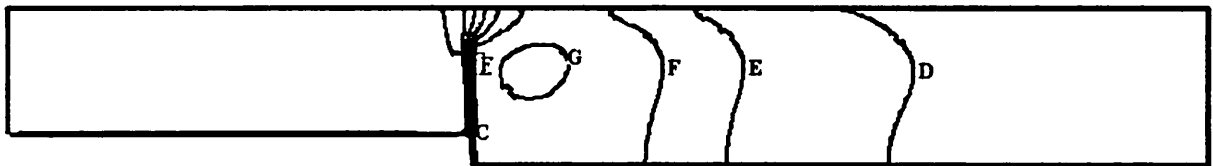
Figure 6.2.9 Geometry of solution domain for flows in pipe with axially-mounted baffle of 50% area reduction (all dimensions in mm)



a) computational grid



b) velocity vectors

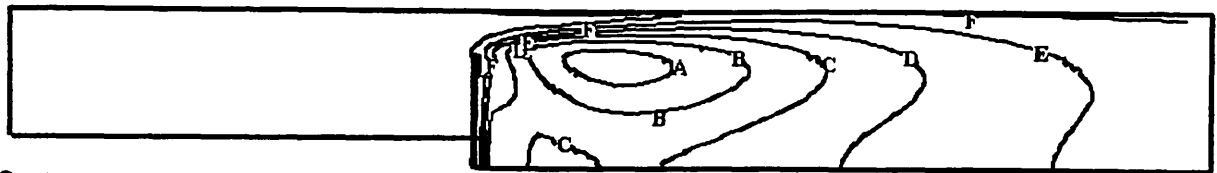


Contour values

A	1.7
B	1.1
C	0.5
D	-0.1
E	-0.7
F	-1.3
G	-2.1

c) normalised pressure ($p/\rho U^2$)

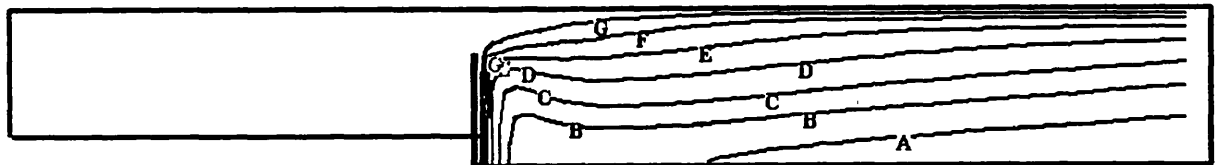
Figure 6.2.10 Details of predictions for turbulent flow of Newtonian fluid in pipe with axially-mounted baffle



Contour values

A	0.60
B	0.49
C	0.38
D	0.27
E	0.16
F	0.05

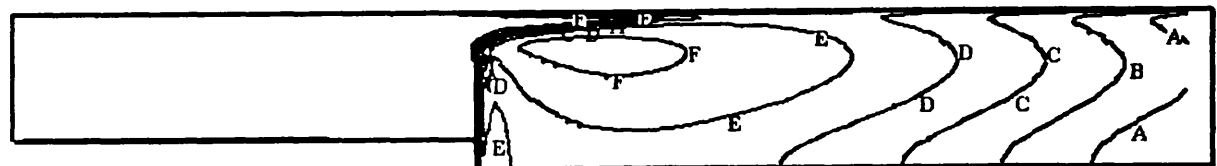
d) normalised turbulence kinetic energy (k/U^2)



Contour values

A	4.70×10^{-3}
B	4.05×10^{-3}
C	3.50×10^{-3}
D	2.85×10^{-3}
E	2.20×10^{-3}
F	1.55×10^{-3}
G	0.90×10^{-3}

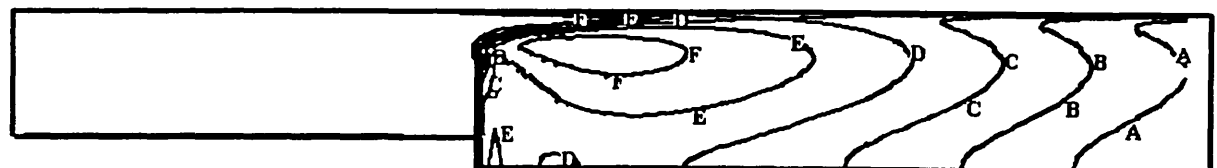
e) normalised length scales of turbulence ($C_\mu^{3/4} k^{3/2} / \epsilon D$)



Contour values (s)

A	6.6×10^{-5}
B	5.6×10^{-5}
C	4.6×10^{-5}
D	3.6×10^{-5}
E	2.6×10^{-5}
F	1.6×10^{-5}

f) Kolmogorov time scales (s)



Contour values (m)

A	8.0×10^{-6}
B	7.2×10^{-6}
C	6.4×10^{-6}
D	5.6×10^{-6}
E	4.8×10^{-6}
F	4.0×10^{-6}

g) Kolmogorov length scales (m)

Figure 6.2.10 continued

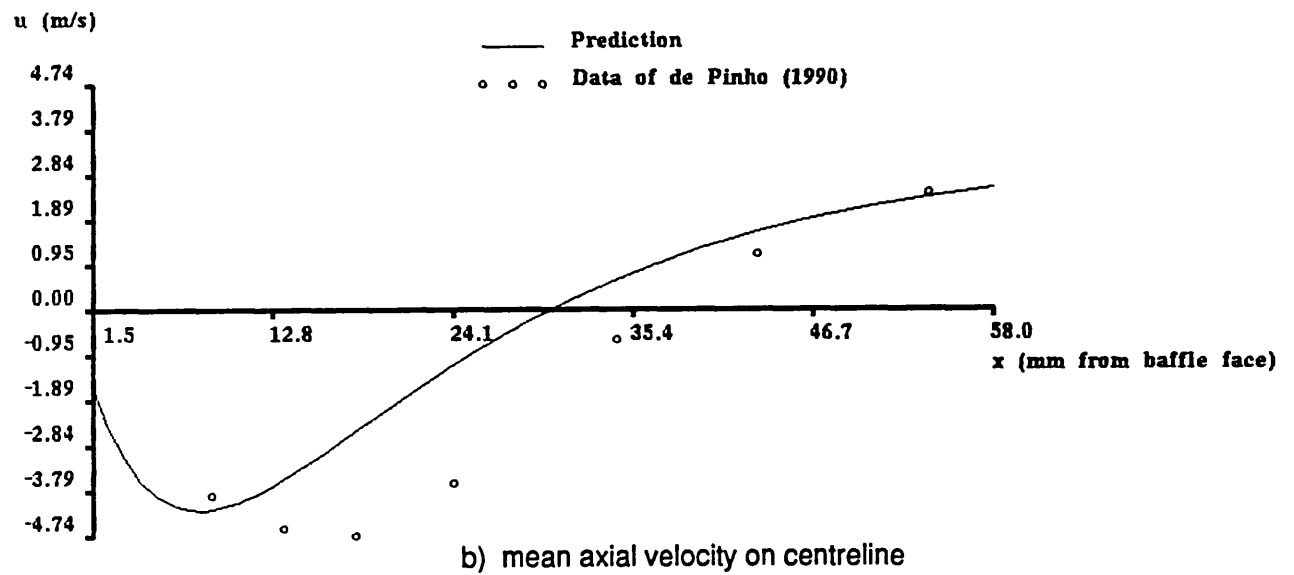
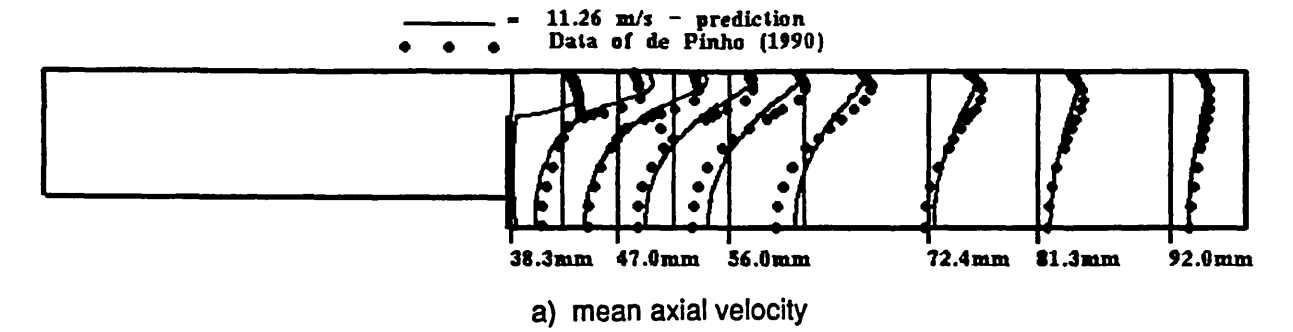
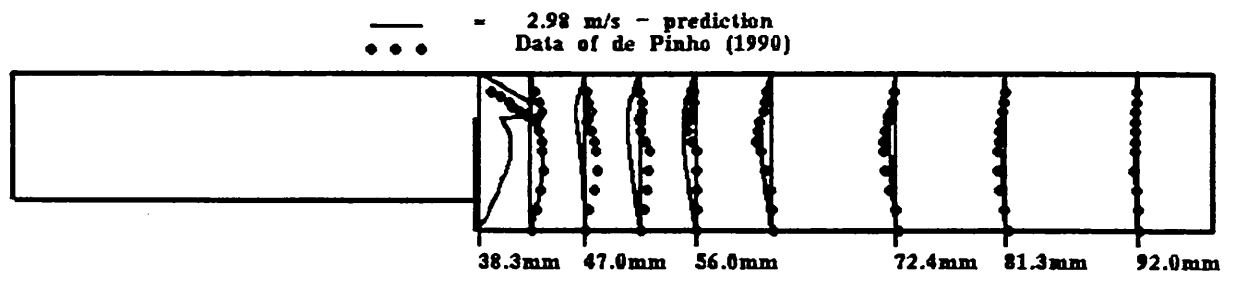
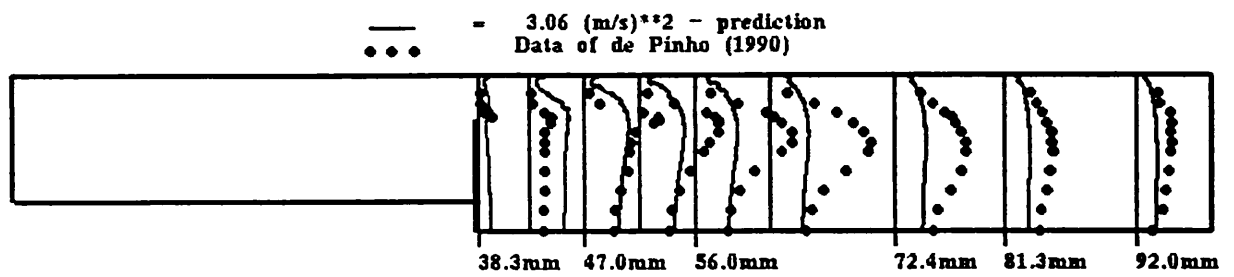


Figure 6.2.11 Comparison of prediction with experimental data of de Pinho (1990), turbulent flow of Newtonian fluid in pipe with axially-mounted baffle

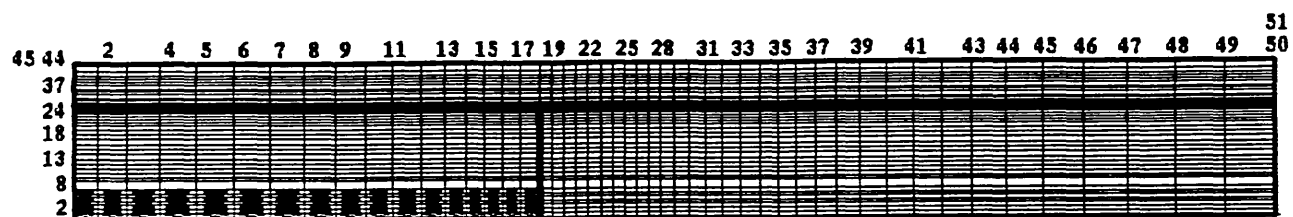


c) mean radial velocity

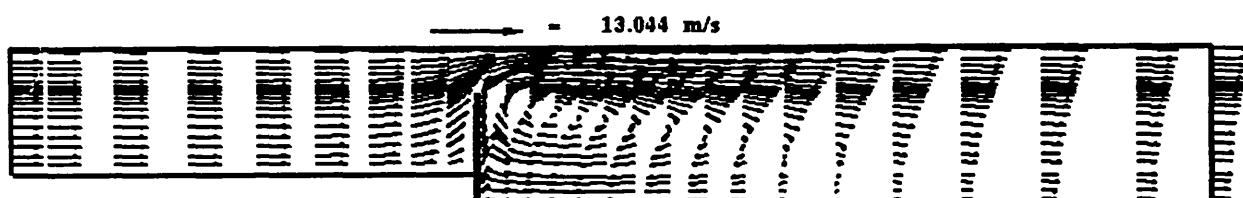


d) turbulence kinetic energy

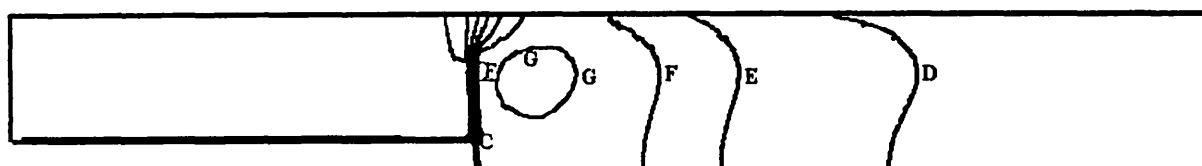
Figure 6.2.11 continued



a) computational grid



b) velocity vectors

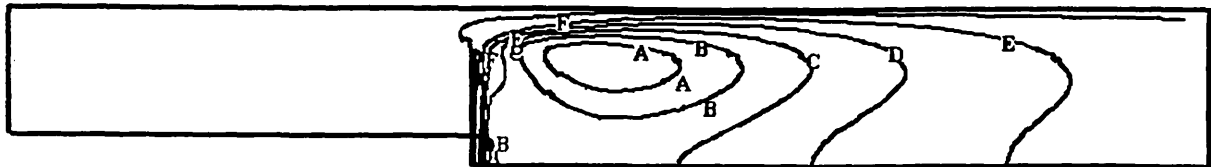


Contour values

A	1.7
B	1.1
C	0.5
D	-0.1
E	-0.7
F	-1.3
G	-2.1

c) normalised pressure (p/pU^2)

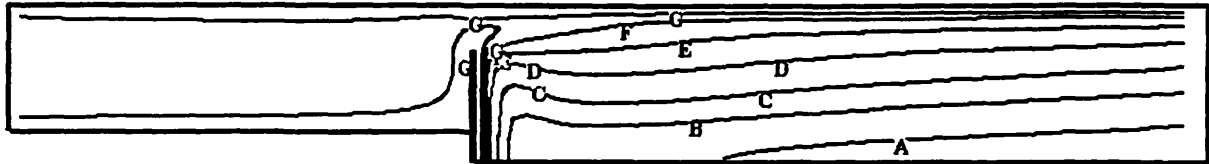
Figure 6.2.12 Details of predictions for turbulent flow of shear-thinning 0.1% CMC solution ($n=0.905$) in pipe with axially-mounted baffle



Contour values

A	0.60
B	0.49
C	0.38
D	0.27
E	0.16
F	0.05

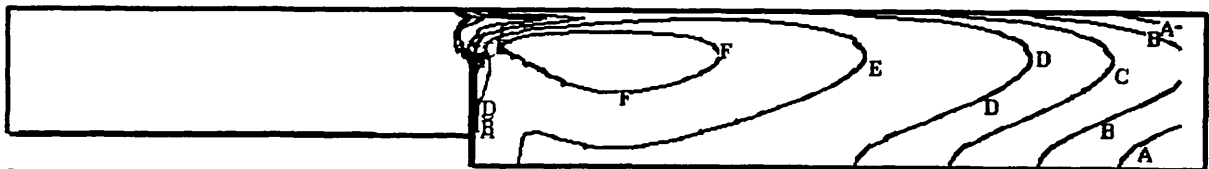
d) normalised turbulence kinetic energy (k/U^2)



Contour values

A	4.70×10^{-3}
B	4.05×10^{-3}
C	3.50×10^{-3}
D	2.85×10^{-3}
E	2.20×10^{-3}
F	1.55×10^{-3}
G	0.90×10^{-3}

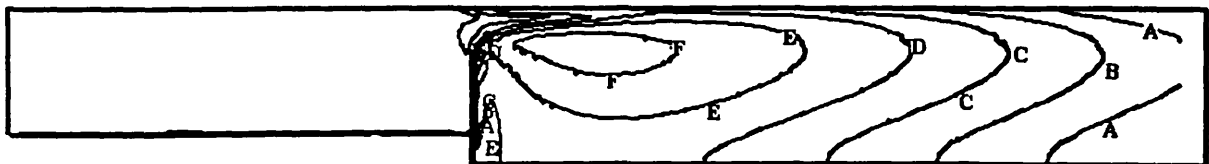
e) normalised length scales of turbulence ($C_\mu^{3/4} k^{3/2} / \epsilon D$)



Contour values (s)

A	11.0×10^{-5}
B	9.5×10^{-5}
C	8.0×10^{-5}
D	6.5×10^{-5}
E	4.0×10^{-5}
F	2.5×10^{-5}

f) Kolmogorov time scales



Contour values (m)

A	1.8×10^{-5}
B	1.6×10^{-5}
C	1.4×10^{-5}
D	1.2×10^{-5}
E	1.0×10^{-5}
F	0.8×10^{-5}

g) Kolmogorov length scales

Figure 6.2.12 continued

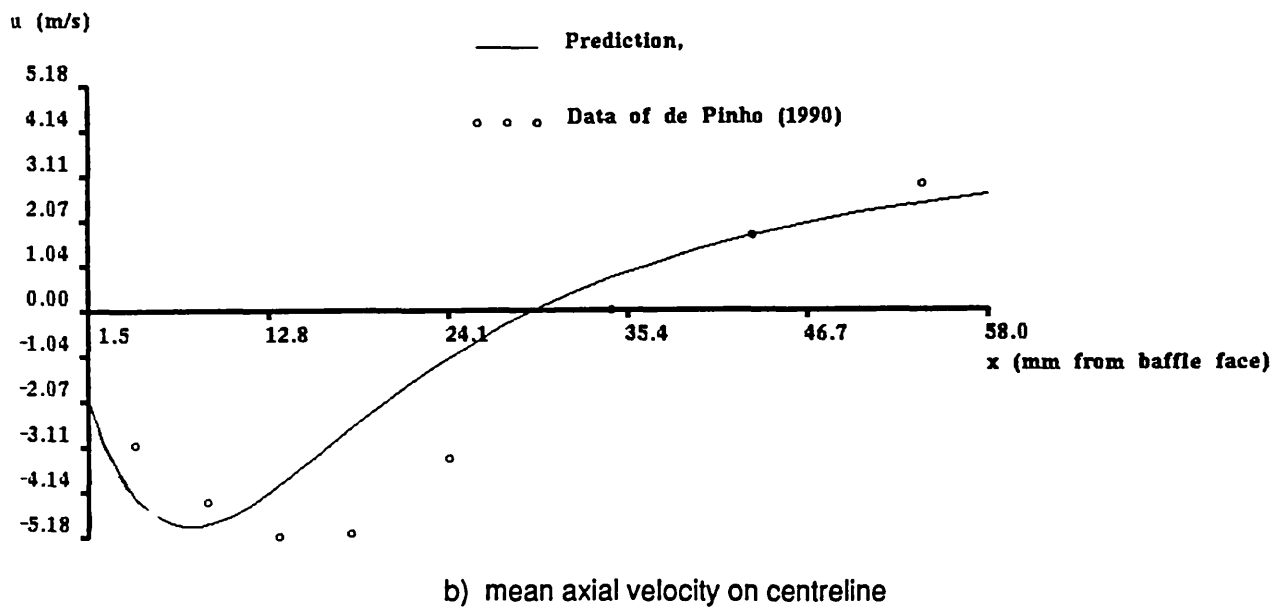
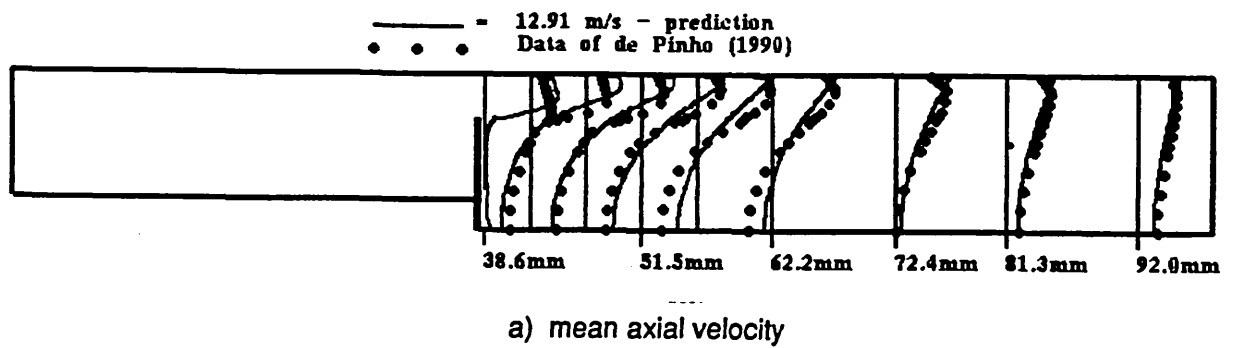
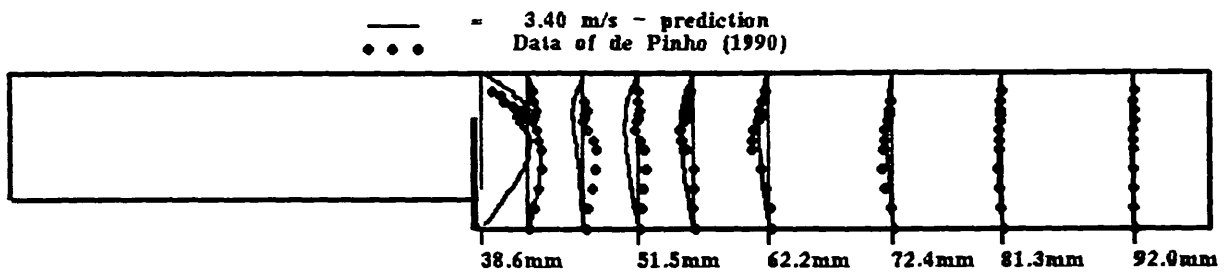
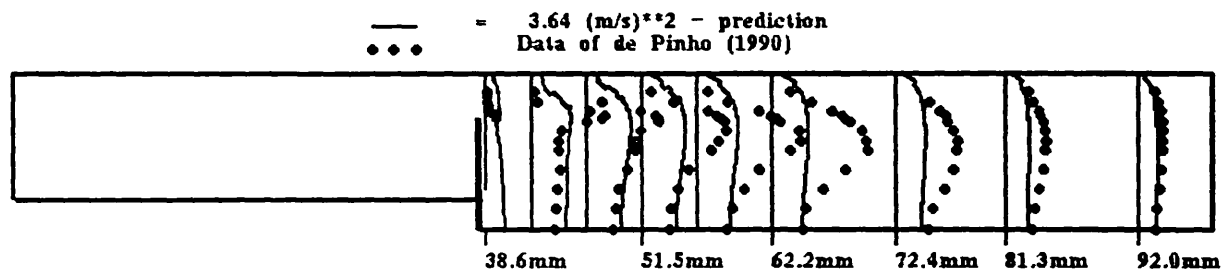


Figure 6.2.13 Comparison of prediction with experimental data of de Pinho (1990), turbulent flow of shear-thinning 0.1% CMC solution ($n=0.905$) in pipe with axially-mounted baffle

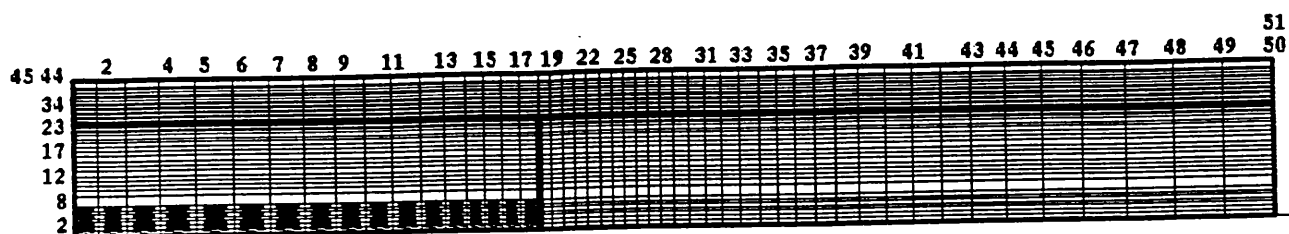


c) mean radial velocity

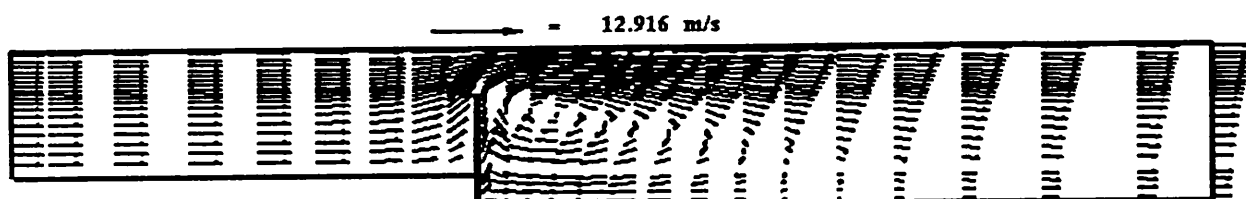


d) turbulence kinetic energy

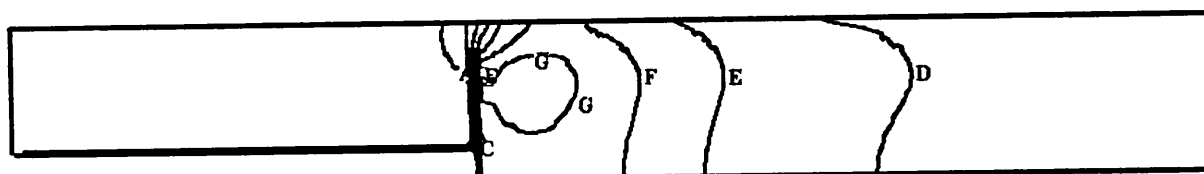
Figure 6.2.13 continued



a) computational grid



b) velocity vectors

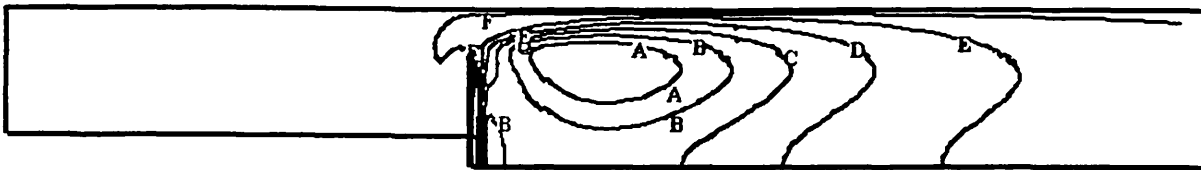


Contour values

A	1.7
B	1.1
C	0.5
D	-0.1
E	-0.7
F	-1.3
G	-2.1

c) normalised pressure ($p/\rho U^2$)

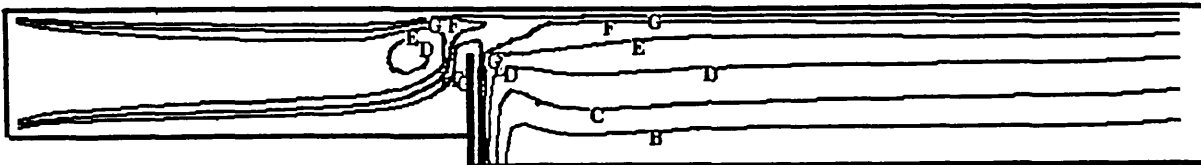
Figure 6.2.14 Details of predictions for turbulent flow of shear-thinning 0.2% CMC solution ($n=0.73$) in pipe with axially-mounted baffle



Contour values

A	0.60
B	0.49
C	0.38
D	0.27
E	0.16
F	0.05

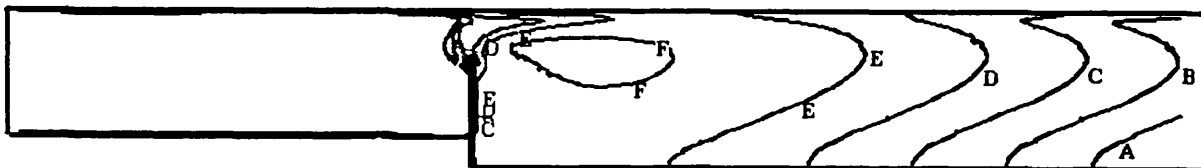
d) normalised turbulence kinetic energy (k/U^2)



Contour values

A	4.70×10^{-3}
B	4.05×10^{-3}
C	3.50×10^{-3}
D	2.85×10^{-3}
E	2.20×10^{-3}
F	1.55×10^{-3}
G	0.90×10^{-3}

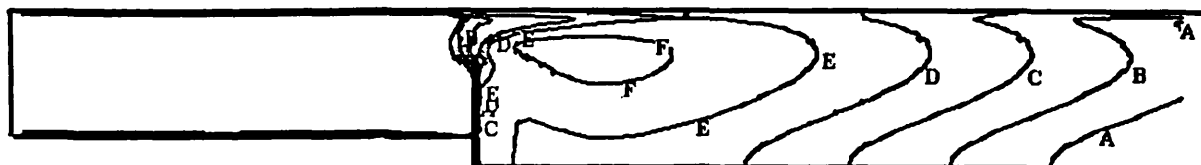
e) normalised length scales of turbulence ($C_\mu^{3/4} k^{3/2} / \epsilon D$)



Contour values (s)

A	14.4×10^{-5}
B	12.0×10^{-5}
C	9.6×10^{-5}
D	7.2×10^{-5}
E	4.8×10^{-5}
F	2.4×10^{-5}

f) Kolmogorov time scales

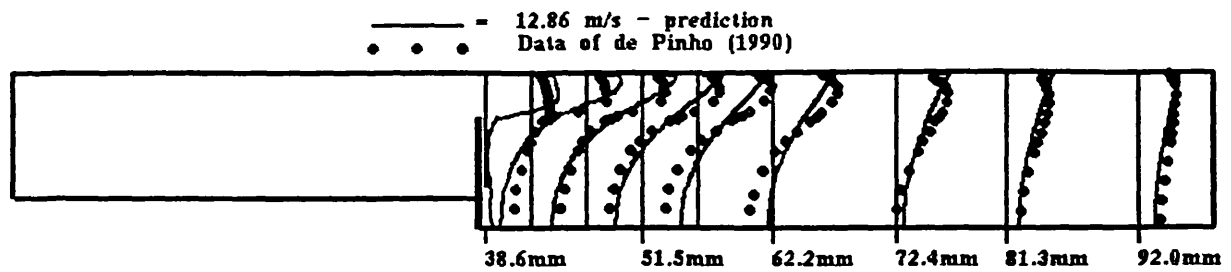


Contour values (m)

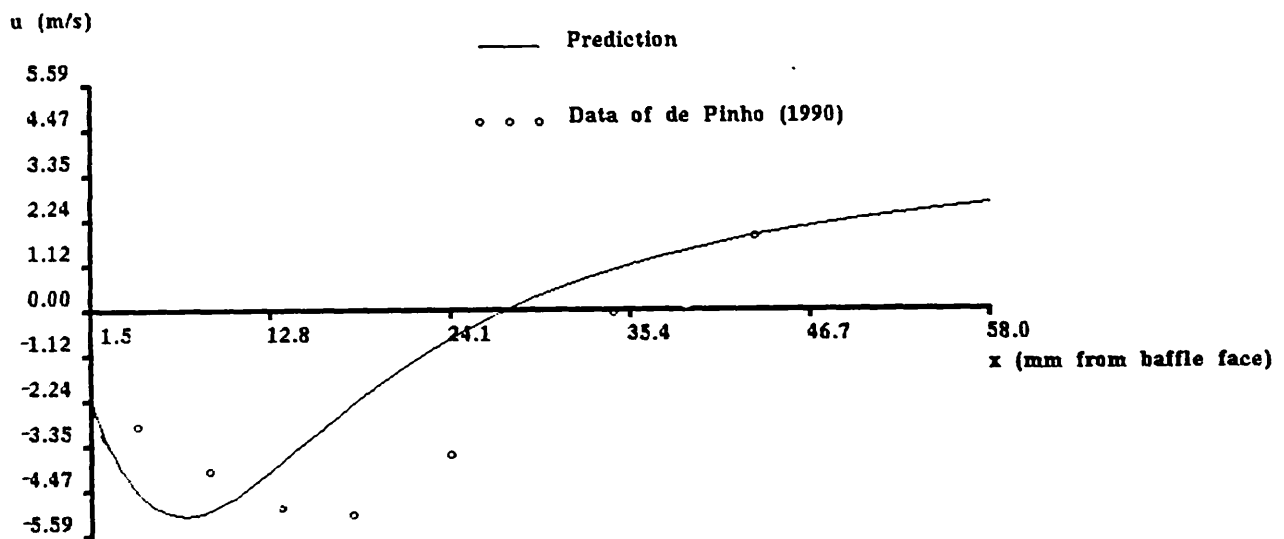
A	2.65×10^{-5}
B	2.30×10^{-5}
C	1.95×10^{-5}
D	1.60×10^{-5}
E	1.25×10^{-5}
F	0.90×10^{-5}

g) Kolmogorov length scales

Figure 6.2.14 continued

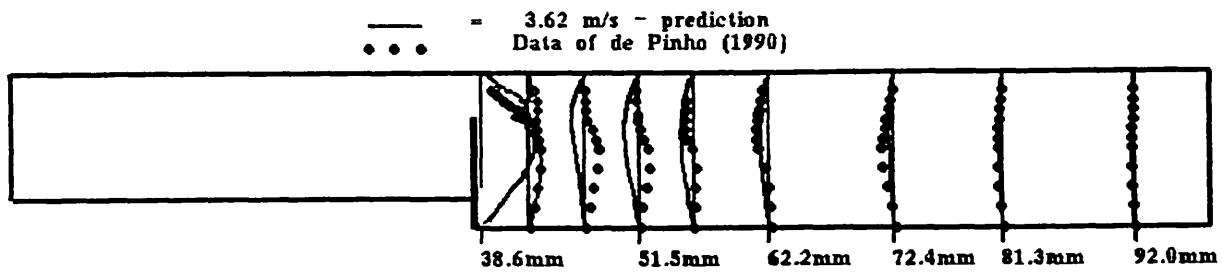


a) mean axial velocity

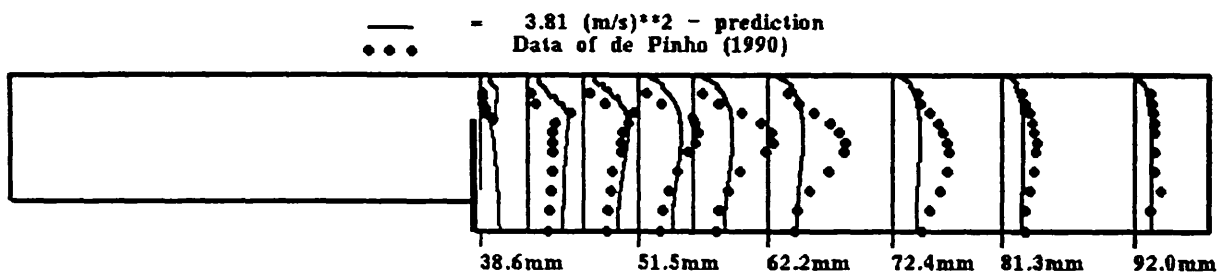


b) mean axial velocity on centreline

Figure 6.2.15 Comparison of prediction with experimental data of de Pinho (1990), turbulent flow of shear-thinning 0.2% CMC solution ($n=0.73$) in pipe with axially-mounted baffle



c) mean radial velocity



d) turbulence kinetic energy

Figure 6.2.15 continued

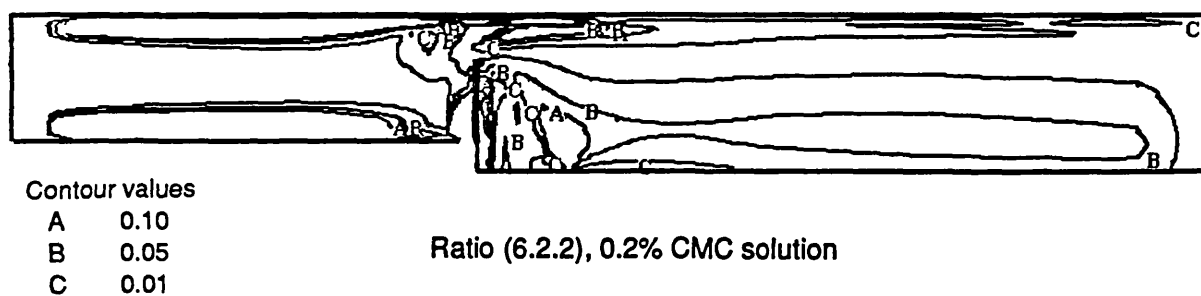
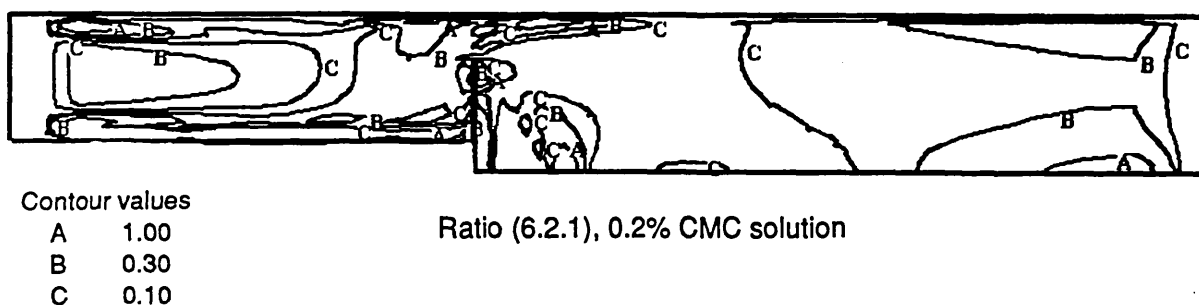
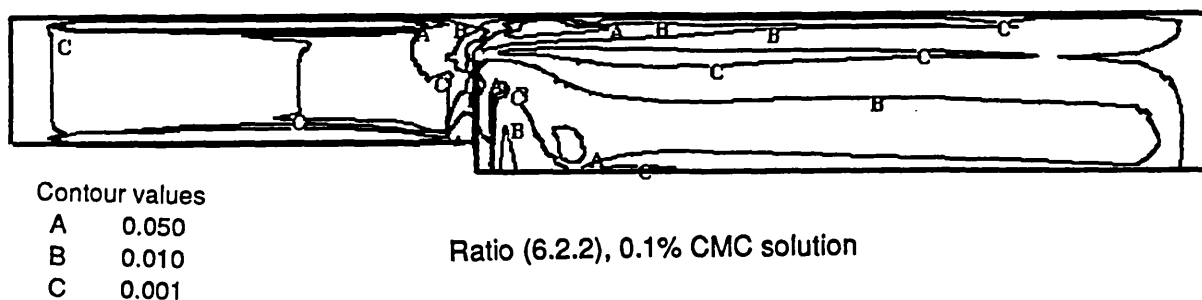
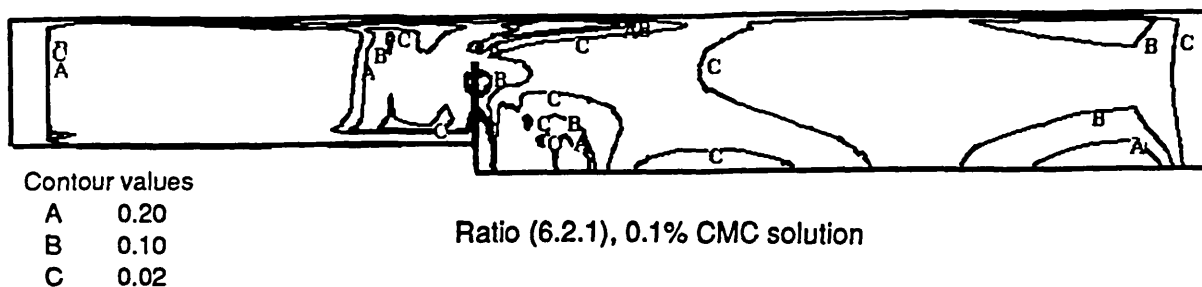


Figure 6.2.16 Relative magnitude of extra ϵ -equation source terms, CMC solutions in pipe with axially-mounted baffle

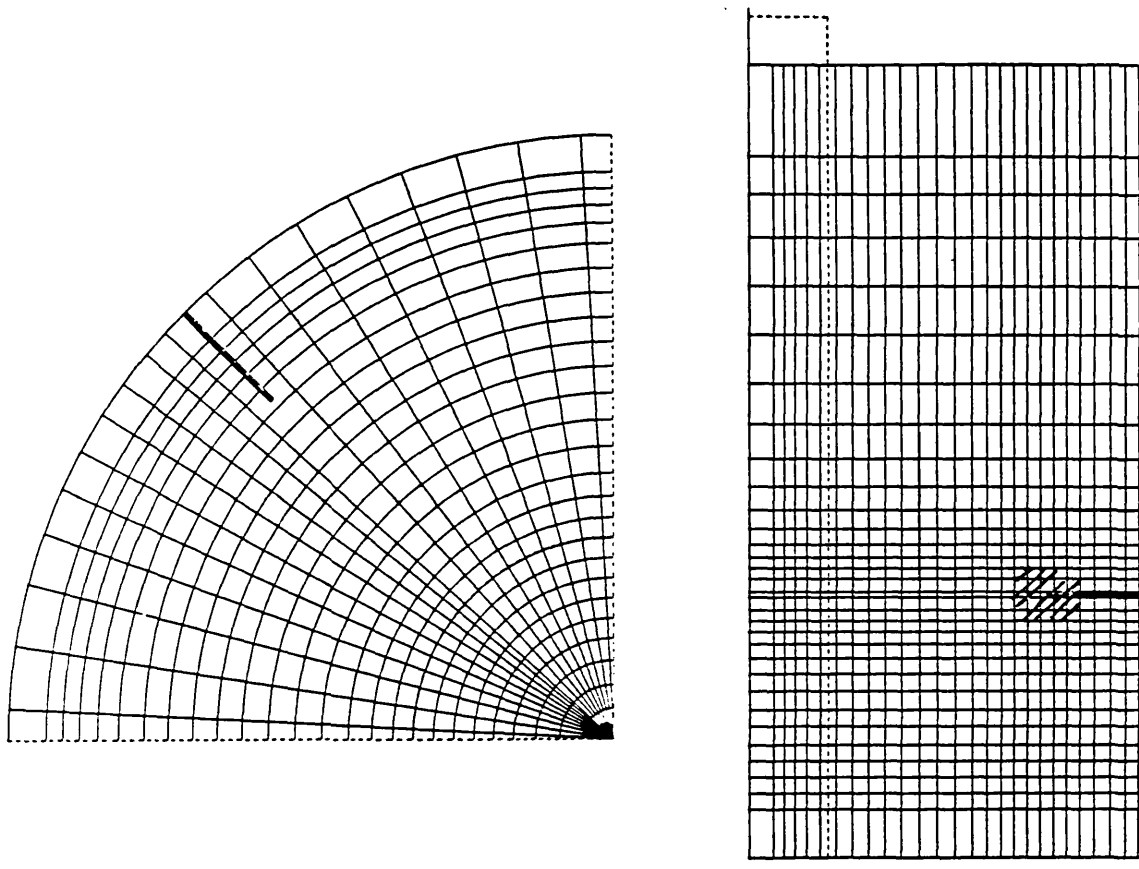


Figure 6.3.1 Computational grid, CMC solution in mixing vessel (15,314 cells)

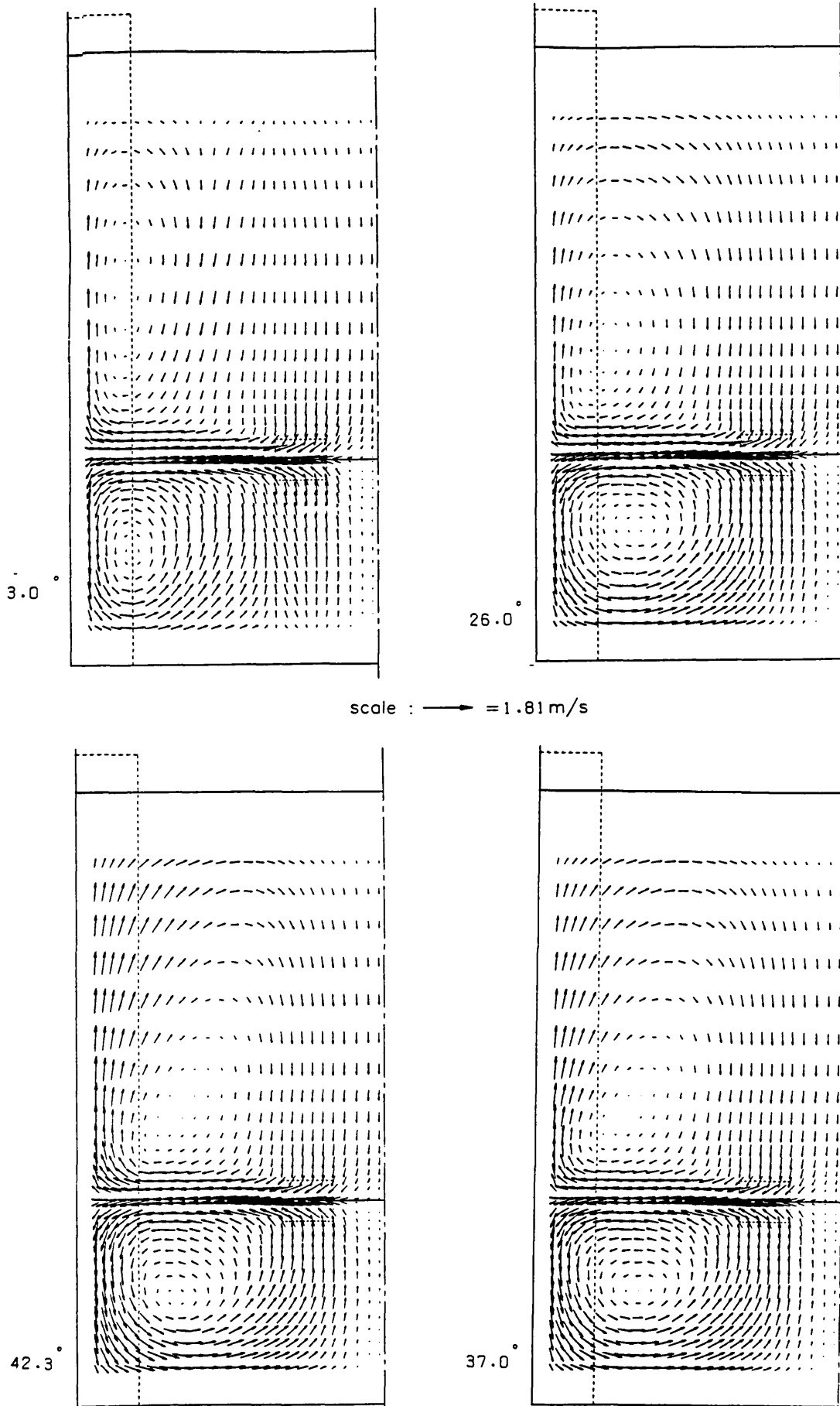


Figure 6.3.2 Velocity vectors in $x-r$ planes, CMC solution in mixing vessel

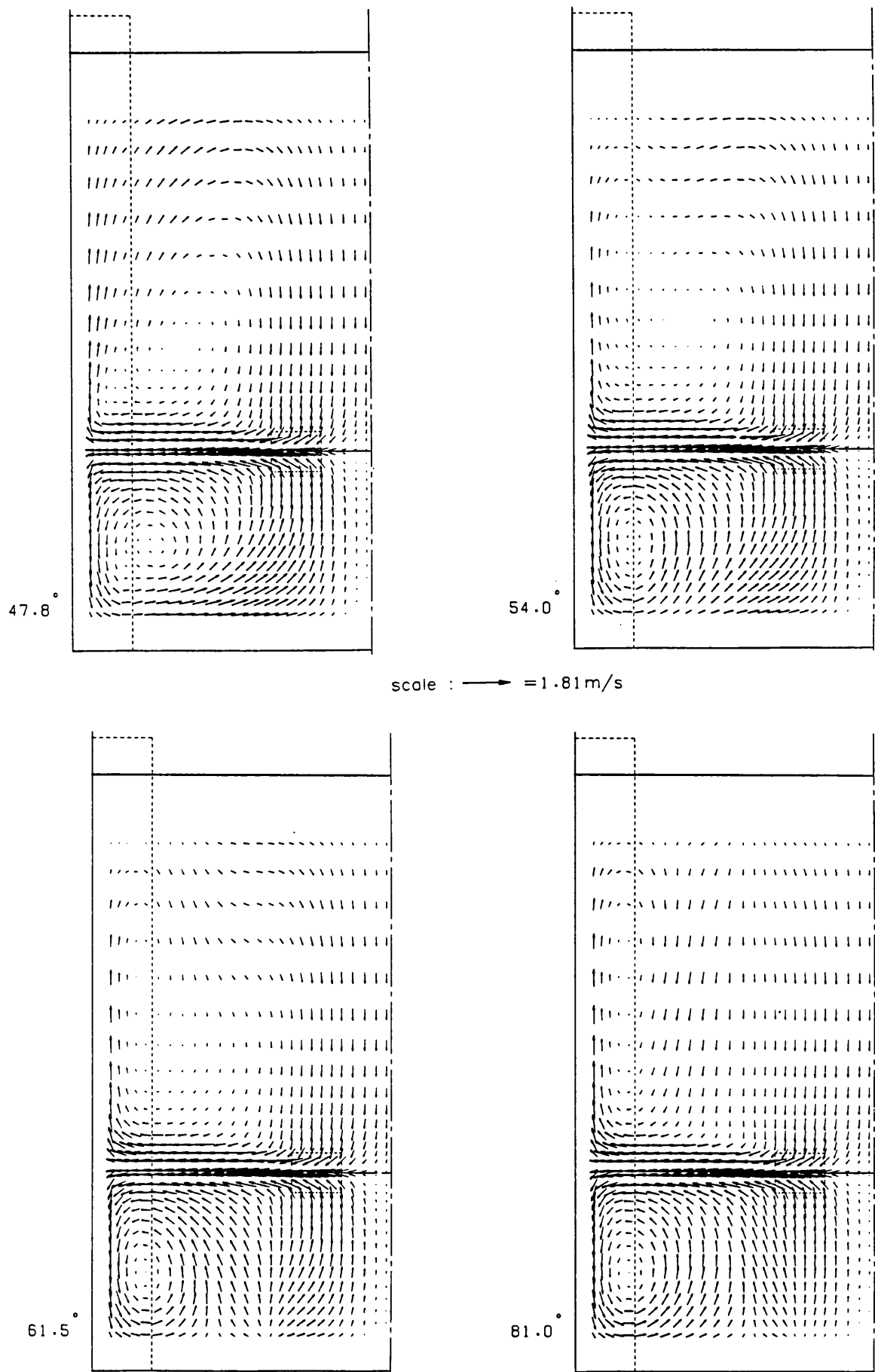


Figure 6.3.2 Velocity vectors in $x - r$ planes, CMC solution in mixing vessel

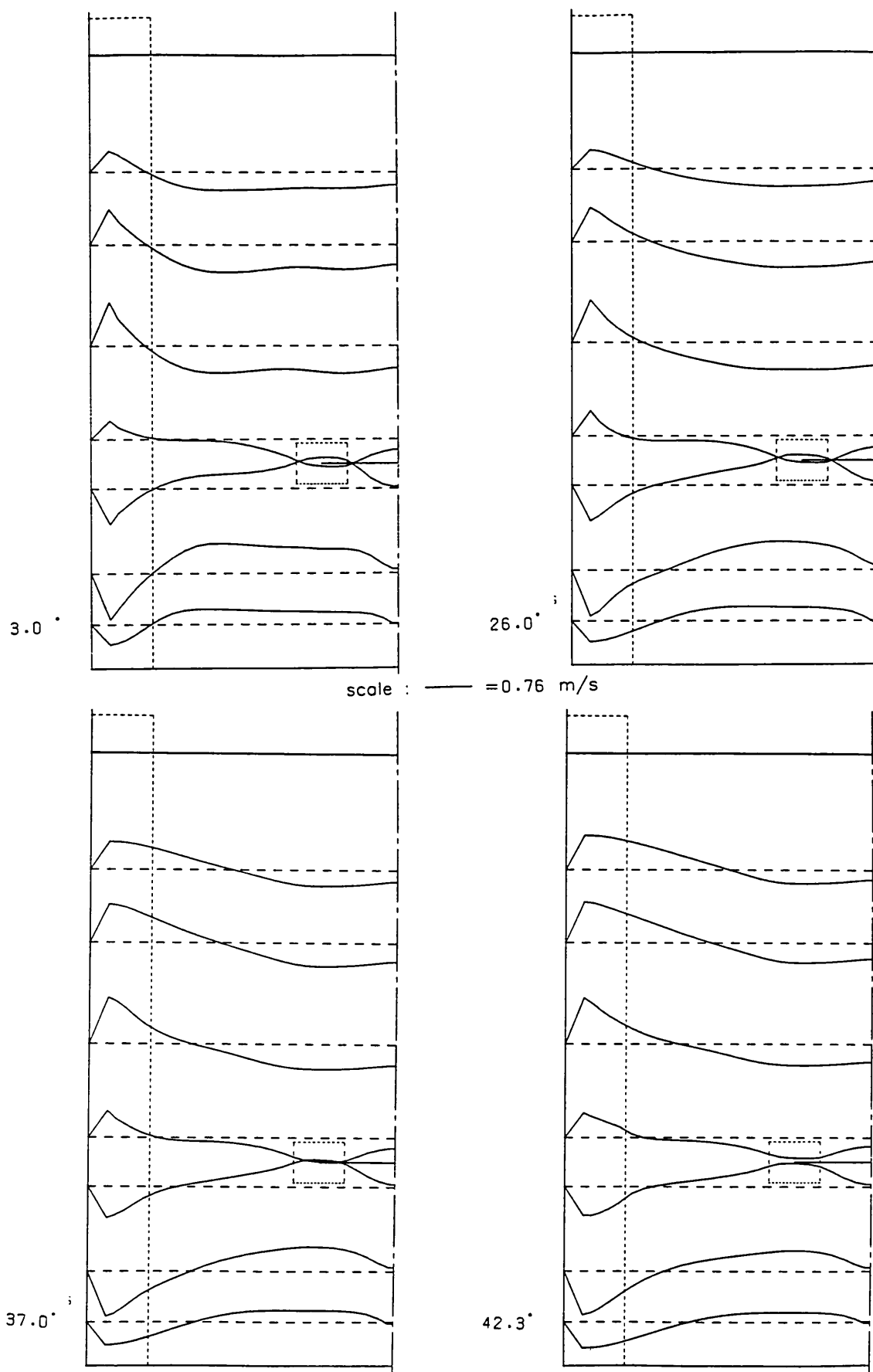


Figure 6.3.3 Axial velocity profiles in $x-r$ planes, CMC solution in mixing vessel

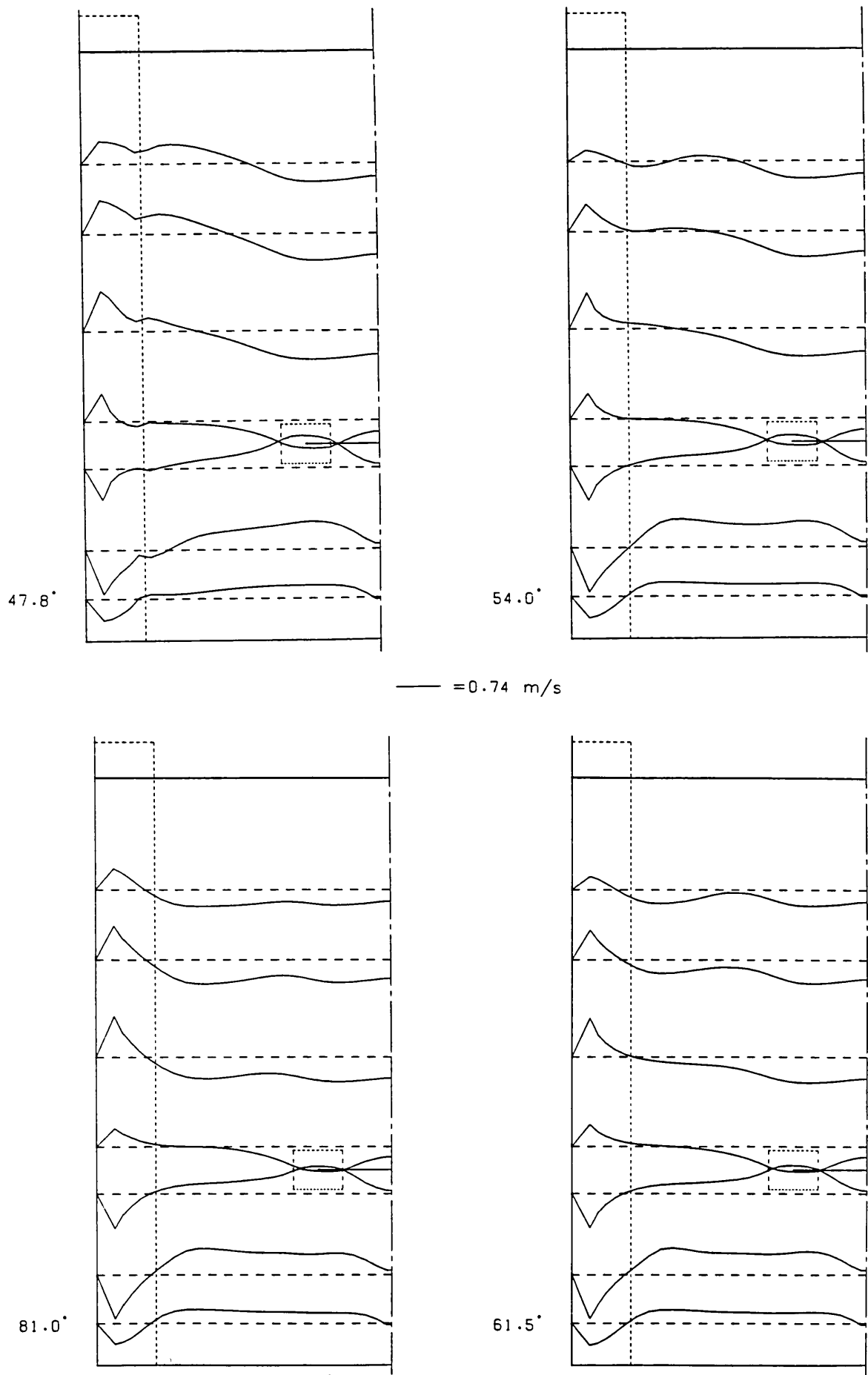


Figure 6.3.3 Axial velocity profiles in $x-r$ planes, CMC solution in mixing vessel

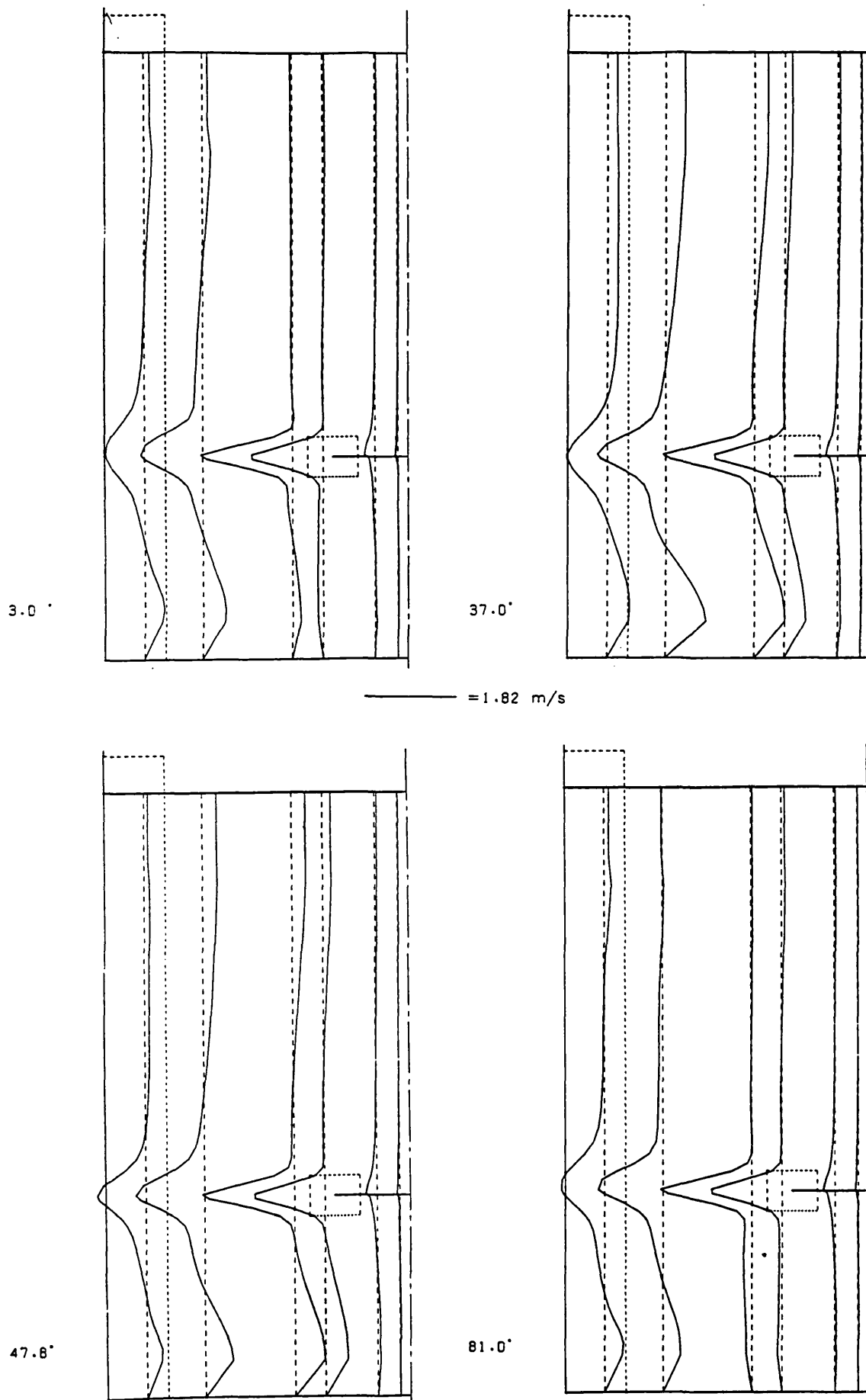


Figure 6.3.4 Radial velocity profiles in $x-r$ planes, CMC solution in mixing vessel

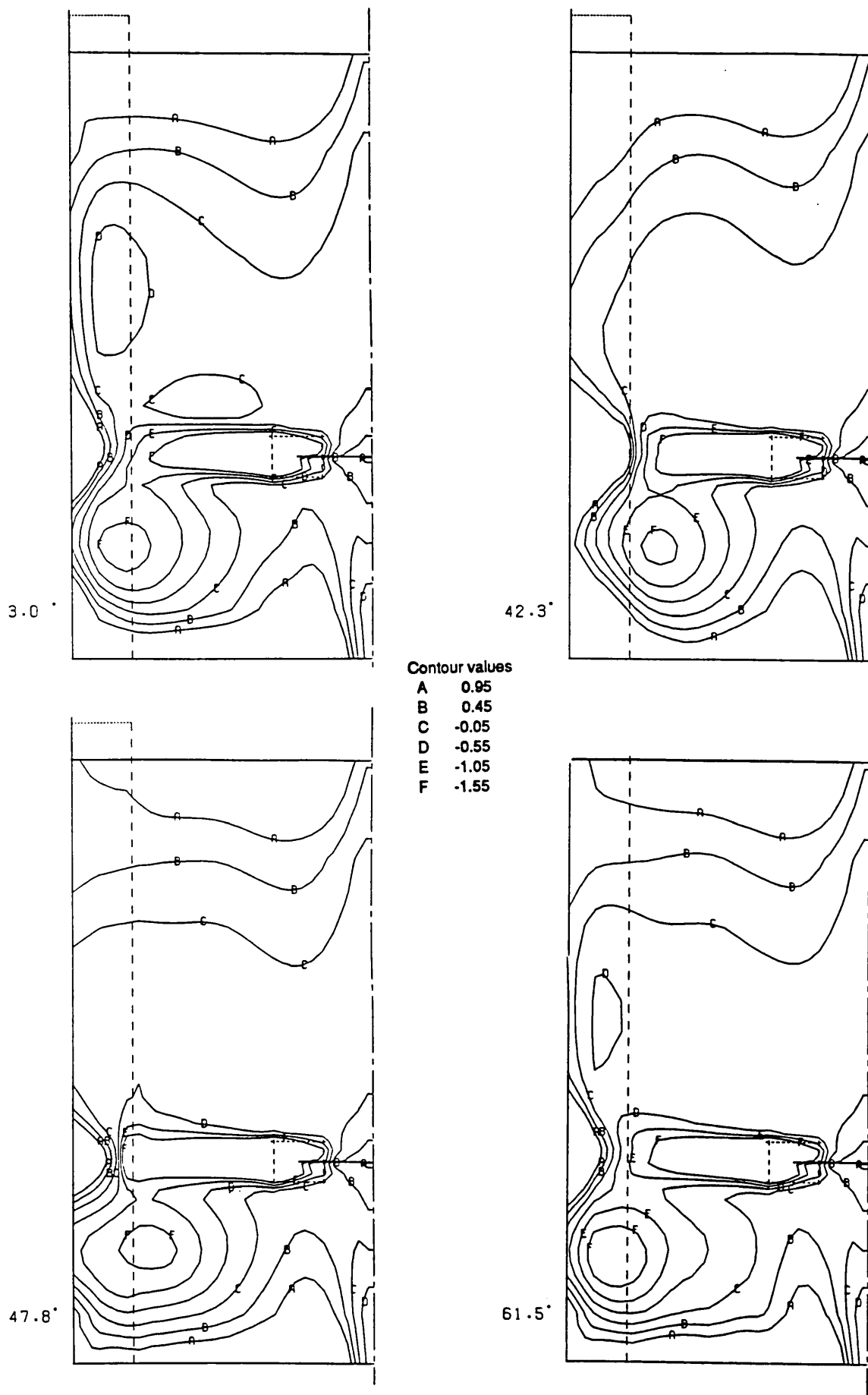


Figure 6.3.5 Normalised pressure in $x - r$ planes, CMC solution in mixing vessel

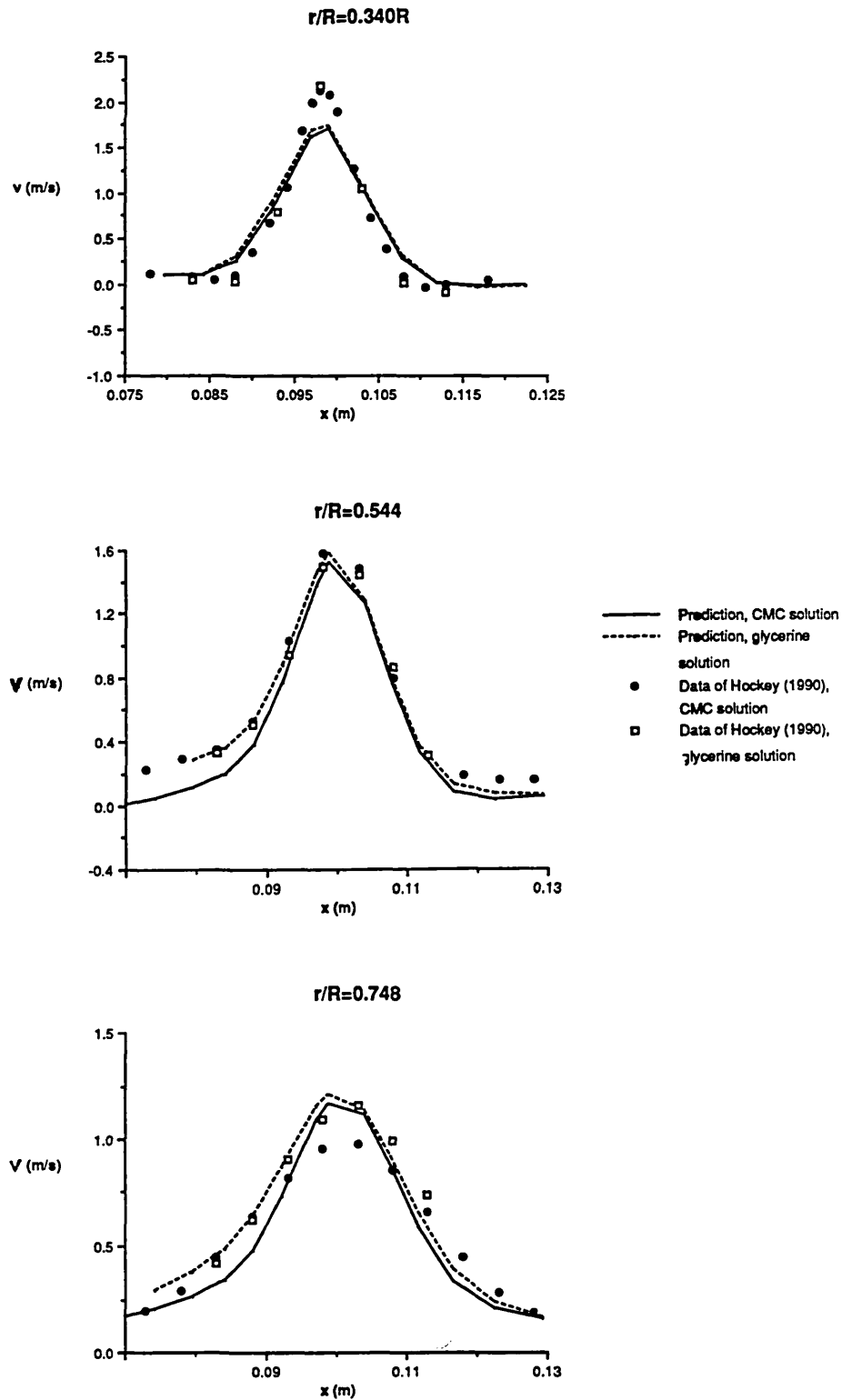


Figure 6.3.6 Impeller-jet radial velocity comparisons, 0° plane, CMC and glycerine solutions in mixing vessel

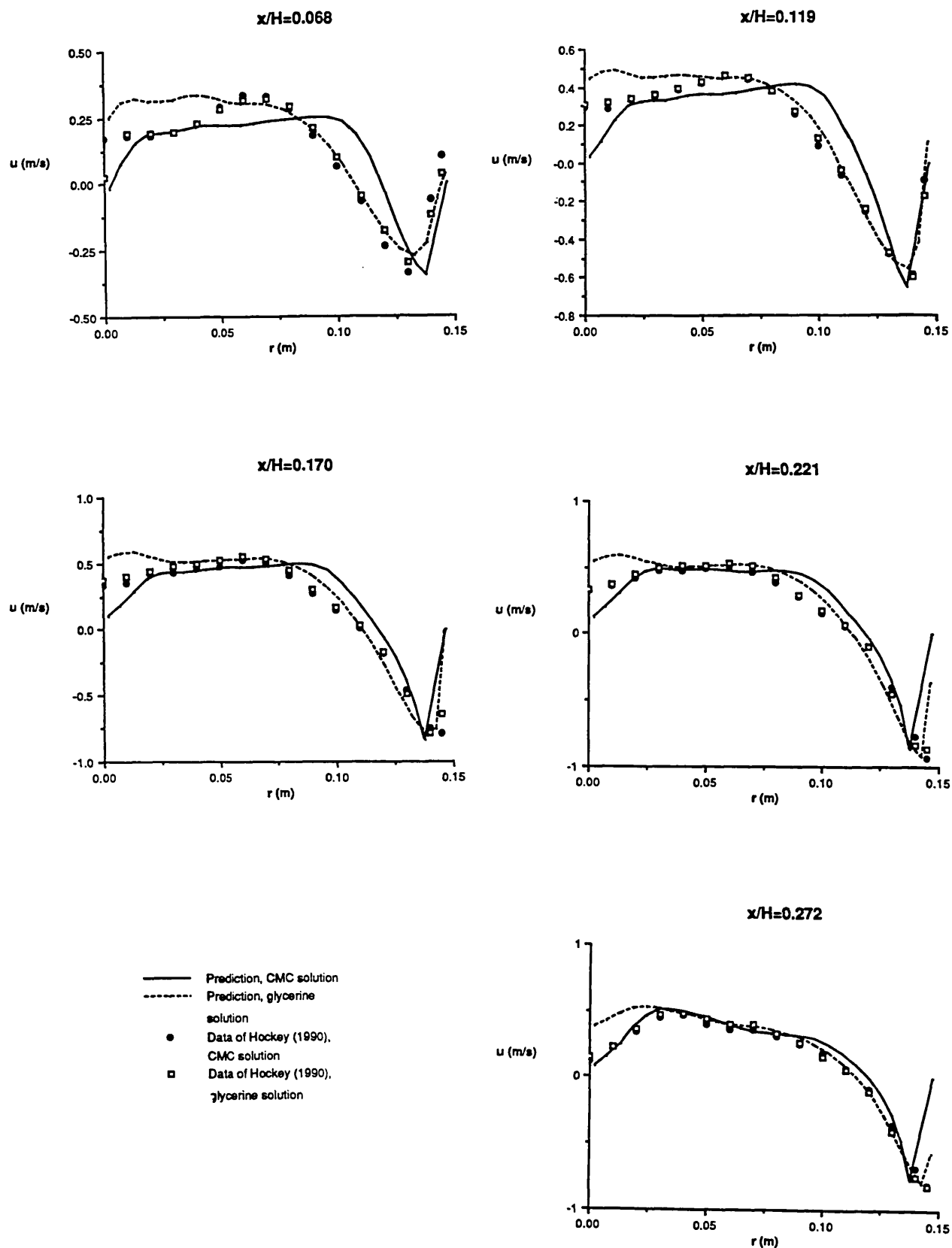


Figure 6.3.7 Below-impeller axial velocity comparisons, 0° plane, CMC and glycerine solutions in mixing vessel

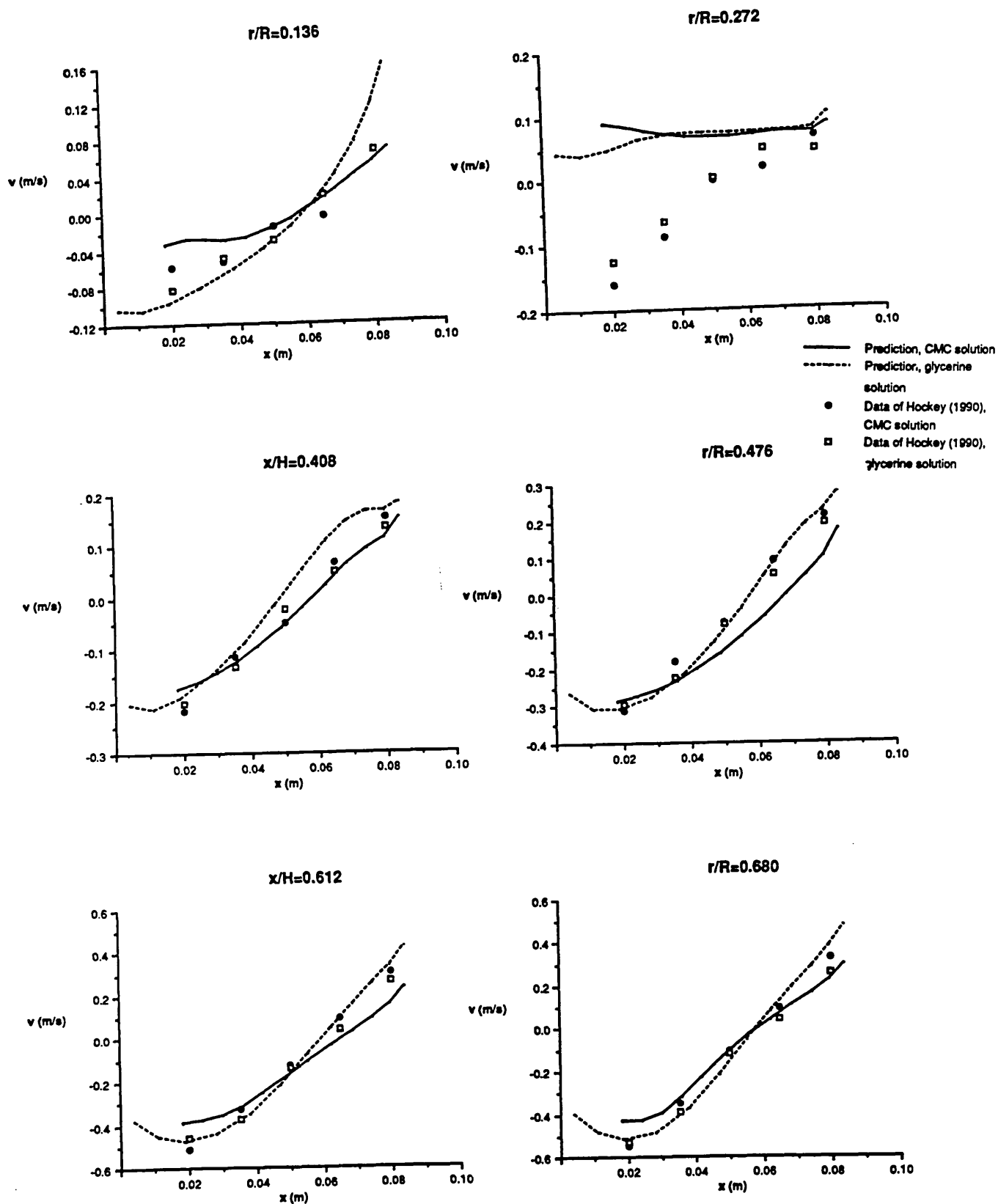


Figure 6.3.8 Below-impeller radial velocity comparisons, 0° plane, CMC and glycerine solutions in mixing vessel

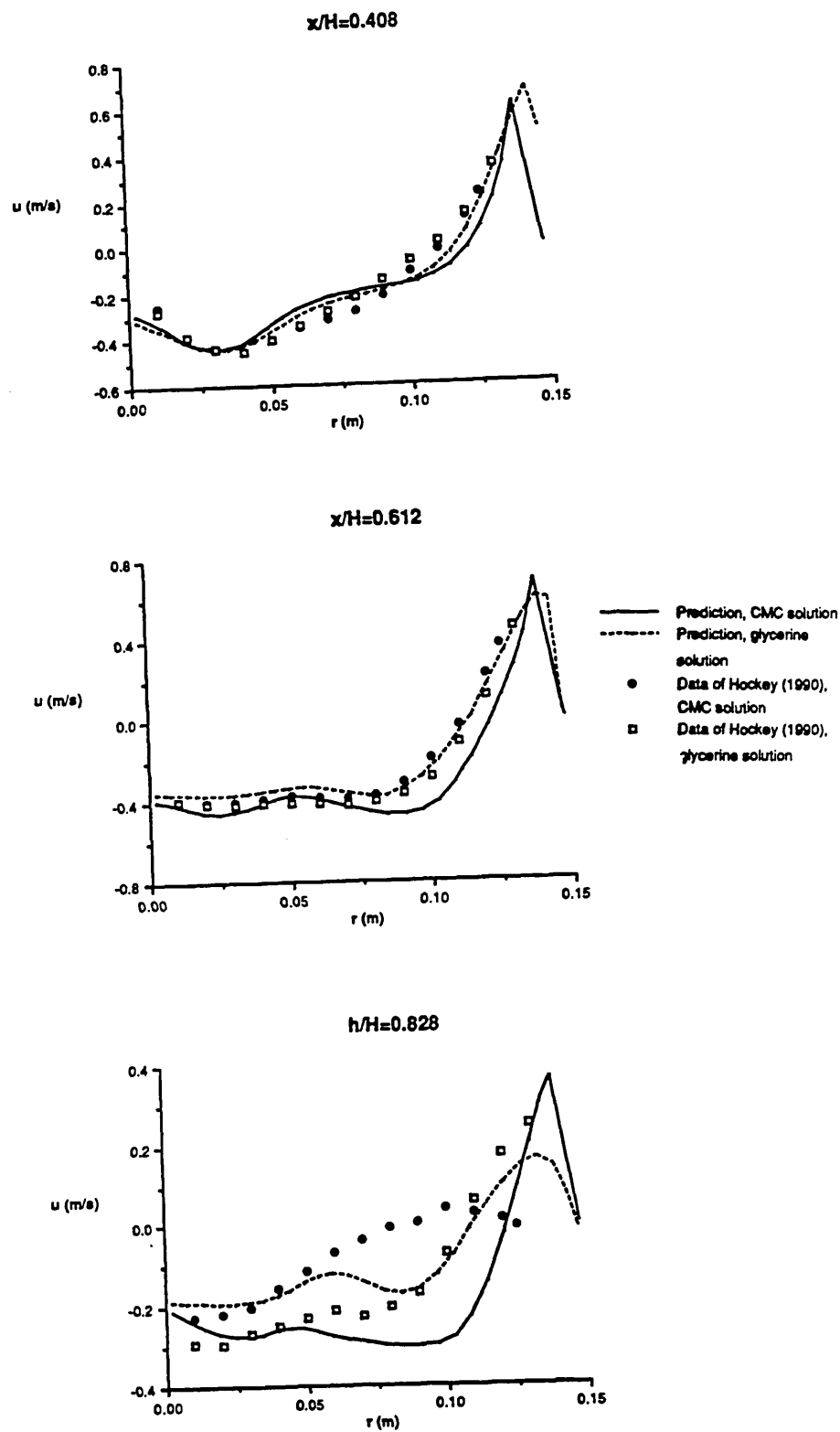


Figure 6.3.9 Above-impeller axial velocity comparisons, 0° plane, CMC and glycerine solutions in mixing vessel

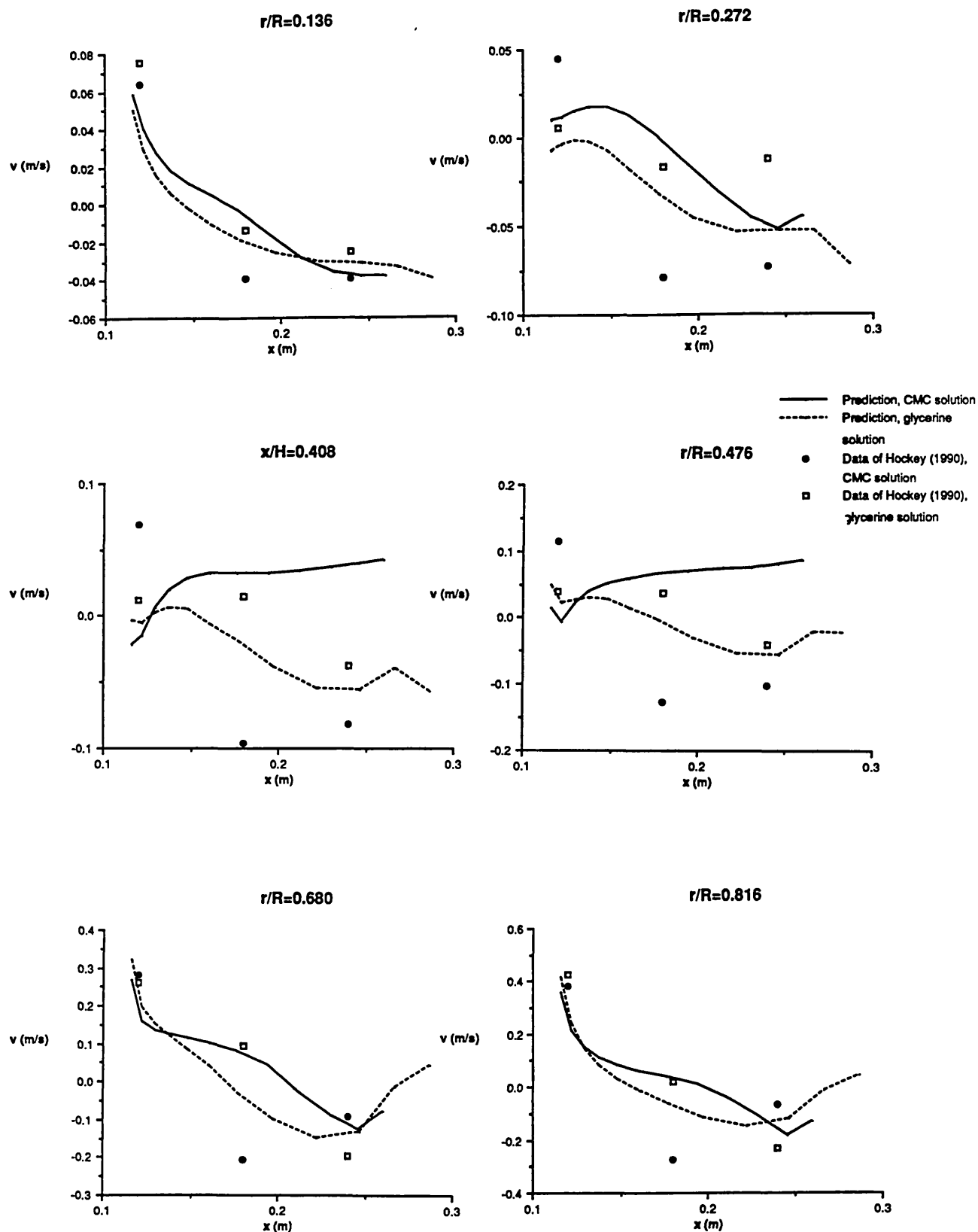
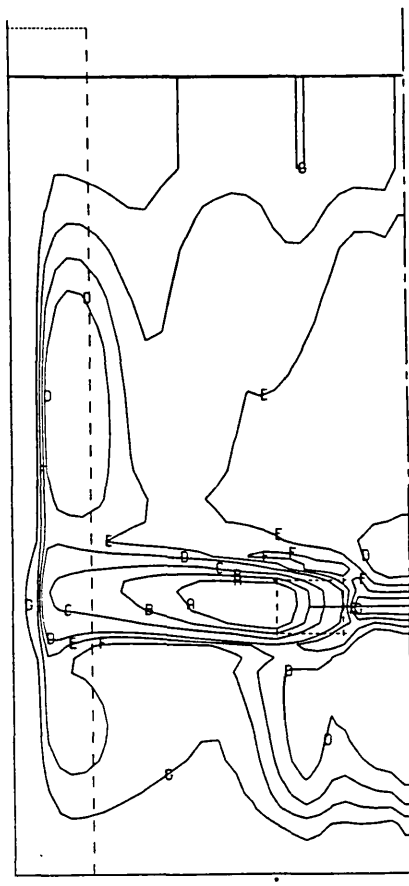
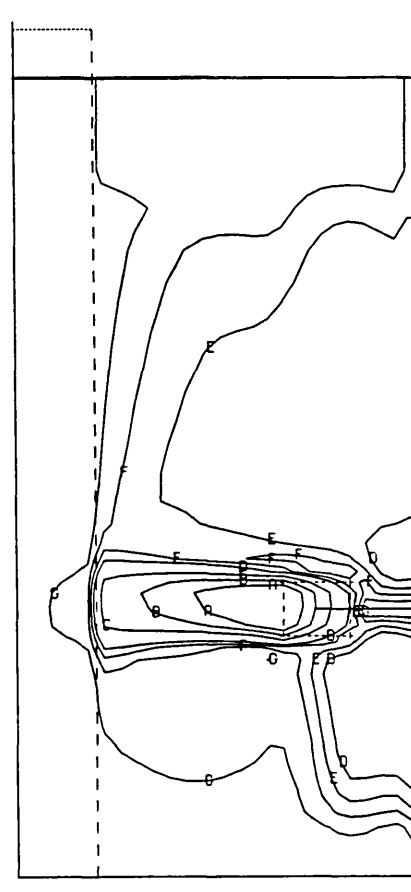


Figure 6.3.10 Above-impeller radial velocity comparisons, 0° plane, CMC and glycerine solutions in mixing vessel

3.0°



42.3°



Contour Values

A : 1300.

B : 1000.0

C : 700.0

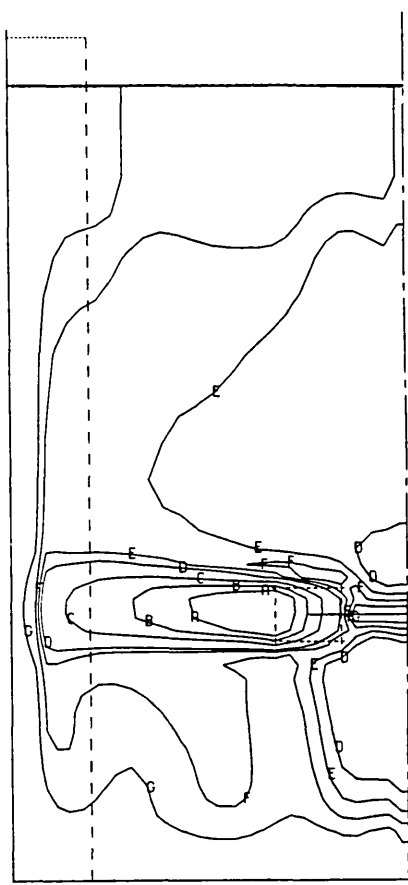
D : 400.0

E : 300.0

F : 200.0

G : 100.0

54.0°



65.5°

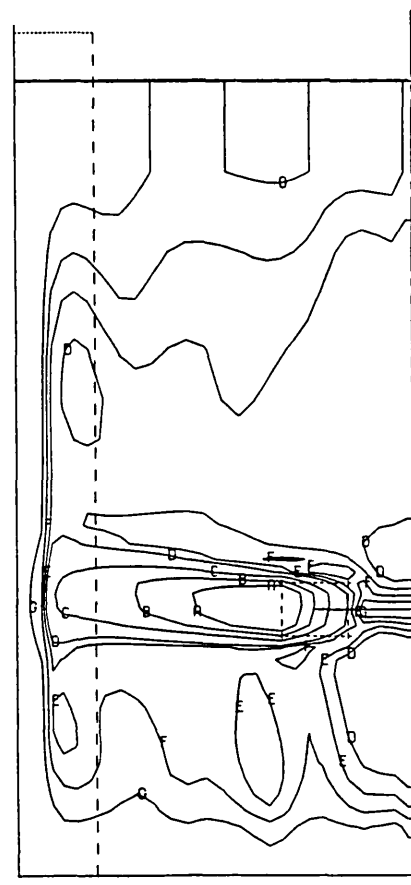


Figure 6.3.11 Local Reynolds number of turbulence in $x - r$ planes,
CMC solution in mixing vessel

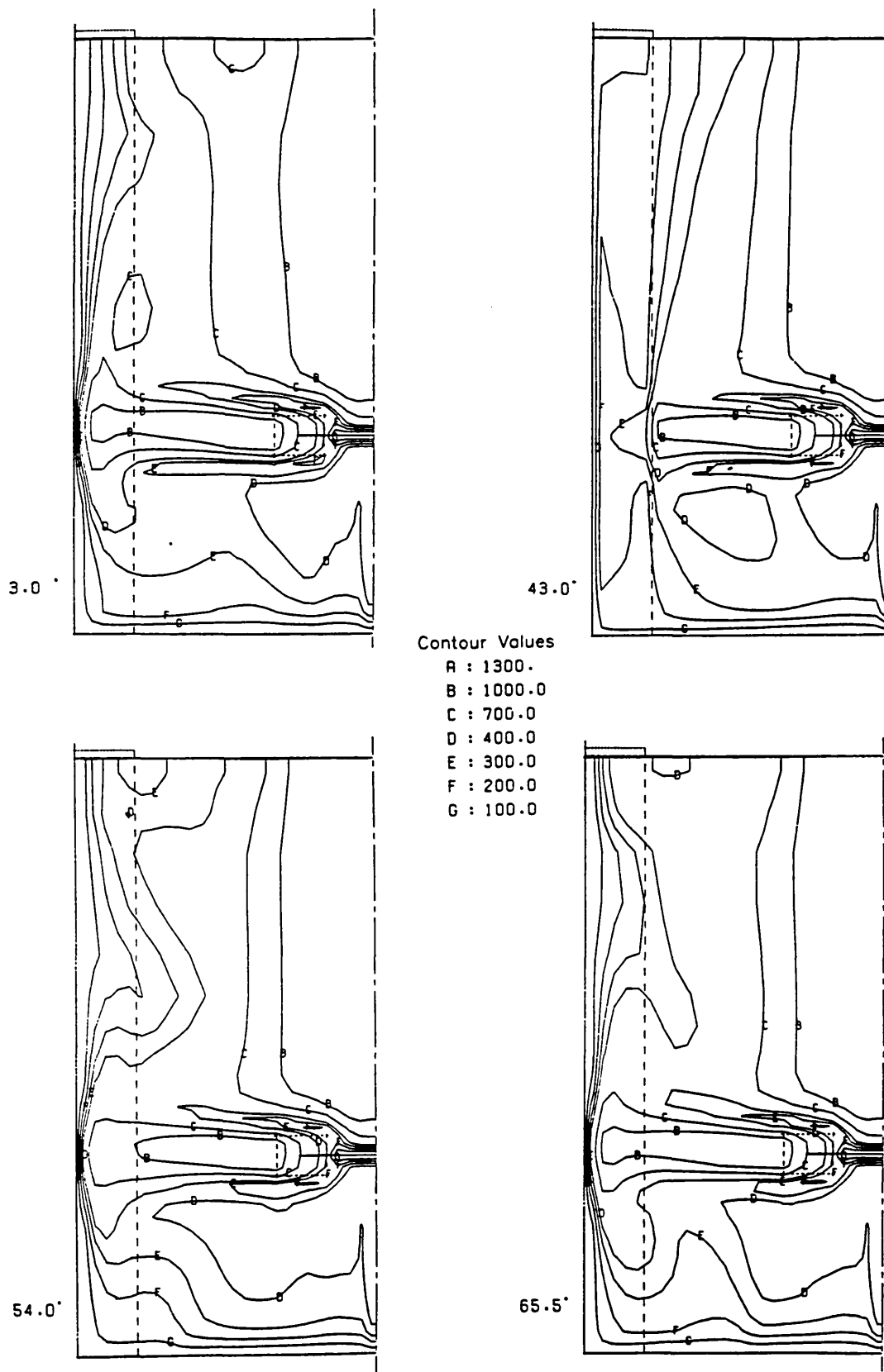


Figure 6.3.12 Local Reynolds number of turbulence in $x - r$ planes, glycerine solution in mixing vessel

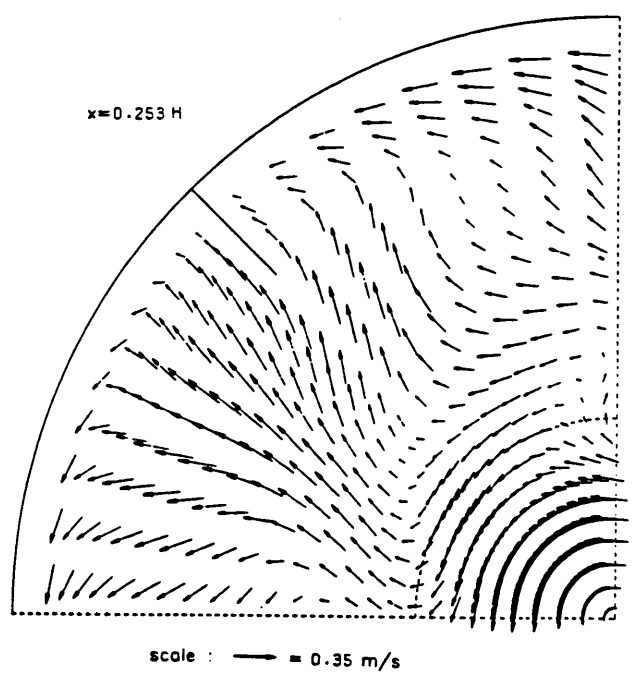
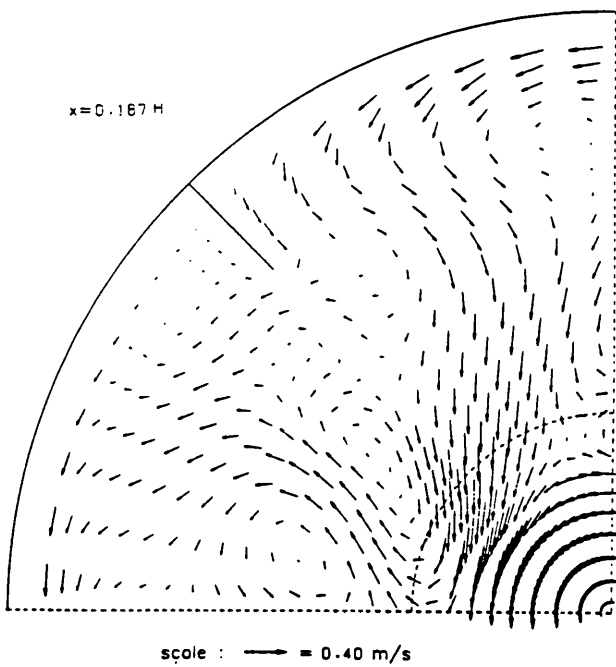
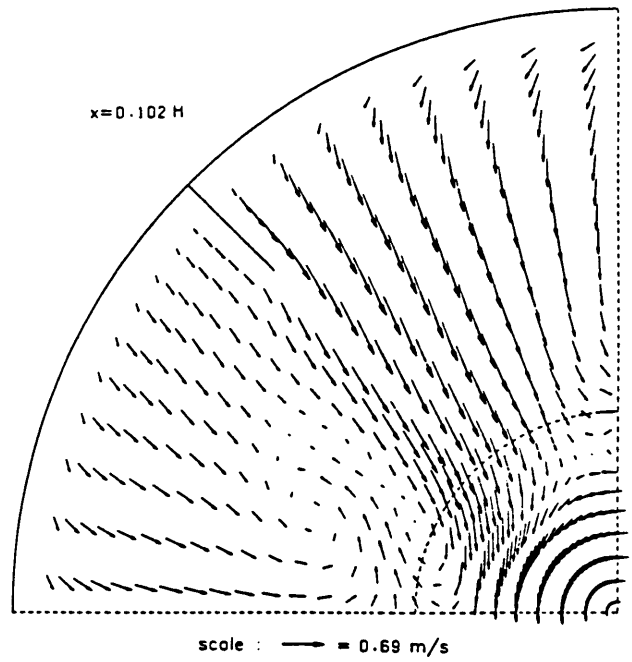
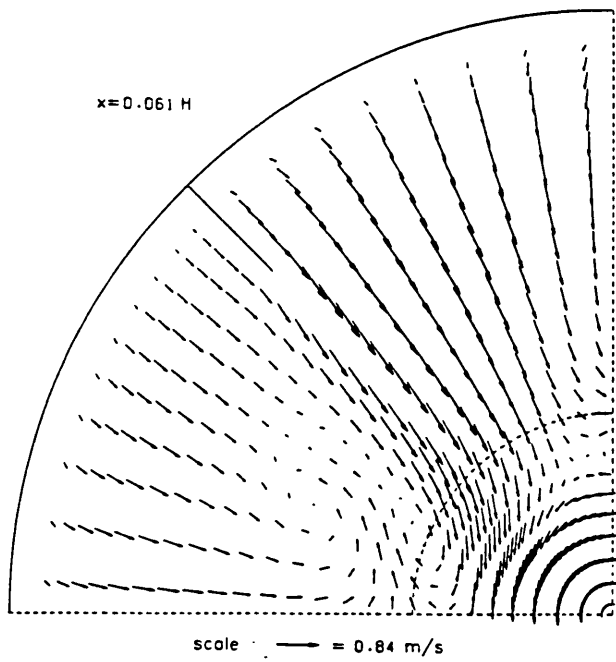


Figure 6.3.13 Velocity vectors in $r - \theta$ planes, CMC solution in mixing vessel

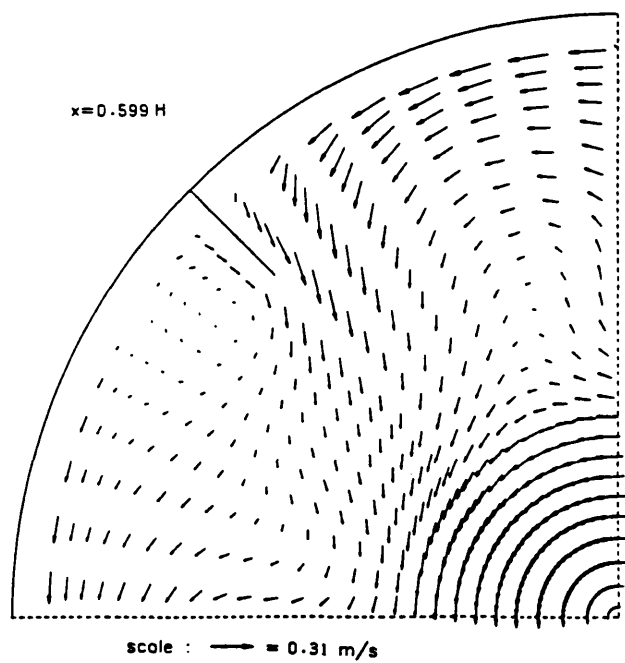
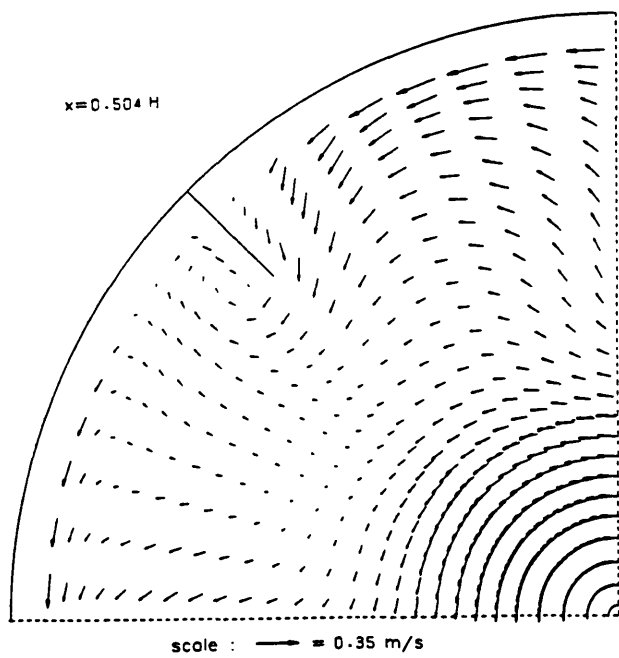
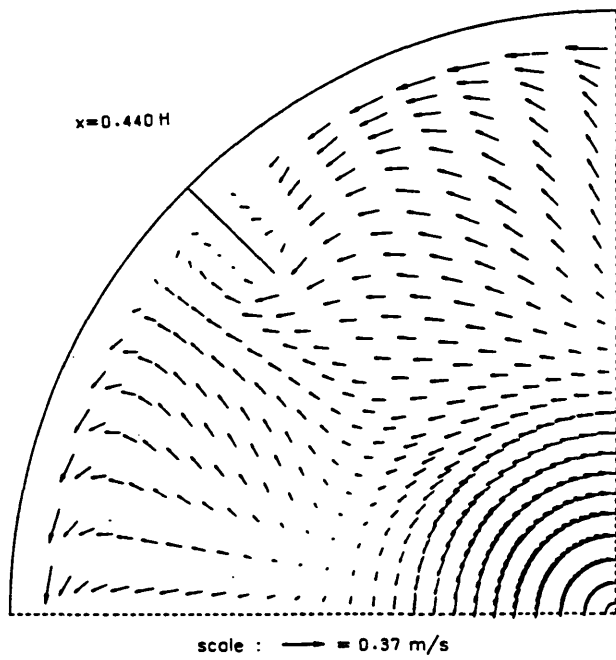
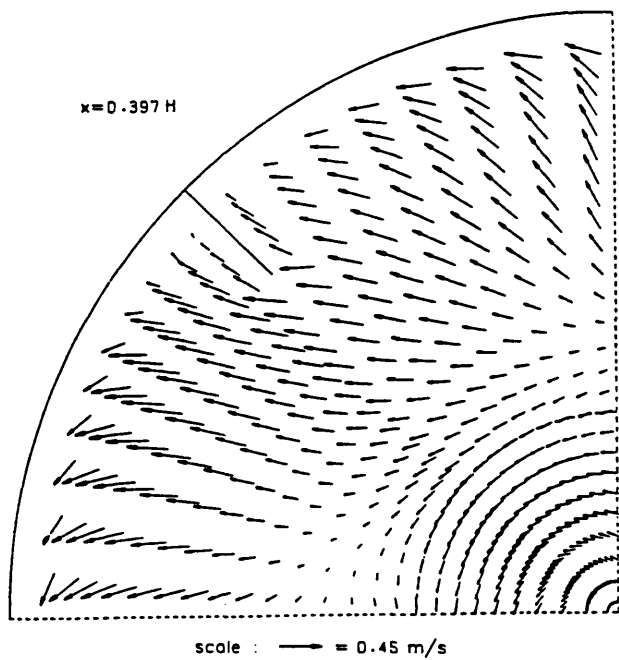
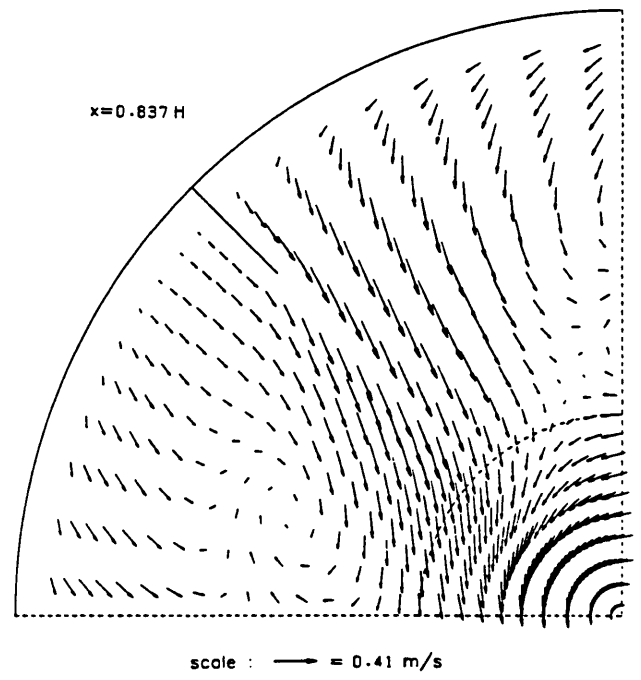
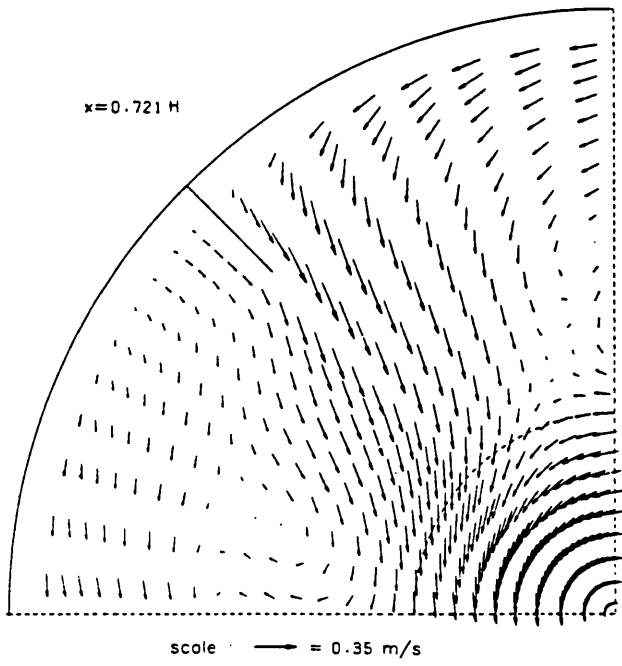


Figure 6.3.13 Velocity vectors in $r - \theta$ planes, CMC solution in mixing vessel



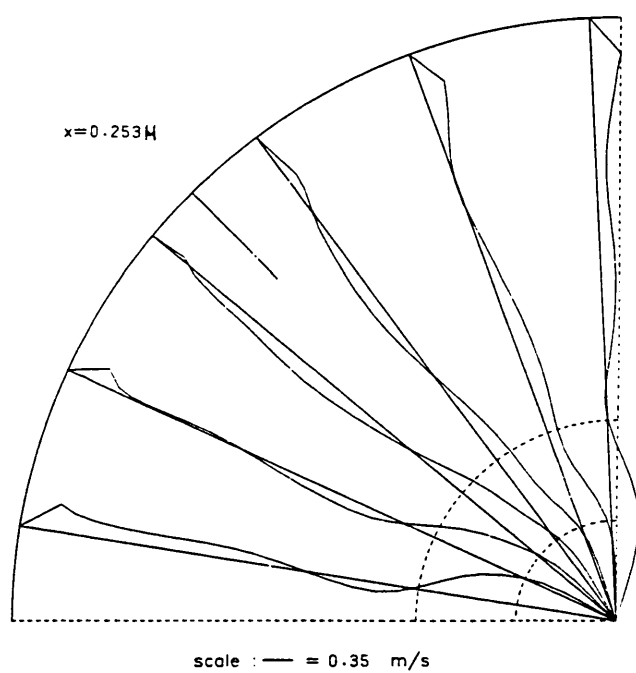
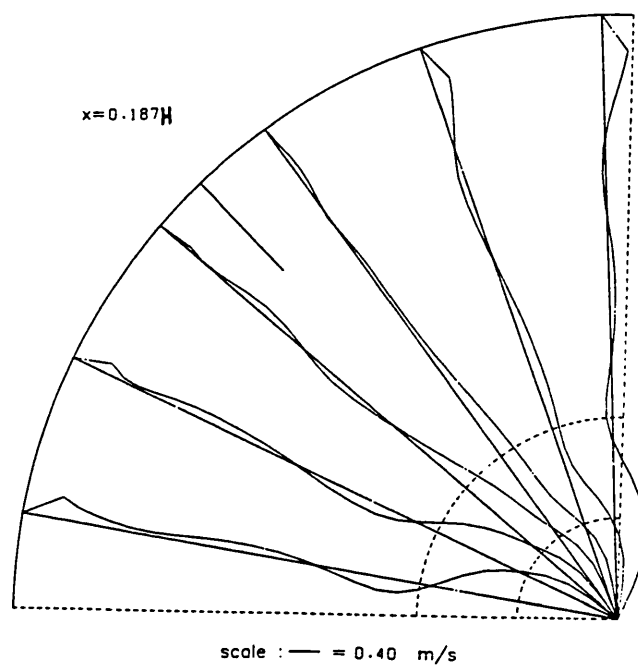
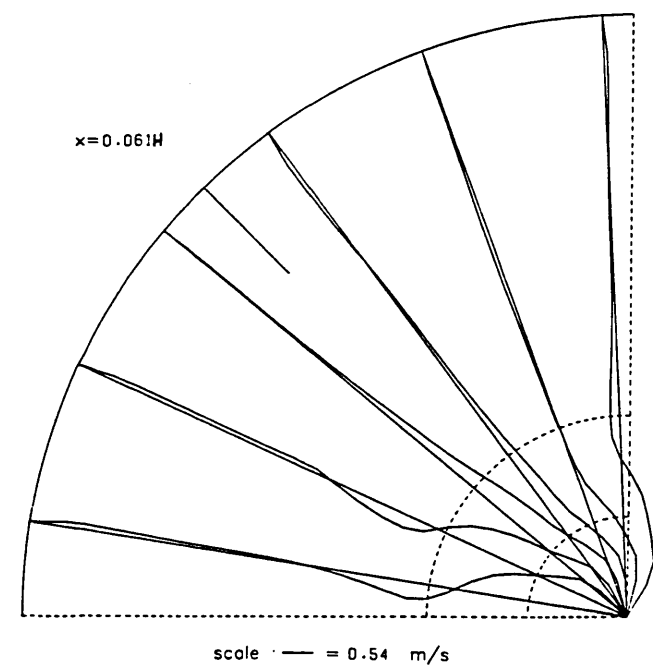
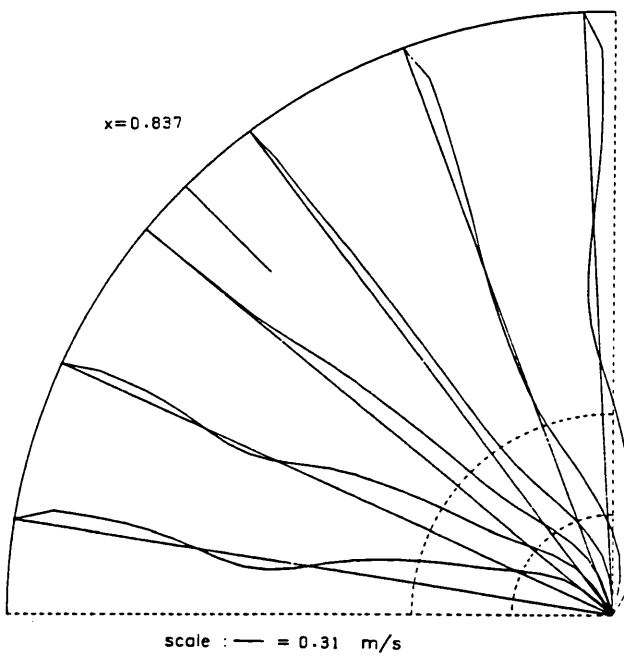
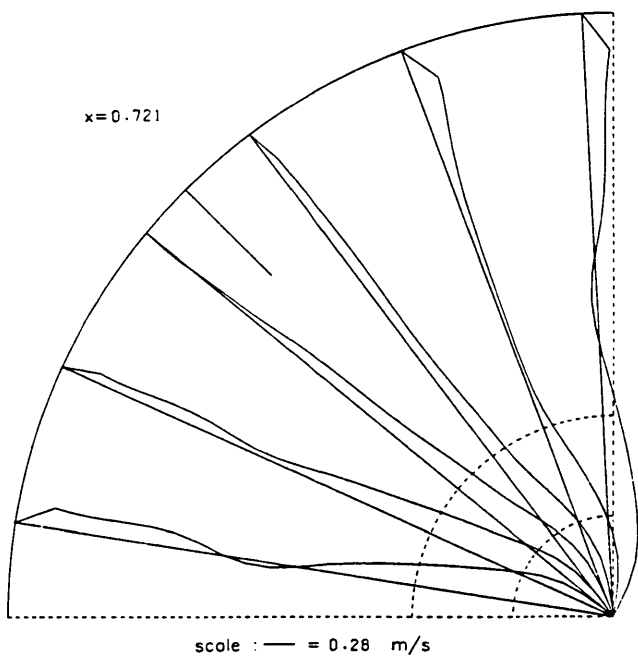
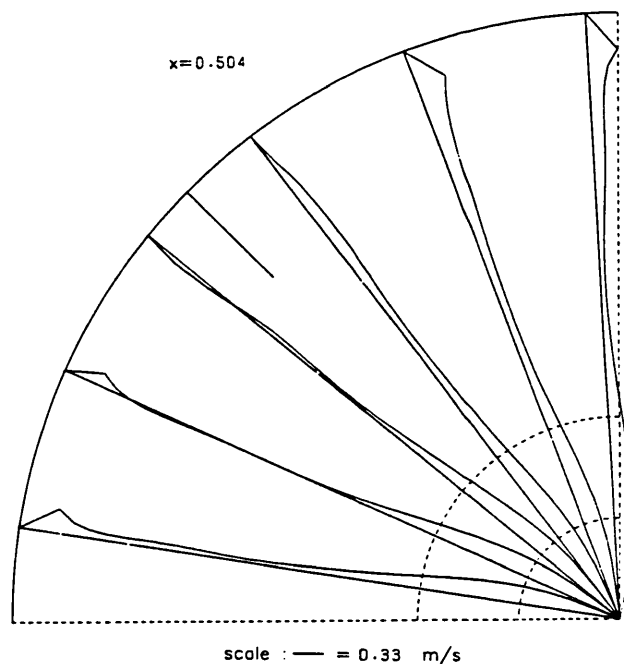
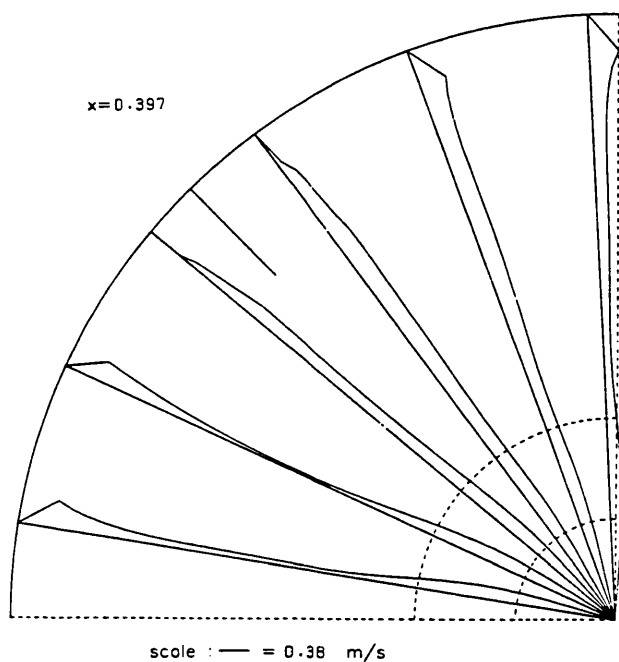


Figure 6.3.14 Swirl velocity profiles in $r - \theta$ planes, CMC solution in mixing vessel



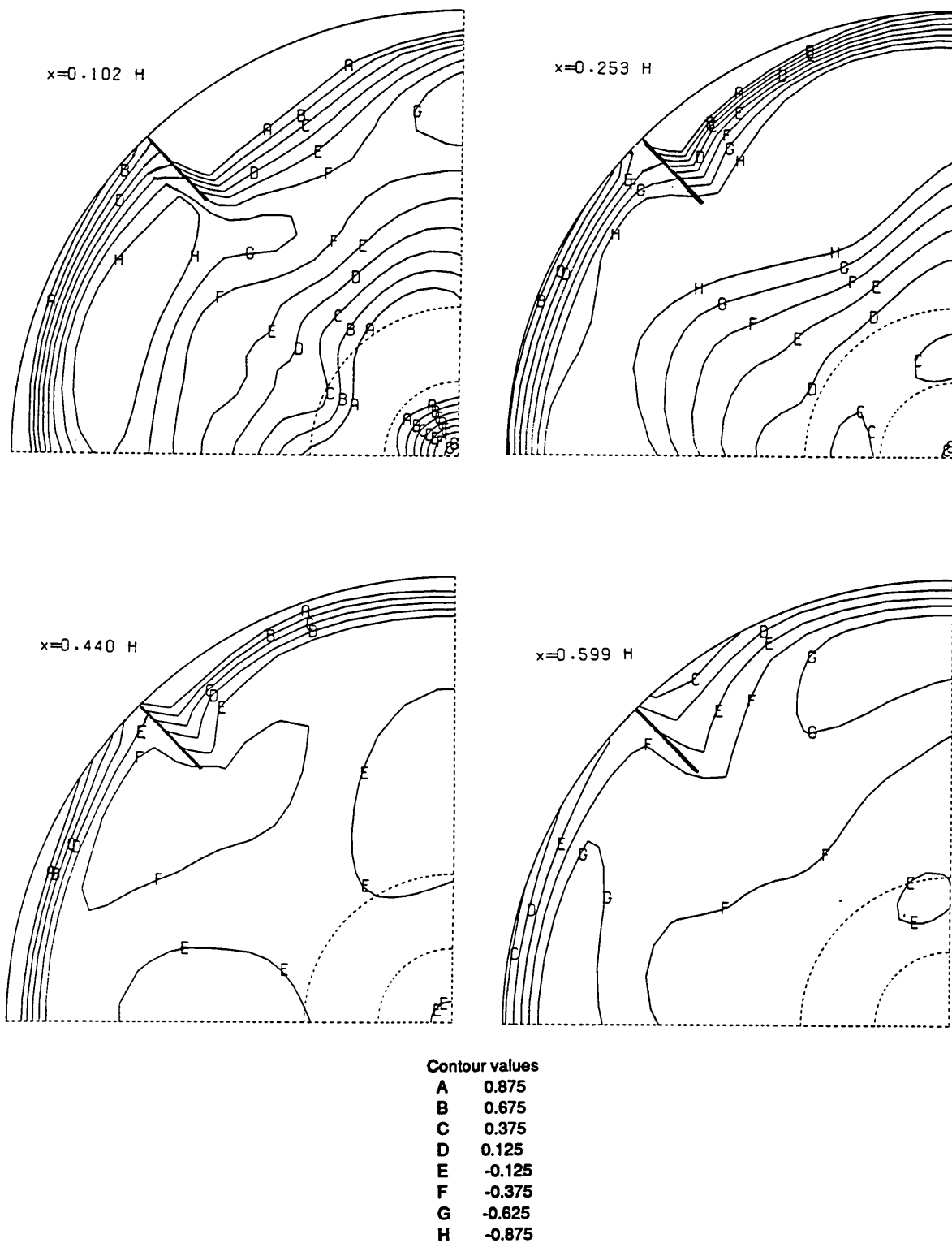


Figure 6.3.15 Normalised pressure in $r - \theta$ planes, CMC solution in mixing vessel

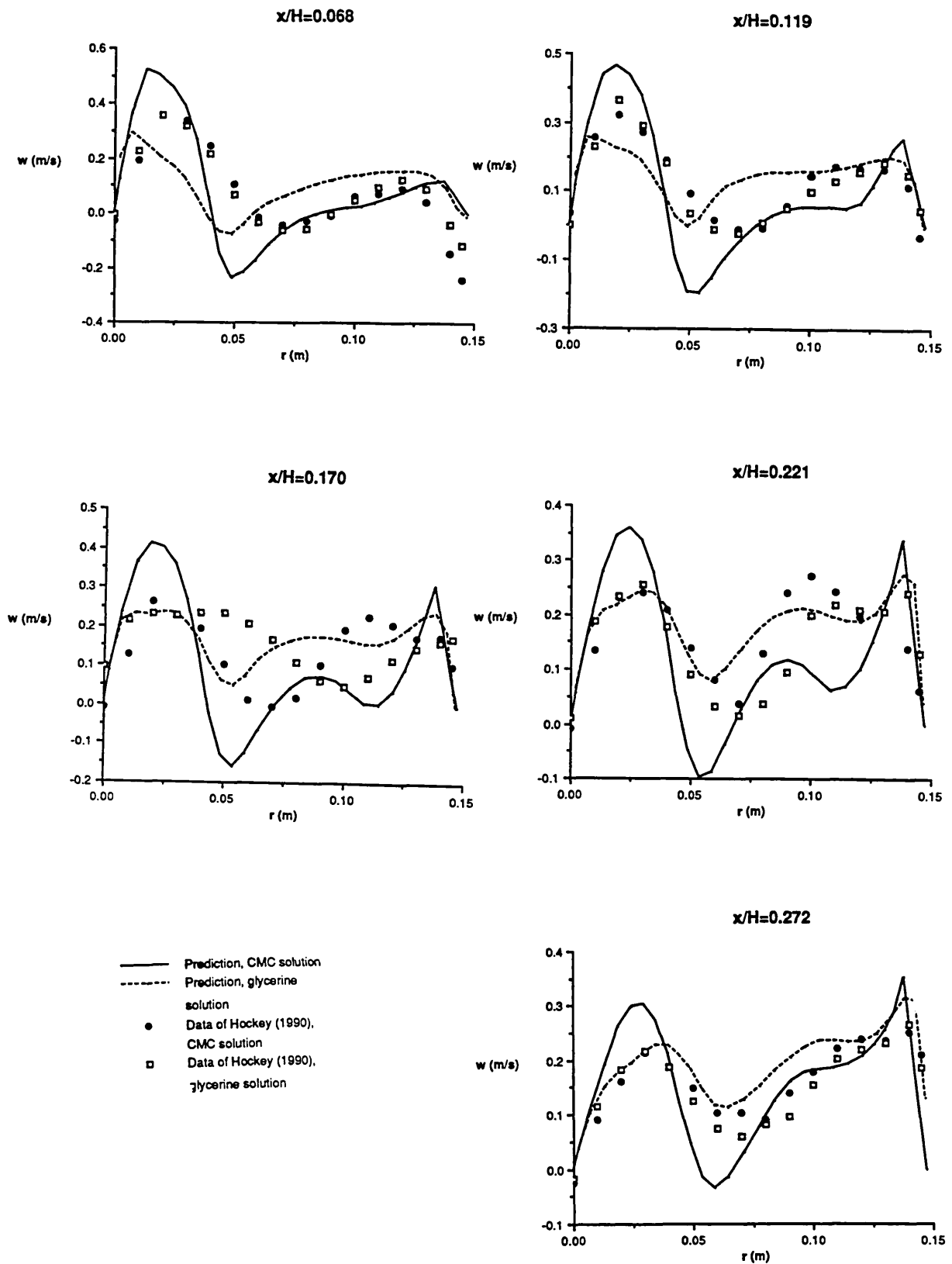


Figure 6.3.16 Below-impeller swirl velocity comparisons, 0° plane, CMC and glycerine solutions in mixing vessel

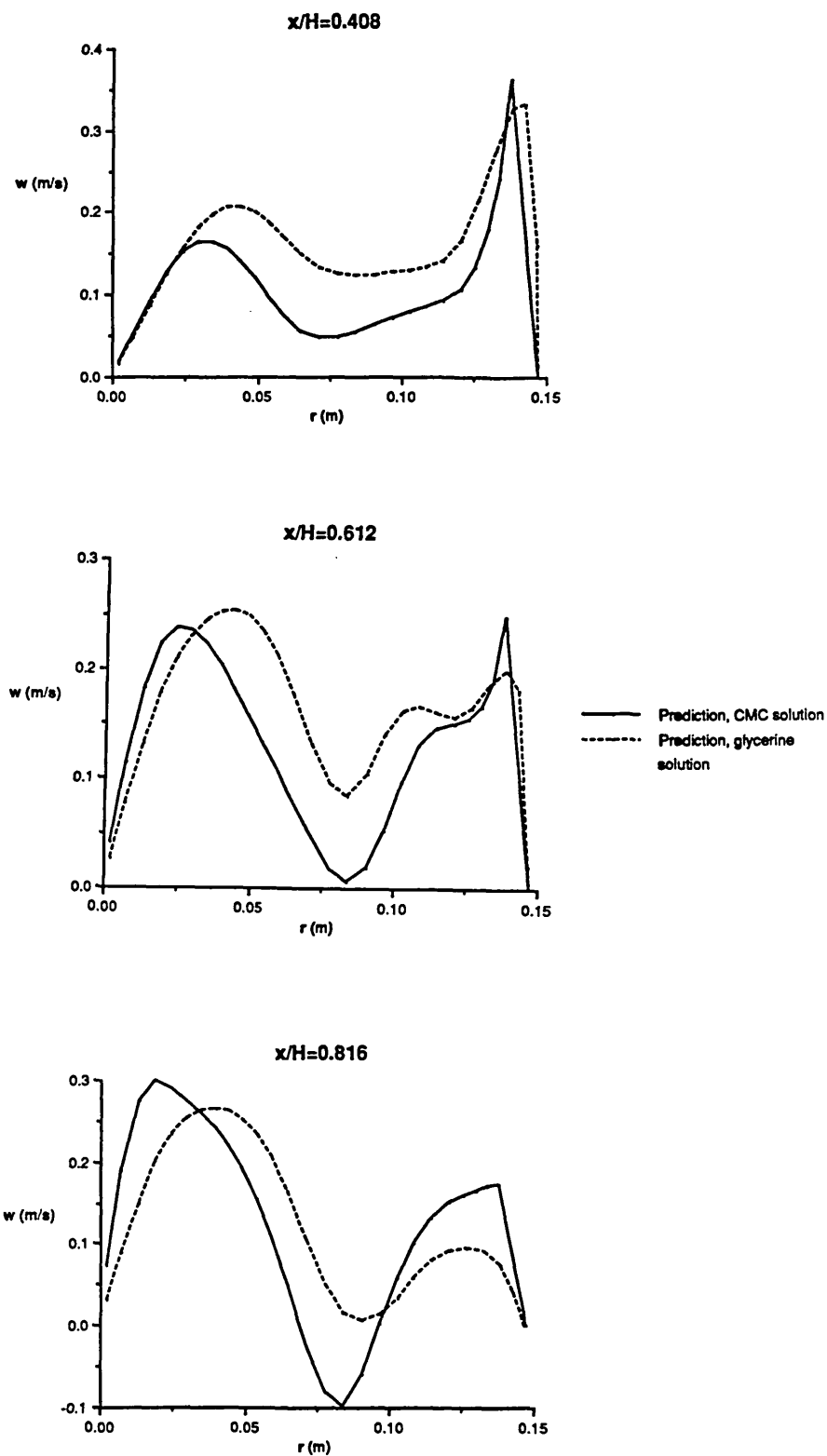


Figure 6.3.17 Above-impeller swirl velocity comparisons, 0° plane, CMC and glycerine solutions in mixing vessel

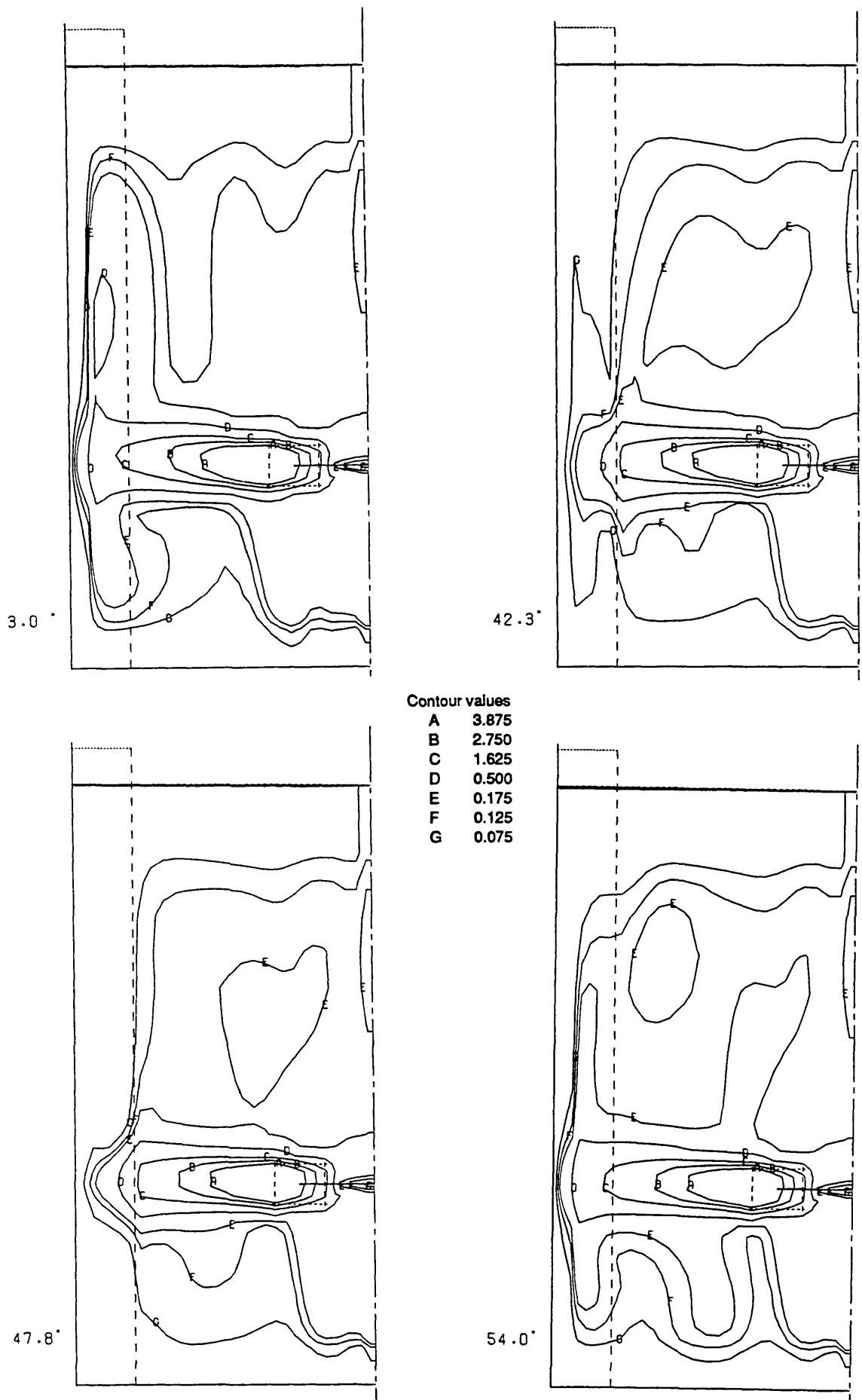


Figure 6.3.18 Normalised turbulence kinetic energy in $x-r$ planes, CMC solution in mixing vessel

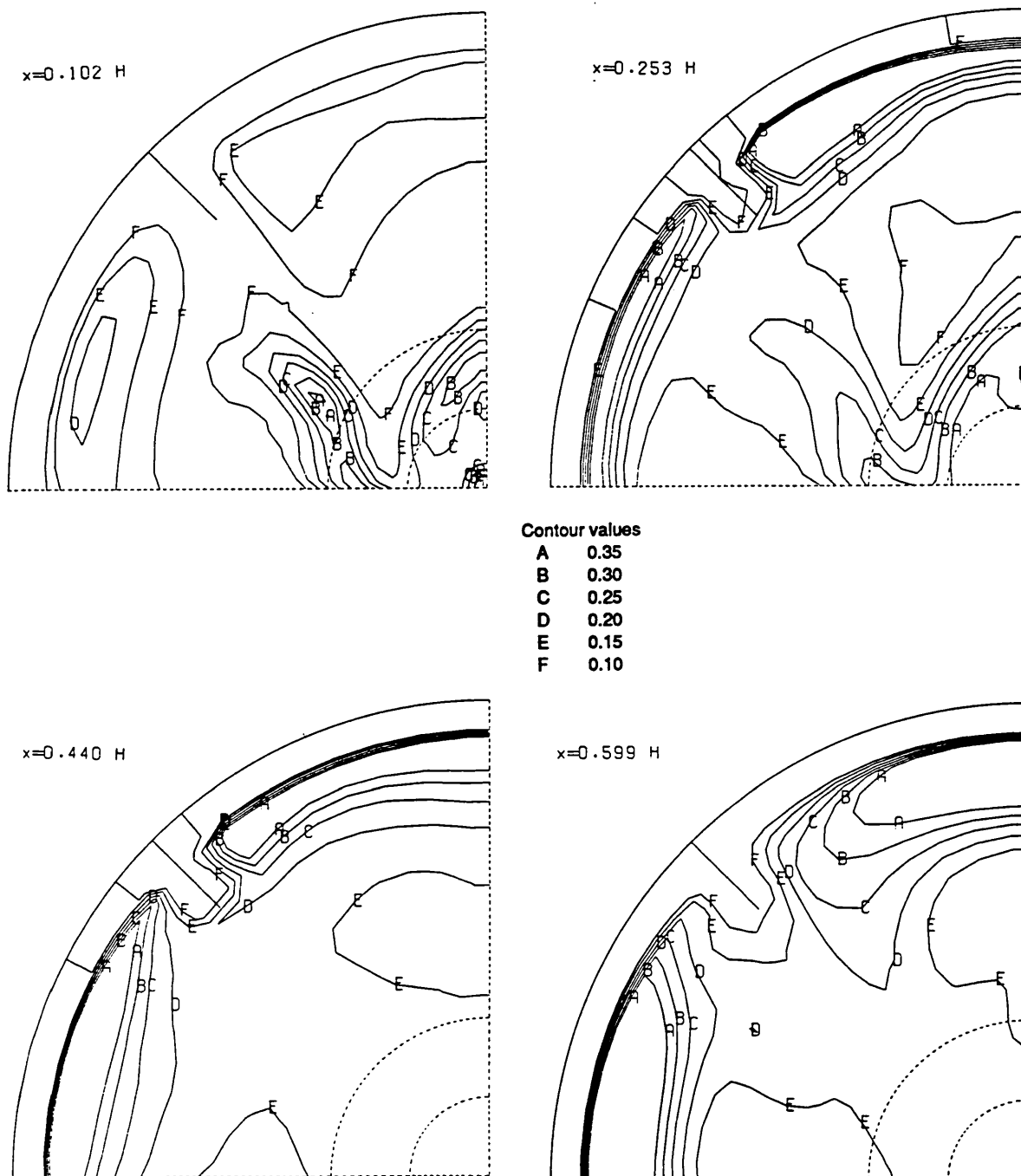


Figure 6.3.19 Normalised turbulence kinetic energy in $r - \theta$ planes,
CMC solution in mixing vessel

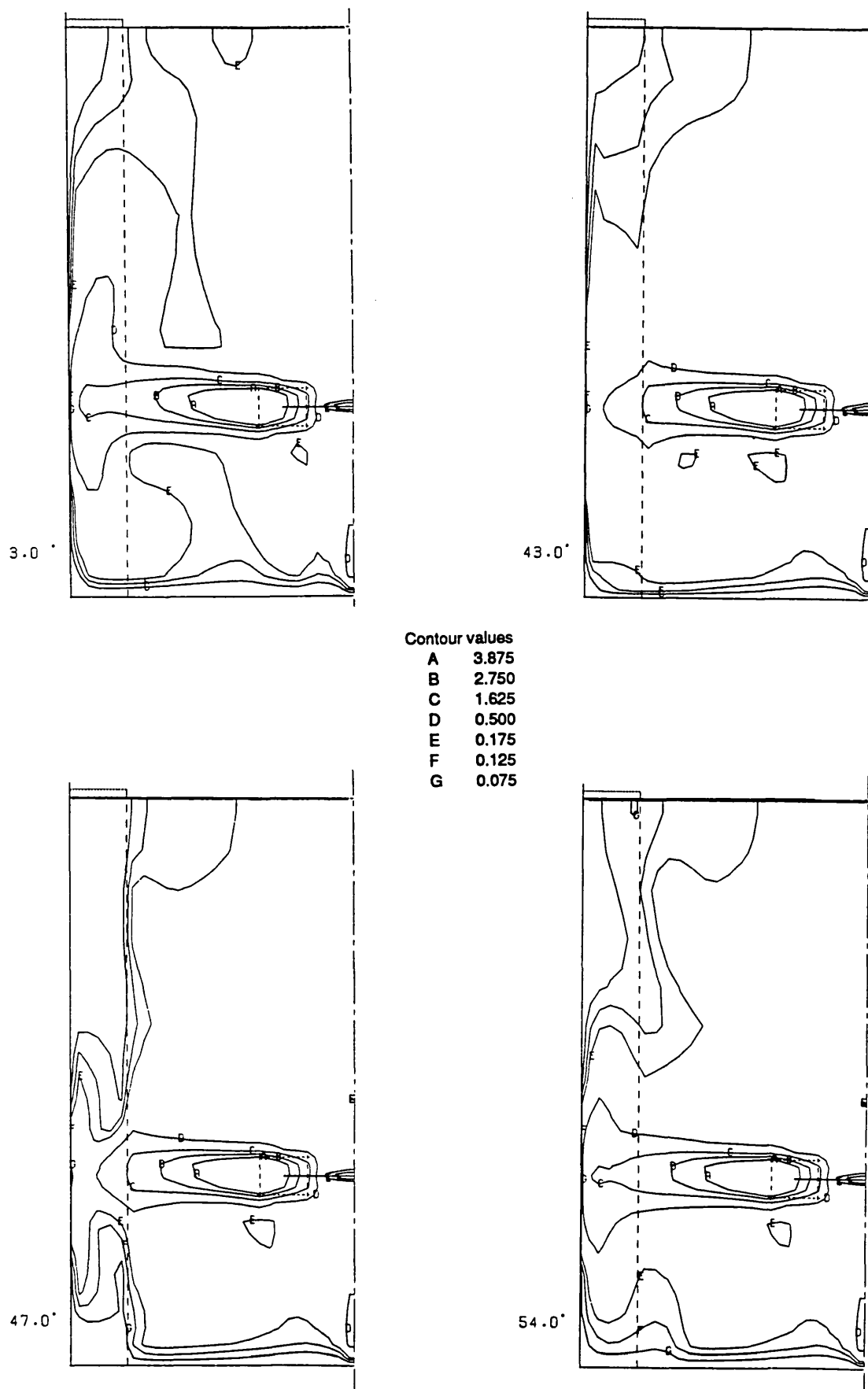


Figure 6.3.20 Normalised turbulence kinetic energy in $x - r$ planes, glycerine solution in mixing vessel

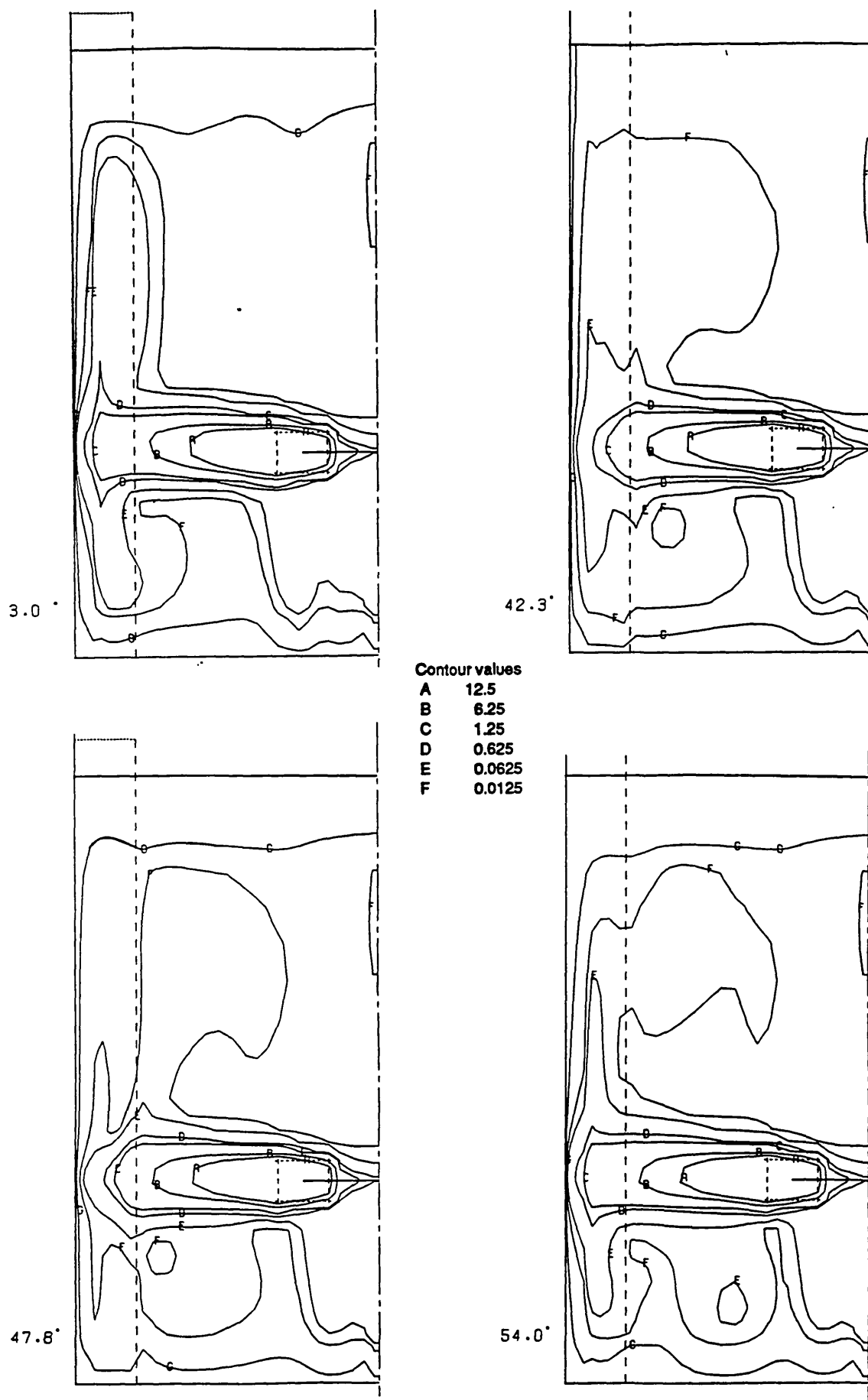


Figure 6.3.21 Normalised turbulence energy dissipation rate in $x - r$ planes, CMC solution in mixing vessel

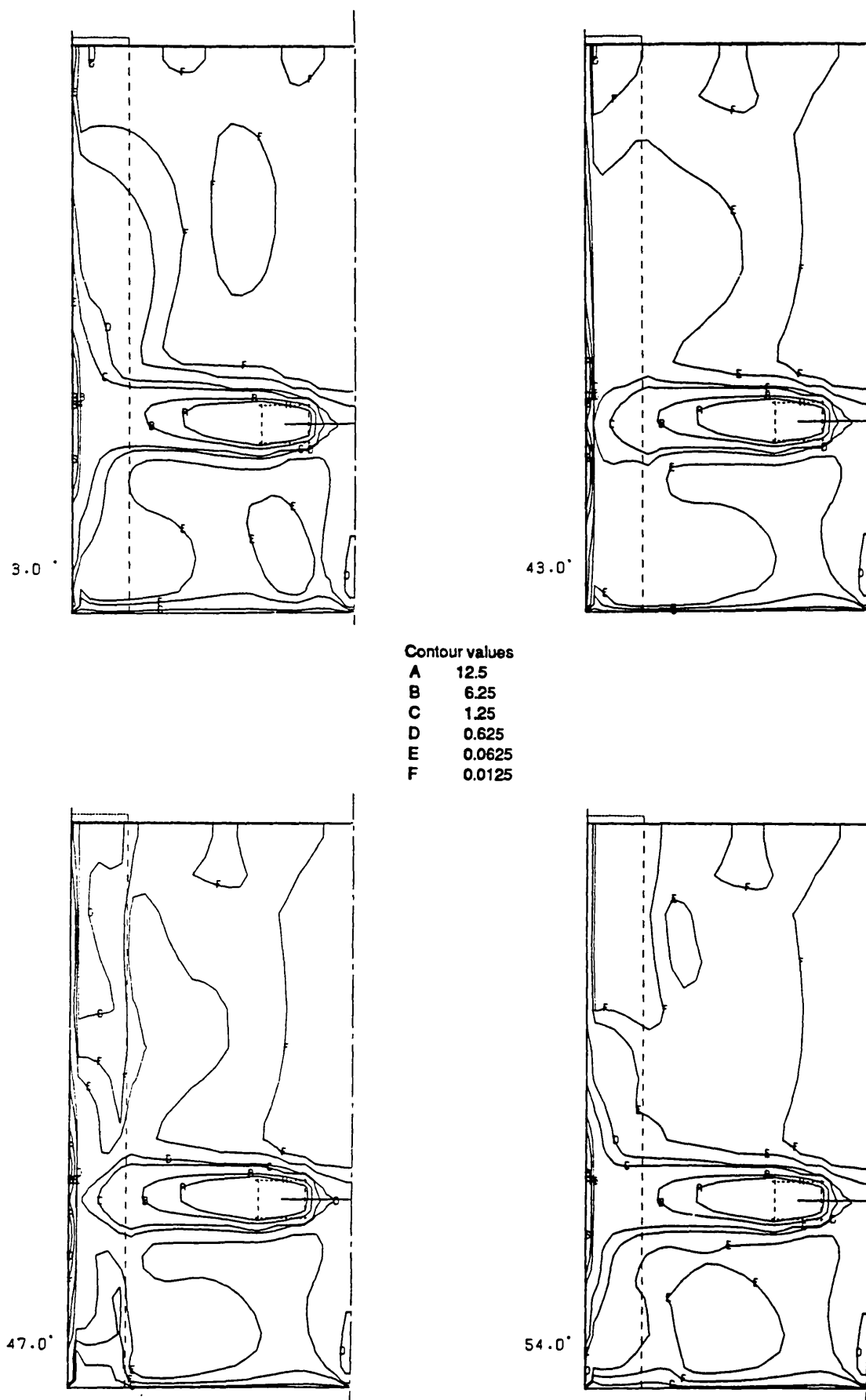
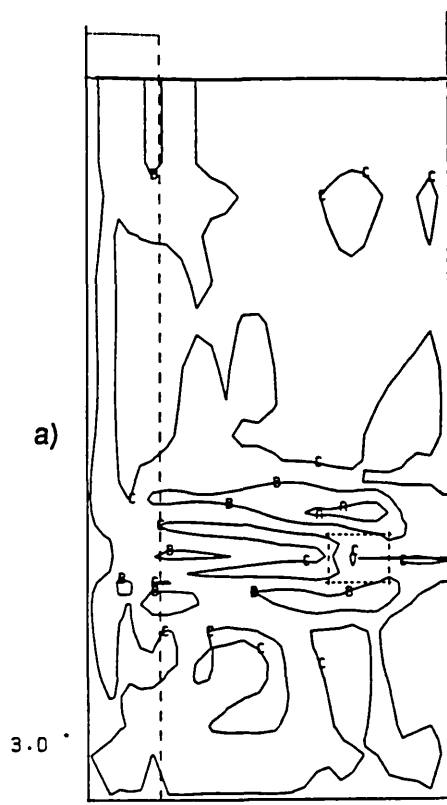
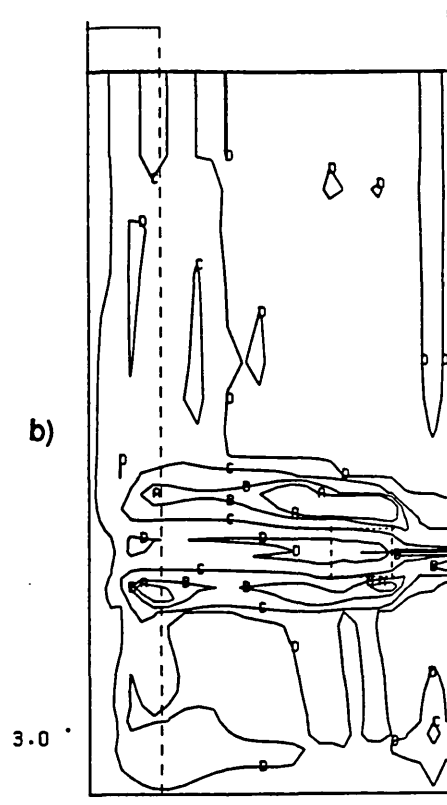


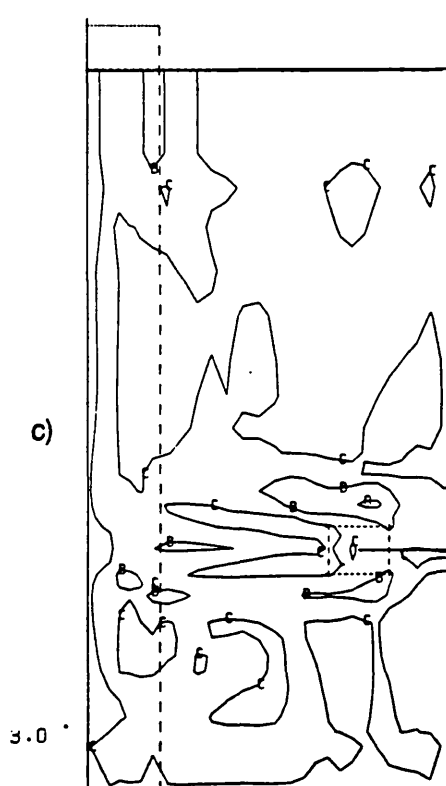
Figure 6.3.22 Normalised turbulence energy dissipation rate in $x - r$ planes, glycerine solution in mixing vessel



Contour Values
 A : 5.000
 B : 1.000
 C : 0.100



Contour Values
 A : 1.000
 B : 0.500
 C : 0.100
 D : 0.01000



Contour Values
 A : 5.000
 B : 1.000
 C : 0.100

a) Relative magnitude of first
 extra term, ratio (6.2.1)

b) Relative magnitude of second
 extra term, ratio (6.2.2)

c) Relative magnitude of
 sum of extra terms

6.3.23 Relative magnitude of extra ϵ equation source terms, CMC solution in mixing vessel

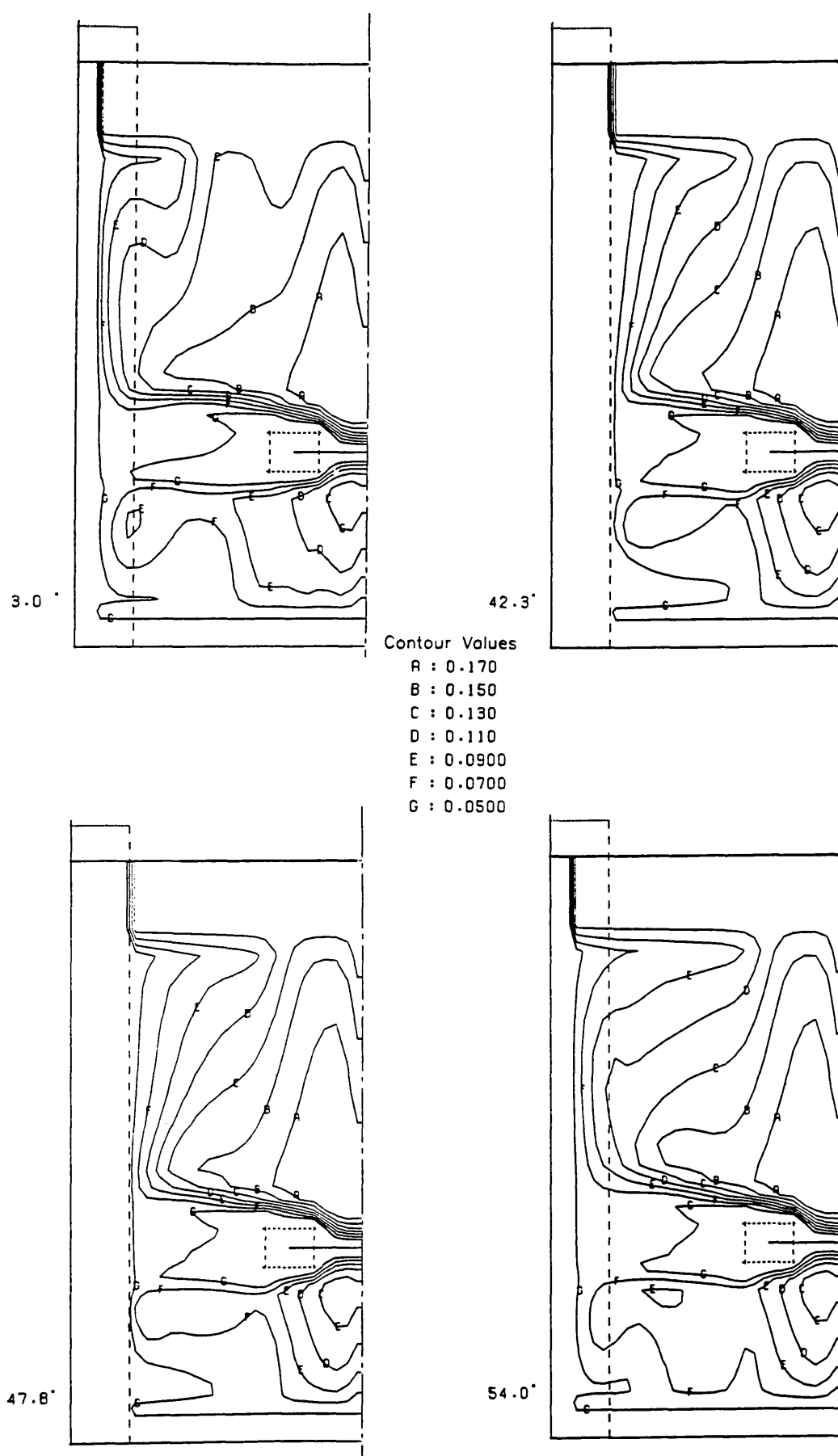


Figure 6.3.24 Normalised turbulence length scales in $x - r$ planes,
CMC solution in mixing vessel

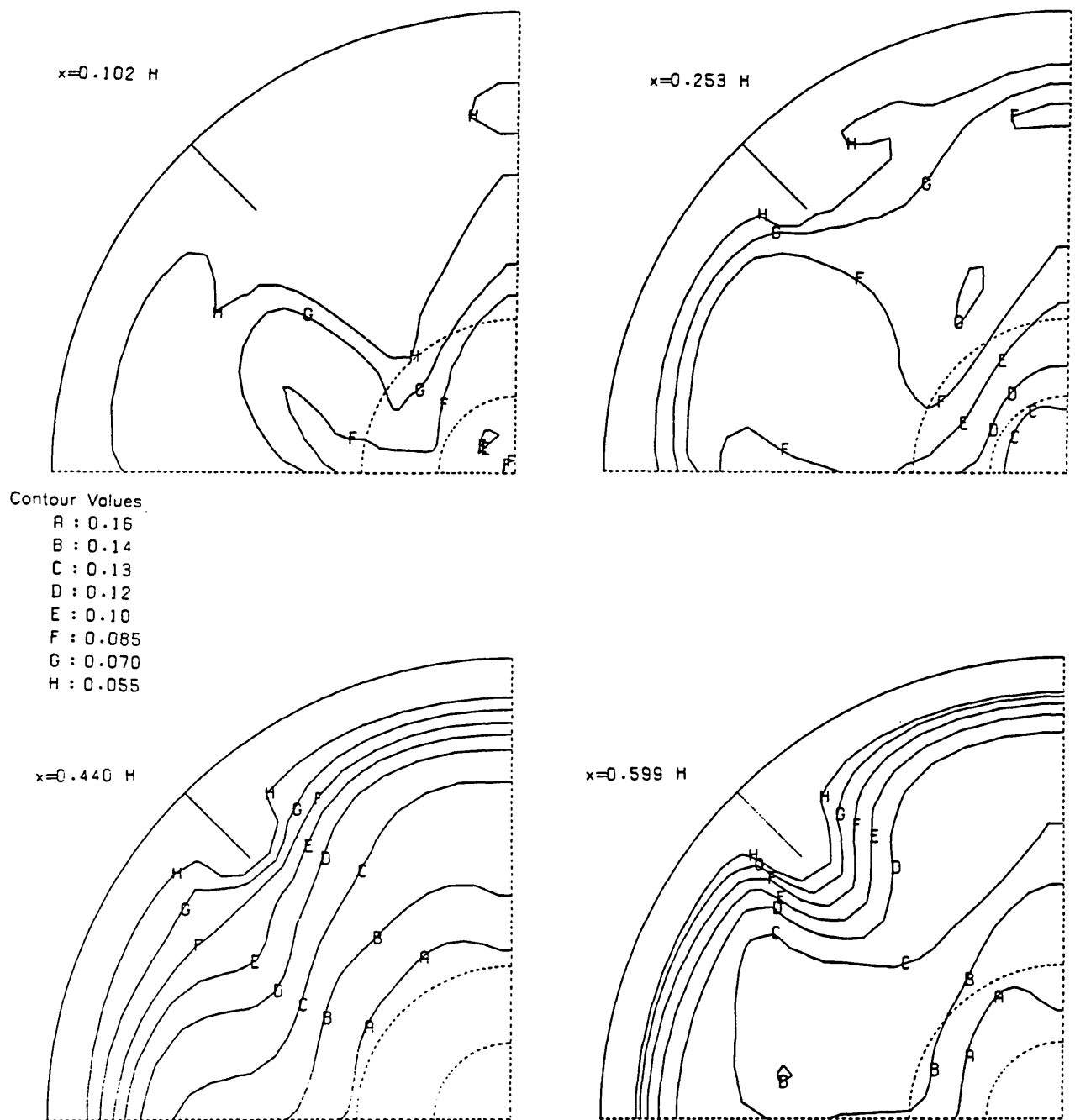


Figure 6.3.25 Normalised turbulence length scales in $r - \theta$ planes,
CMC solution in mixing vessel

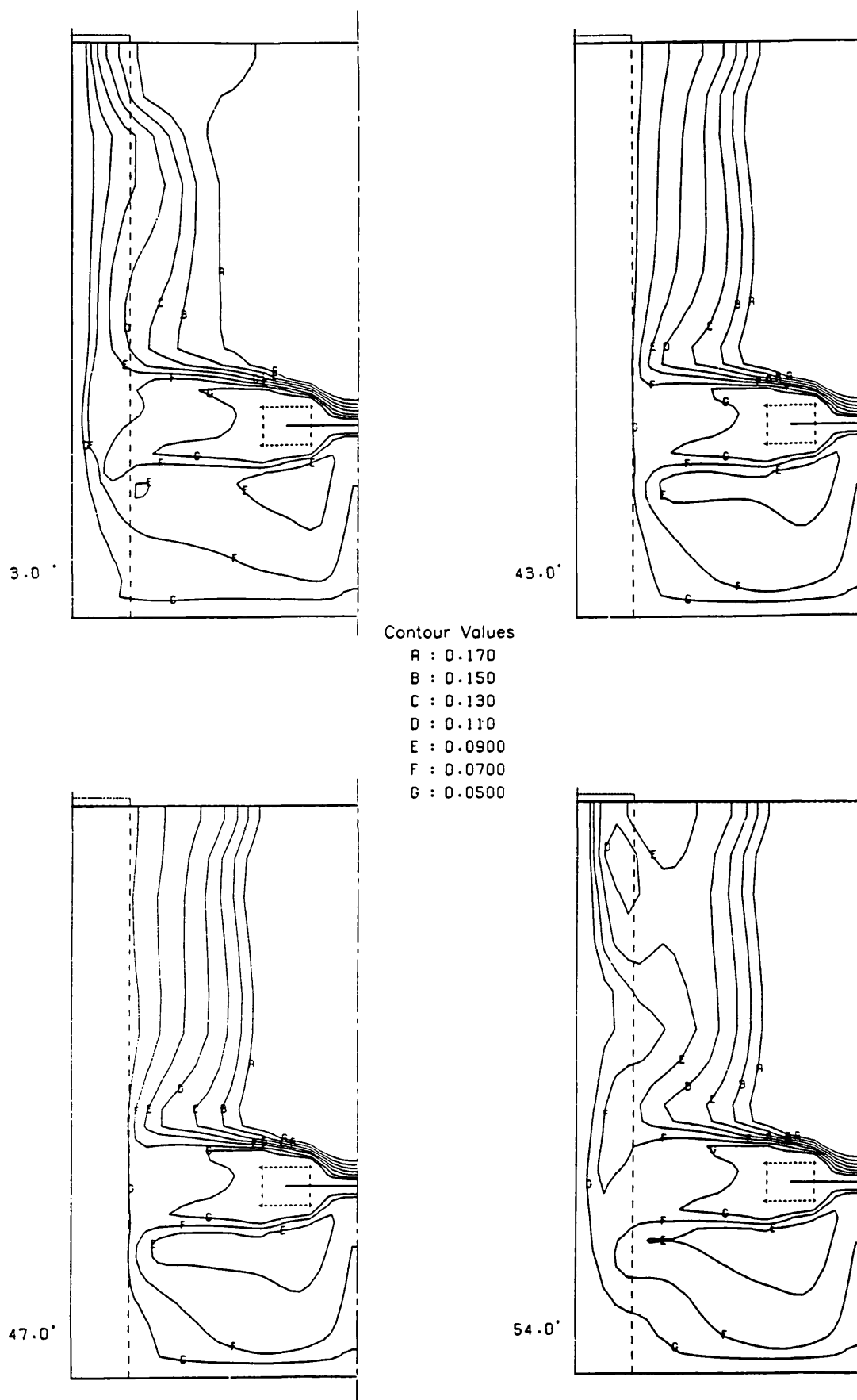


Figure 6.3.26 Normalised turbulence length scales in $x - r$ planes, glycerine solution in mixing vessel

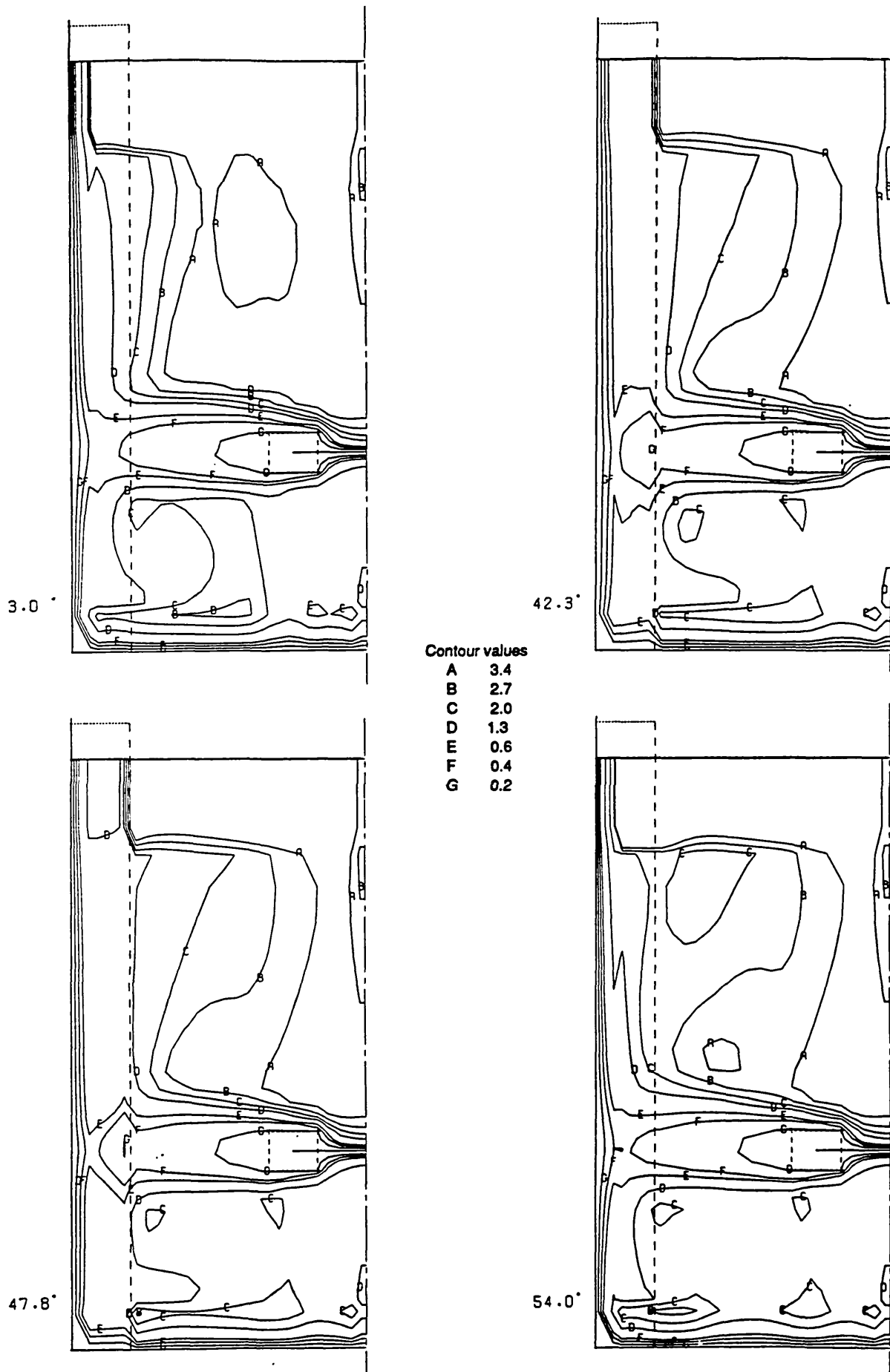


Figure 6.3.27 Normalised turbulence time scales in $x - r$ planes, CMC solution in mixing vessel

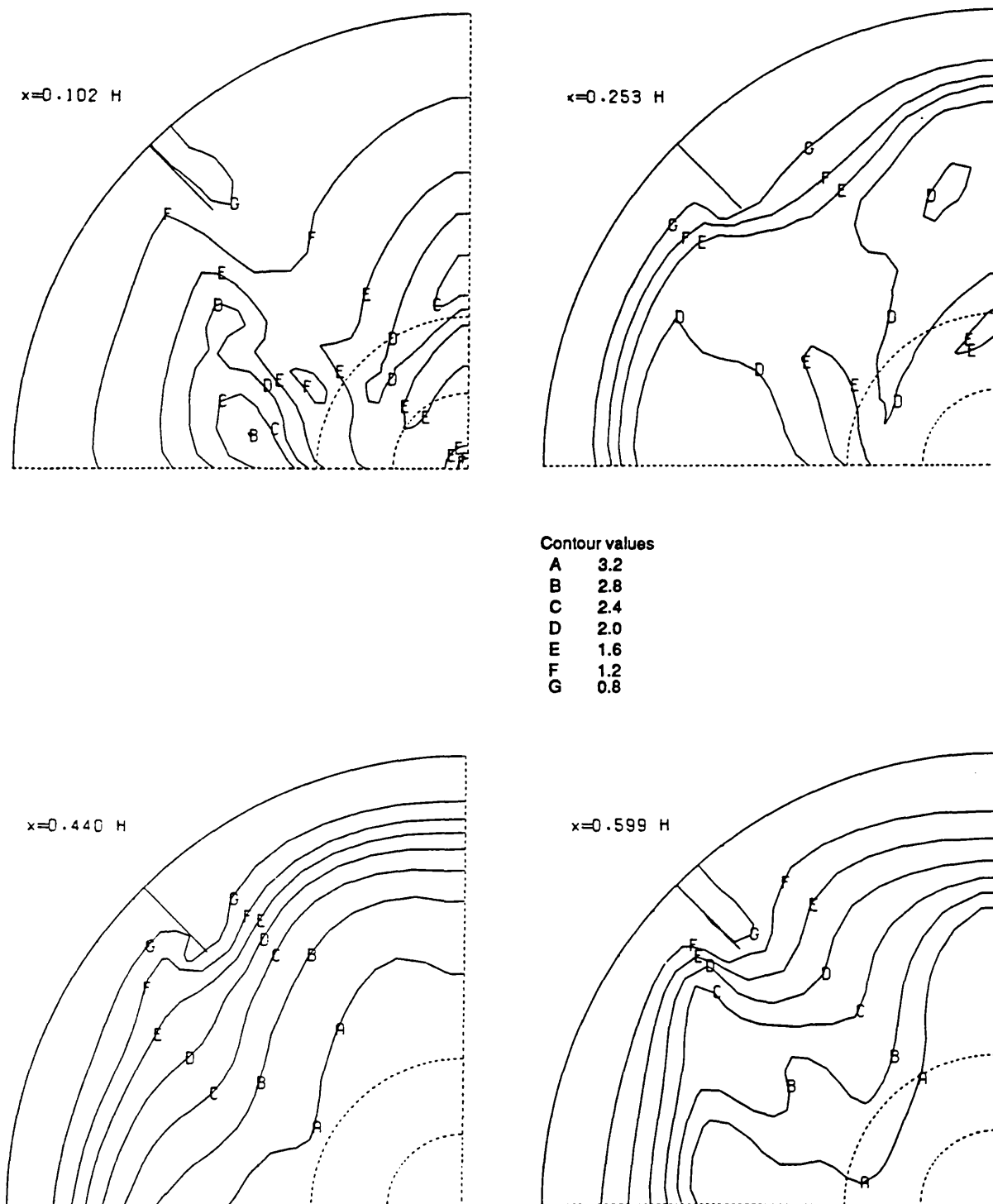


Figure 6.3.28 Normalised turbulence time scales in $r - \theta$ planes, CMC solution in mixing vessel

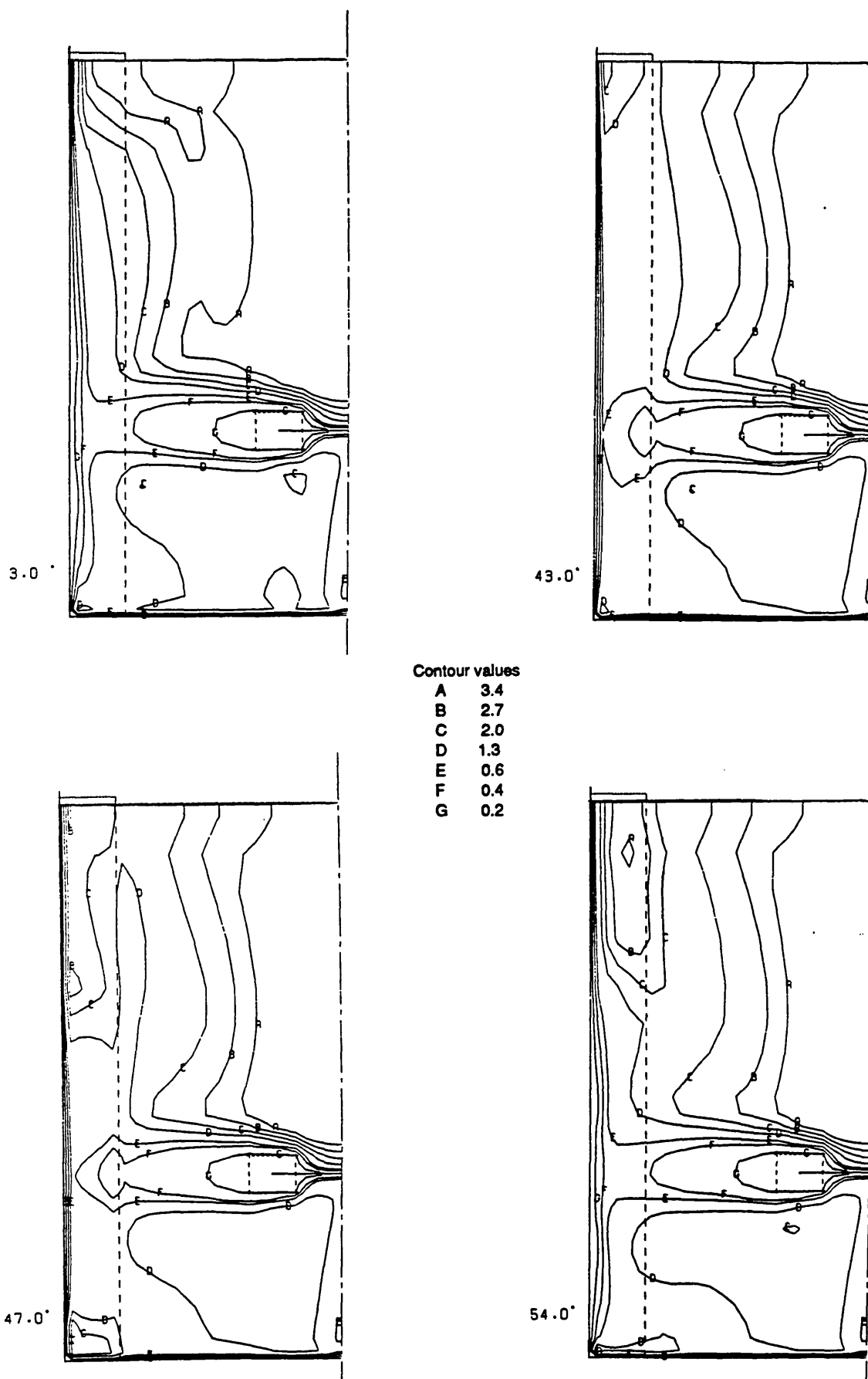


Figure 6.3.29 Normalised turbulence time scales in $x - r$ planes, glycerine solution in mixing vessel

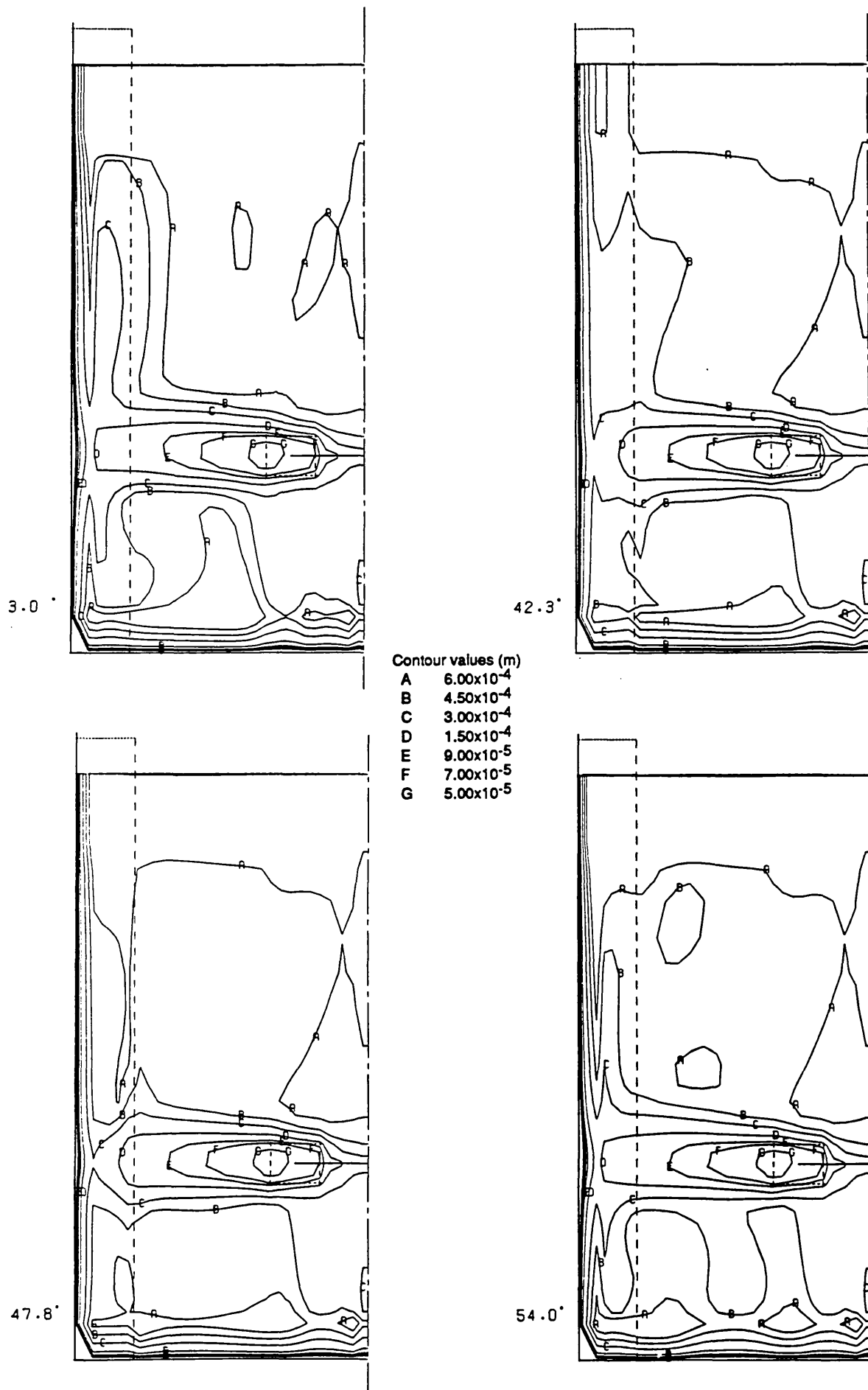


Figure 6.3.30 Kolmogorov length scales (m) in $x - r$ planes,
CMC solution in mixing vessel

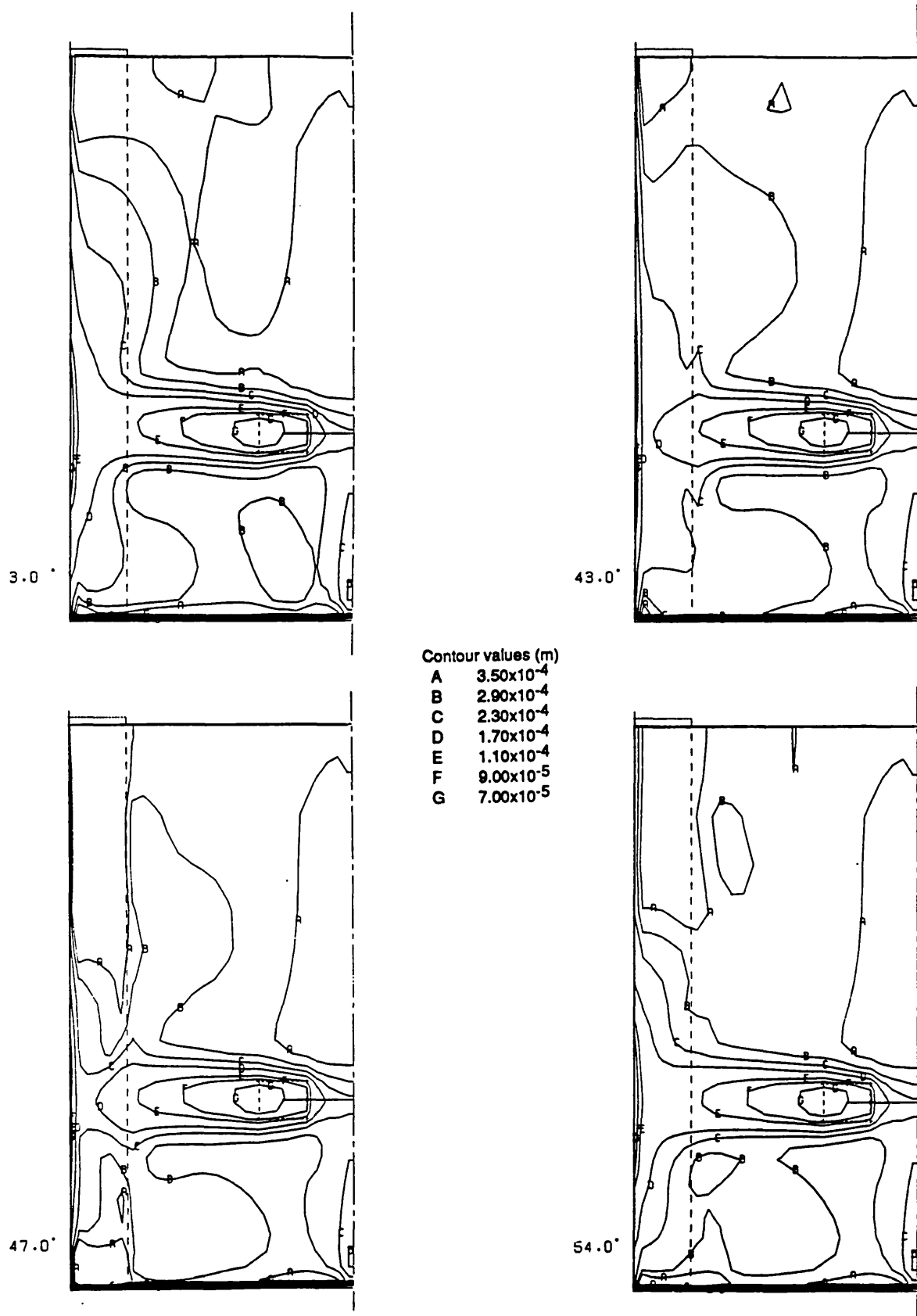


Figure 6.3.31 Kolmogorov length scales (m) in $x - r$ planes,
glycerine solution in mixing vessel

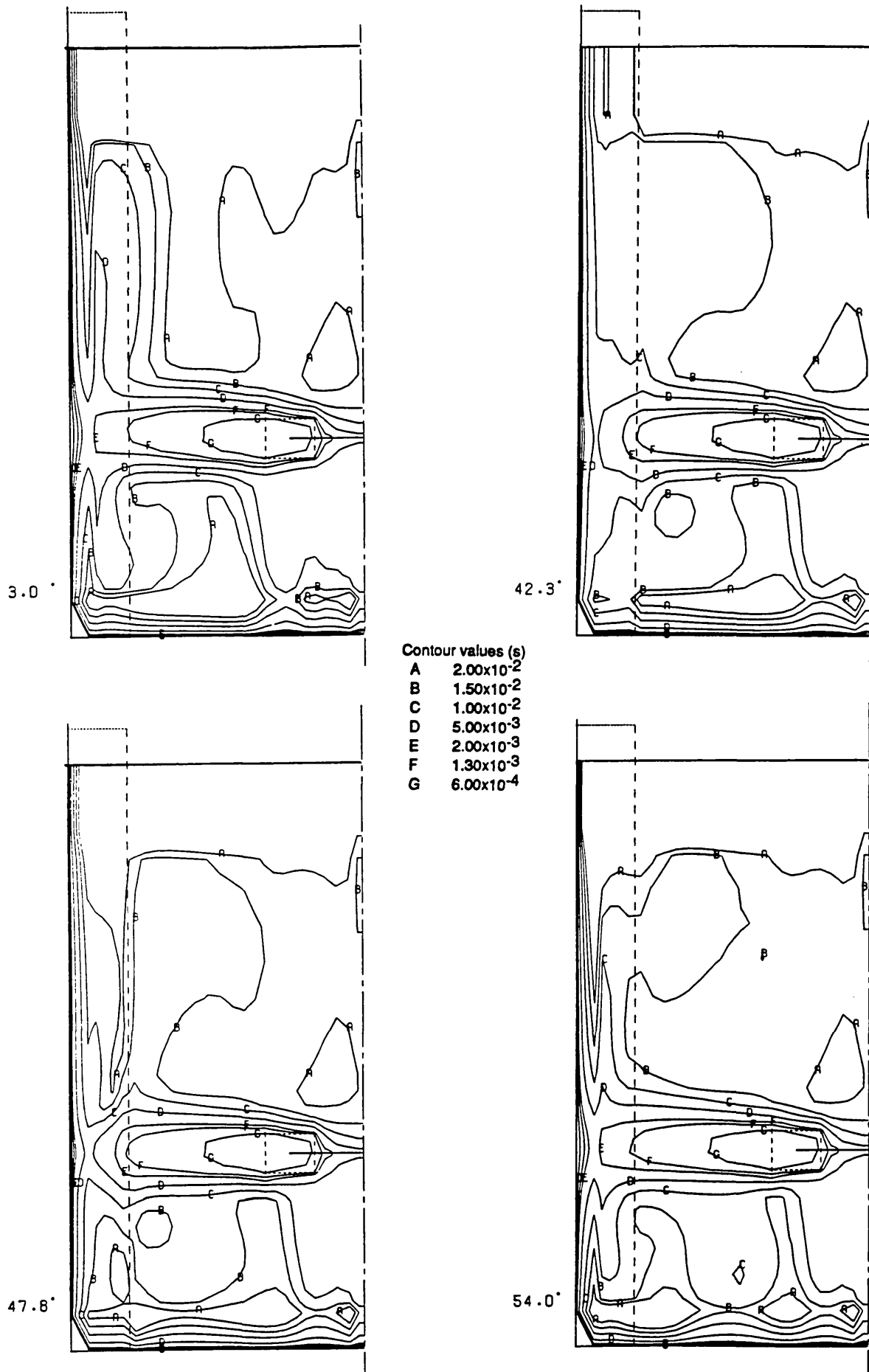
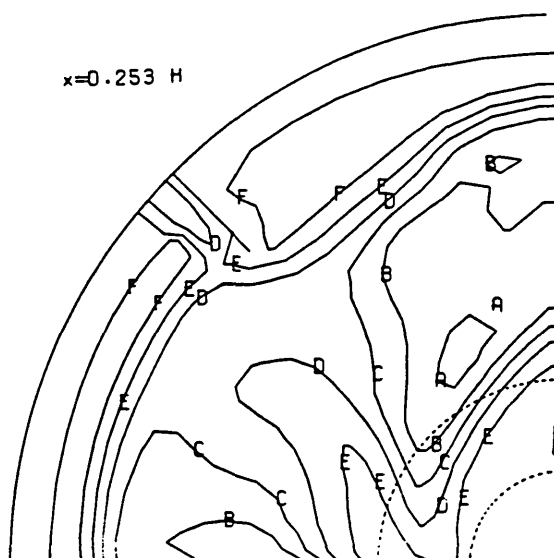
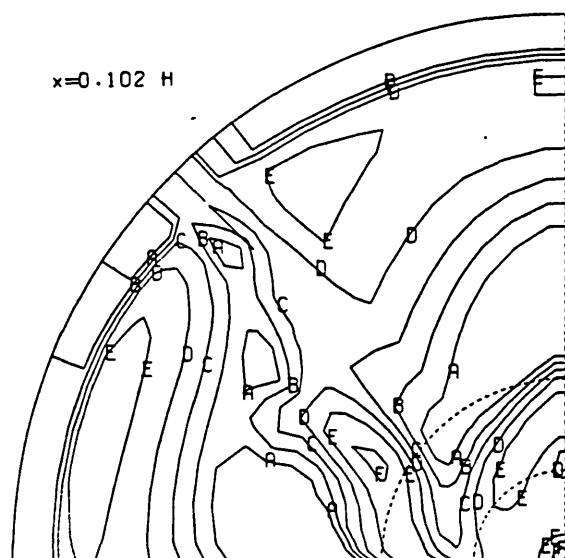


Figure 6.3.32 Kolmogorov time scales (s) in $x - r$ planes, CMC solution in mixing vessel



Contour values (s)

A	1.9×10^{-2}
B	1.6×10^{-2}
C	1.4×10^{-2}
D	1.2×10^{-2}
E	9.0×10^{-3}
F	6.5×10^{-3}

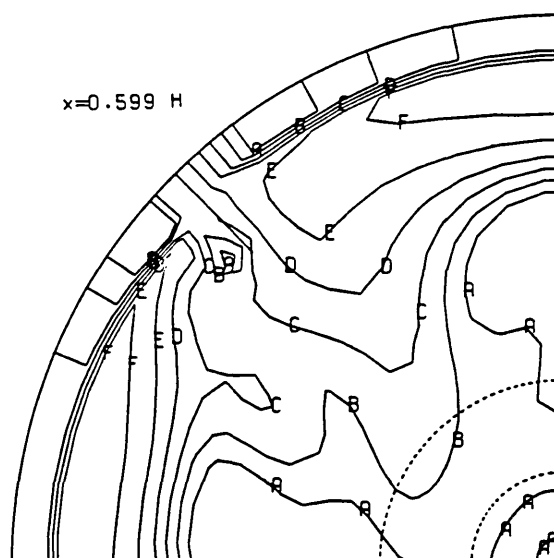
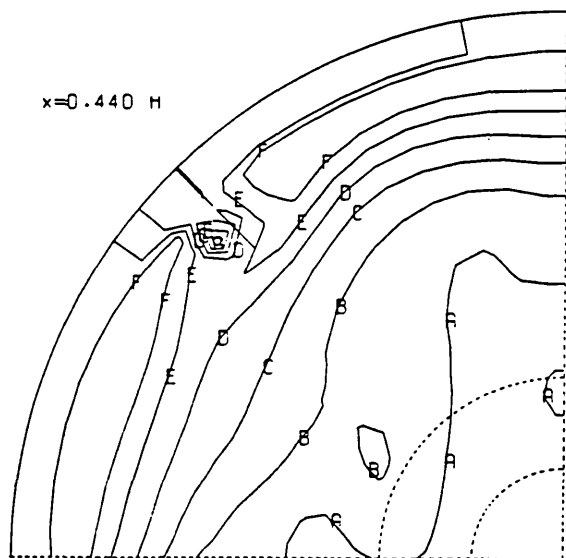


Figure 6.3.33 Kolmogorov time scales (s) in $r - \theta$ planes, CMC solution in mixing vessel

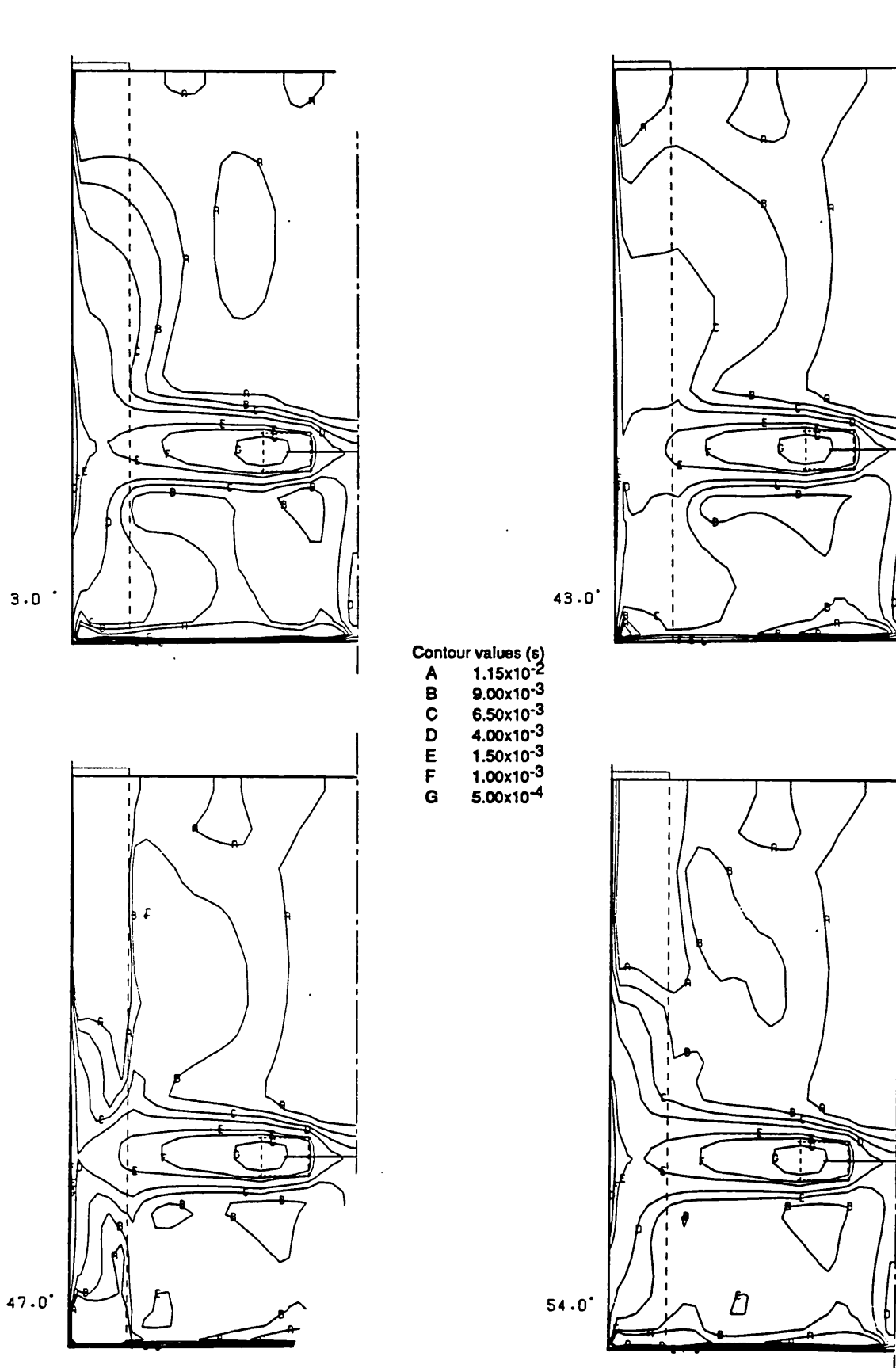


Figure 6.3.34 Kolmogorov time scales (s) in $x - r$ planes, glycerine solution in mixing vessel

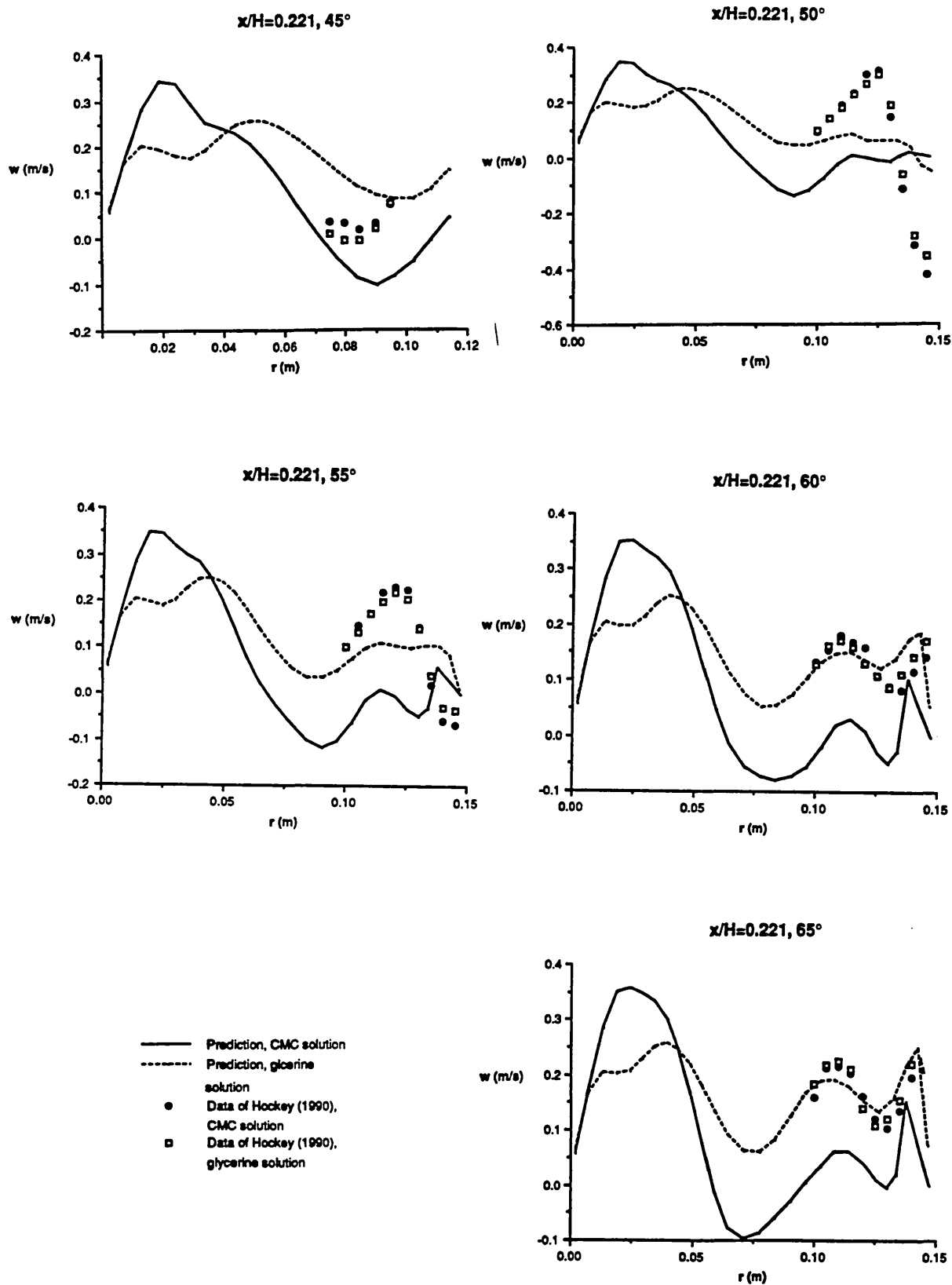


Figure 6.5.1 Swirl velocity comparisons in plane of baffle and baffle wake, at $x = 0.221H$, CMC and glycerine solutions in mixing vessel

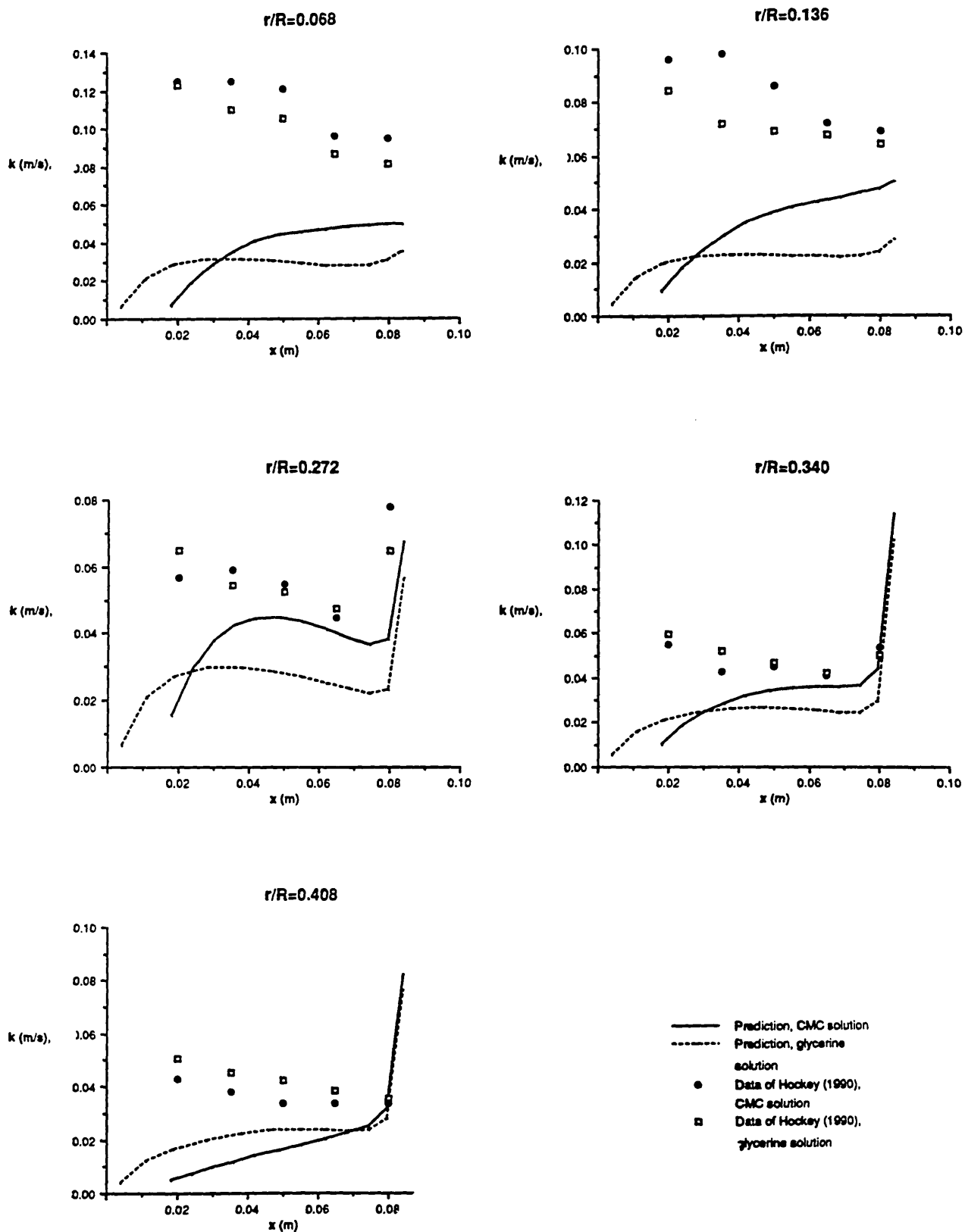


Figure 6.5.2 Below-impeller turbulence kinetic energy comparisons, 0° plane, CMC and glycerine solutions in mixing vessel

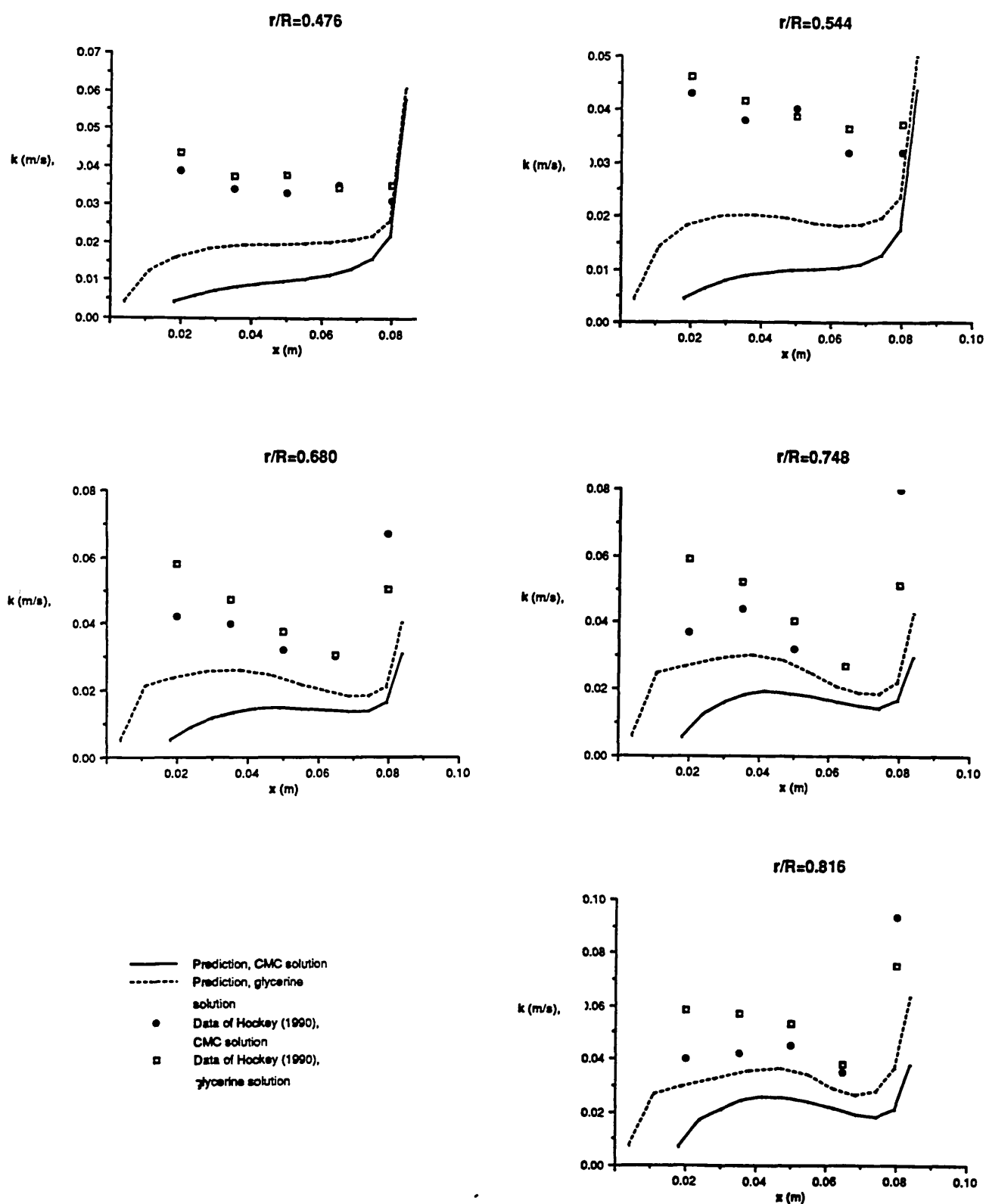


Figure 6.5.2 Below-impeller turbulence kinetic energy comparisons, 0° plane, CMC and glycerine solutions in mixing vessel

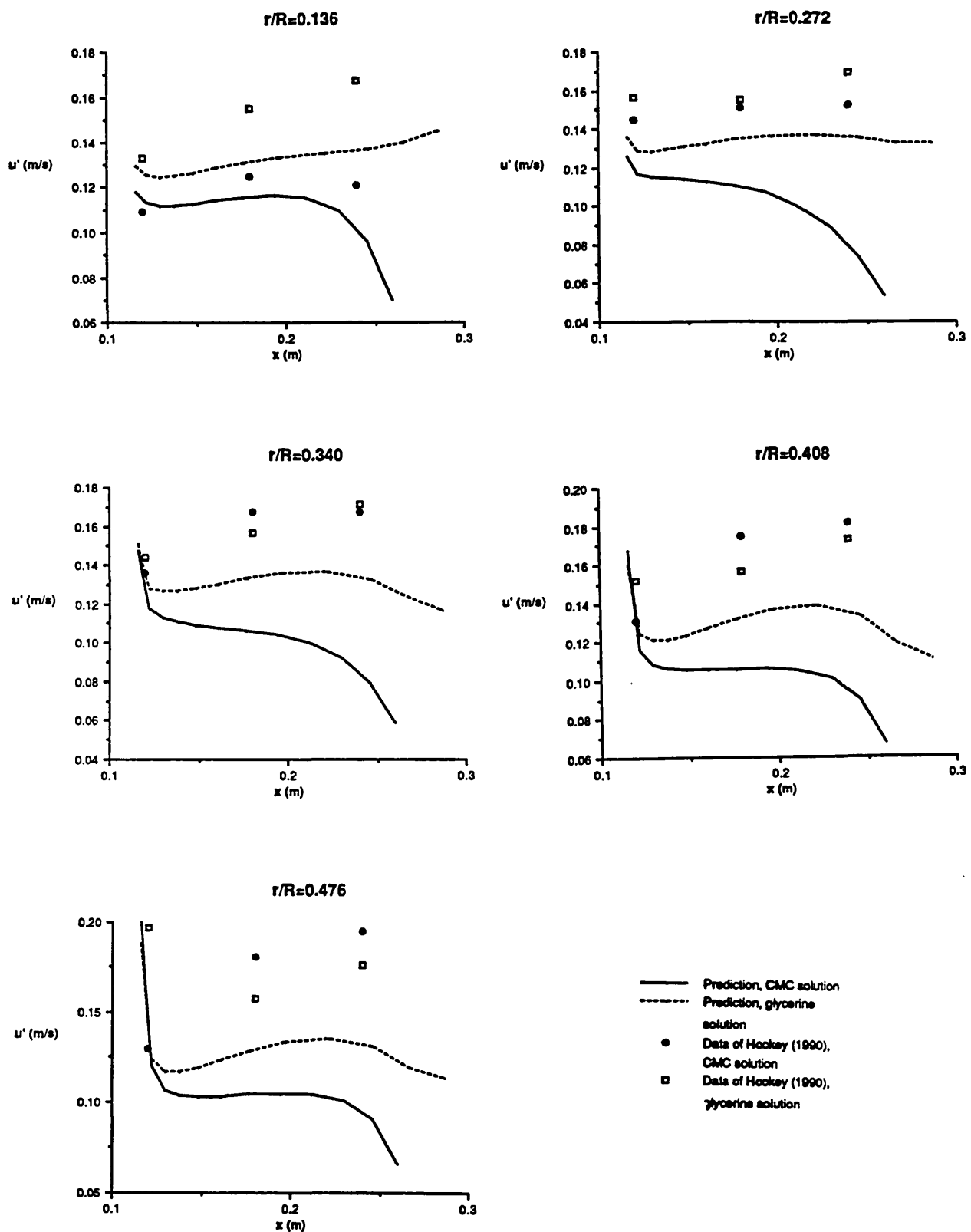


Figure 6.5.3 Above-impeller turbulence kinetic energy comparisons, 0° plane, CMC and glycerine solutions in mixing vessel

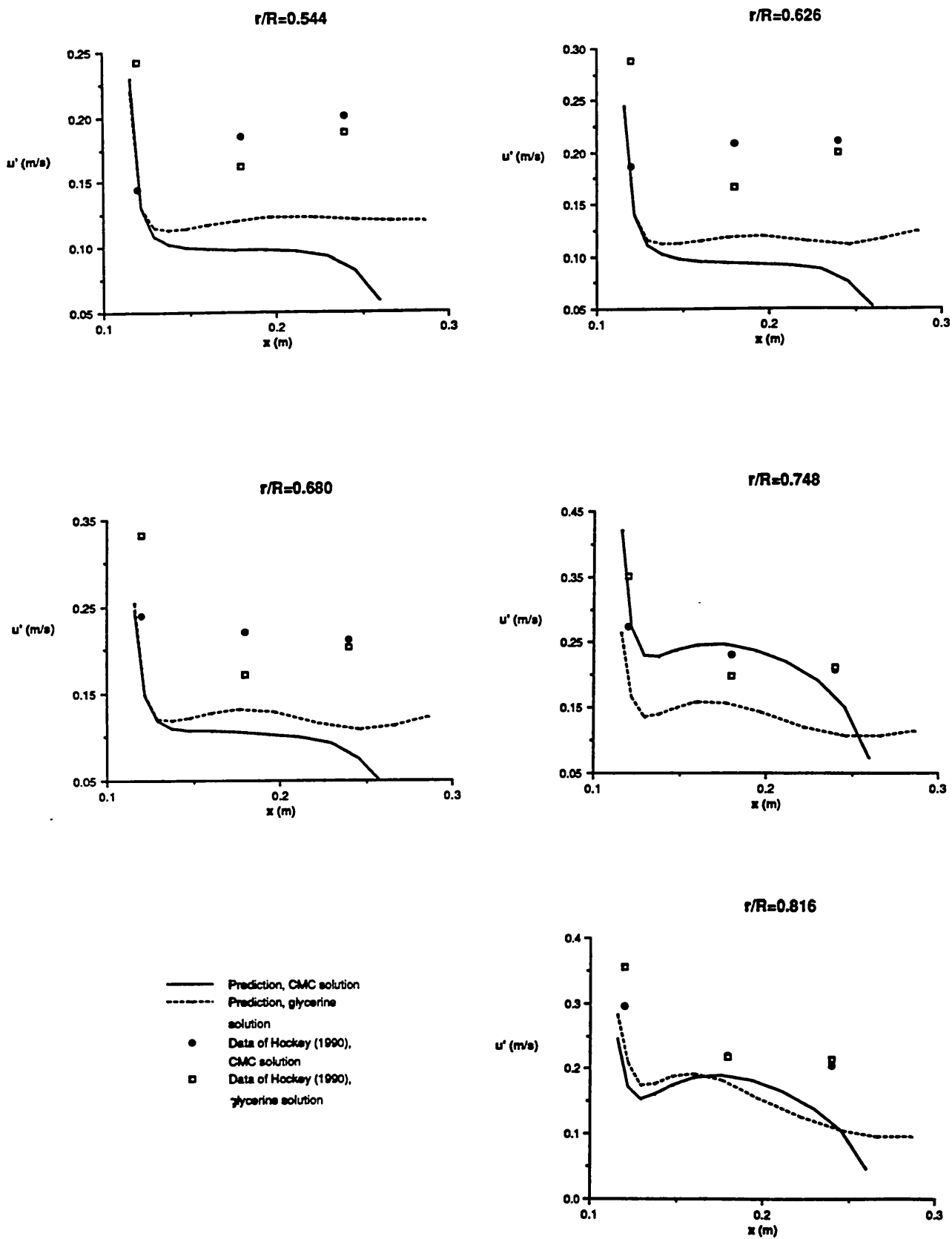


Figure 6.5.3 Above-impeller turbulence kinetic energy comparisons, 0° plane, CMC and glycerine solutions in mixing vessel

Nomenclature

a	Cell face area, m^2
$A\phi$	Coefficients of discretised equations
A, B	Constants in 'law of the wall', (2.5.1)
C_1, C_2, C_μ	Turbulence model coefficients, section 3.8.5
De	Deborah number, defined by (2.2.1)
f	Fanning friction factor, defined by (2.5.9)
G	Rate of generation of turbulence kinetic energy, defined by (3.9.7)
H	Vessel height, m
k	Turbulence kinetic energy, defined by (3.6.2), m^2/s^2
K	Fluid consistency in power law constitutive equation, (2.3.1), kg/ms^{2-n}
L	Length scale characteristic of macro-scale flow, m Turbulence length scale, defined by (5.3.3), m
n	Shear-thinning index in power-law and Carreau constitutive equations, (2.3.1) and (2.3.2)
N	Impeller rotational speed, $1/s$
N_p	Power number, defined by (2.4.15)
p	Pressure, kg/ms^2
Pe	Peclet number, defined (4.4.4)
R	Vessel radius, m
Re	Reynolds number
Re_{gen}	Generalised Reynolds number for pipe flow of Newtonian and shear-thinning fluids, defined by (2.4.8)
Re_{pl}	Reynolds number for pipe flow of Newtonian and shear-thinning fluids, defined by (2.4.12)
$Re_{\mu w}$	Wall viscosity Reynolds number for pipe flow of Newtonian and shear-thinning fluids, defined by (2.4.13)
S	Source term in transport equations
S^1, S^2	Coefficient and component of linearised transport equation source term, respectively, (4.3.10)
t	Characteristic time of flow process in (2.2.1), s
u	Axial velocity, m/s
u_i	Velocity component in the i direction, m/s
U	Velocity characteristic of macro-scale flow, m/s
u^+	Dimensionless velocity, defined by (2.5.3)
$u_\star$	Friction velocity, defined by (2.5.4), m/s
u_K	Velocity characteristic of the Kolmogorov scales, defined by (3.7.19), m/s
v	Radial velocity, m/s
w	Swirl (circumferential) velocity
We	Weissenberg number, defined by (2.4.2)
x	Axial co-ordinate, m
x_i	i direction co-ordinate, m

y	Radial co-ordinate, m
y^+	Dimensionless distance from wall, defined by (2.5.5)
α_ϕ	Under-relaxation factor in discretised equation for ϕ , (4.8.2)
ε	Energy dissipation rate, defined by (3.4.2), m^2/s^3
ζ_{norm}	Maximum tolerable value of normalised residual sums, section 4.9
ϕ	A transported quantity
γ_{ij}	Strain tensor, $1/\text{s}$
Γ	Diffusion coefficient
θ	Circumferential co-ordinate, m
κ	Von Karman constant
λ	Time constant in (2.3.2), s
Λ	Characteristic time of material, s
ρ	Fluid density, kg/m^3
P	Impeller input power, kgm^2/s^3
μ	Molecular viscosity, kg/ms
μ_w	Wall molecular viscosity, kg/ms
μ_t	Turbulent viscosity, kg/ms
μ_∞	Limiting molecular viscosity in upper strain rate limit,
(2.3.2),	kg/ms
μ_0	Limiting molecular viscosity in lower strain rate limit,
	(2.3.2), kg/ms
ν	Kinematic viscosity, m^2/s
η	Length scale characteristic of the Kolmogorov eddies, defined by (3.7.18), m
σ	Standard variation of the p.d.f. of the instantaneous energy dissipation rate, defined by (3.7.37)
τ_{ij}	Stress tensor, kg/ms^2
τ_w	Wall shear stress, kg/ms^2
τ	Time scale characteristic of energy-containing eddies, k/ε , chapters 5 and 6
τ_k	Time scale characteristic of the Kolmogorov eddies, defined by (5.3.6), s
Superscripts	
$\wedge$	Instantaneous quantity
$-$	Mean component of time-averaged quantity
$'$	Fluctuating component of time-averaged quantity
$\sim$	Normalised quantity
$^*, **$	Intermediate values of the appropriate quantity in the PISO algorithm

Errata

Page no.	Line no.	Present	Should read
35	3	(2.4.16)	(2.4.17)
45	5	Appendix D	Appendix E
	18	(D.5)	(E.5)
	31	permissable	permissible
62	14	(3.7.21)	(3.7.22)
64	22	(3.6.3)	(3.6.4)
65	11	(3.6.4)	(3.6.2)
72	13	mat	may
73	13	(3.6.2)	(3.6.3)
88	12	(3.9.1) to (3.9.5)	(3.9.2) to (3.9.6)
110	7	(1985)	(1986)
113	13	(4.6.6) and (4.6.7)	(4.7.6) and (4.7.7)
119	13	discepancy	discrepancy
120	6	wtith	with
144	2	th	the
148	31	5.4.9 to 5.4.14	5.4.29 to 5.4.32
149	1	5.4.15 to 5.4.18	5.4.35 to 5.4.38
161	13	whic	which
162	25	6.2.12b	6.2.11b
163	3,5,8,16	McGurk	McGuirk
190	11	reliability	unreliability
221	10	(1985)	(1986)