Modelling of industrial flow processes: Opportunities for performance enhancement

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Detailed flow modelling of industrial processes offers new possibilities for performance enhancement and innovation in design of process equipment. In this review, we describe the overall methodology of industrial flow modelling. Some examples of applications of flow modelling are described to illustrate the methodology. Challenges and opportunities with reference to the Indian context are discussed.

ALMOST all the processes relevant to the manufacturing industry (chemical, petrochemical, fertilizer, metallurgical, power, cement, etc.) involve flow of fluids in some way or other. The innovation and competitive edge of any manufacturing industry, therefore, rests on how well these flow processes are designed and operated. If the underlying flow processes are adequately studied and controlled, there is always scope for performance enhancement and for evolving innovative design solutions. There are many instances in the past where innovative analysis and clever engineering of flow processes have realized substantial enhancements even in the so-called 'mature' technologies. One of the most striking examples of using knowledge of fluid dynamics to substantially enhance the performance of the reactor is the development of super-condensed mode of operation of fluidized bed polymerization reactors[1]. With the right selection of nozzle design and nozzle locations, it is now possible to increase the capacity of such polymerization reactors by 50 to 100% (this means producing fifty thousand to one lakh tonnes per year of polyethylene more from the existing reactor!)

Performance enhancement of existing or new processes may be realized in a variety of ways such as producing more from existing equipment, producing better quality products, having lower energy consumption and more safety of operations with less pollution and so on. Realization of enhancement in any of the aspects mentioned above requires expertise from various fields ranging from chemistry and catalysis to reaction engineering, fluid dynamics, mixing and heat and mass transfer. For the given fixed chemistry/catalysts, the performance of industrial processes or equipment is a complex function of the underlying transport processes. These transport processes are in turn governed by the fluid dynamics and therefore on a variety of design and operating parameters of process equipment. Specialized techniques and tools (of flow modelling) are therefore required to understand these complex flow processes.

Traditionally, experimental and semi-theoretical methods (like cold flow simulations or tracer studies) have been used to obtain the information about the fluid dynamics and mixing required for the process optimization. The information obtained from these methods is usually described in an overall/global parametric form. This practice conceals detailed local information about turbulence and mixing which may ultimately determine the process/equipment performance. With the emergence of high performance computers and advances in numerical techniques and algorithms, a relatively new approach to flow modelling of process equipment, based on computational fluid dynamics (CFD), is now available to engineers. This approach was mainly used by aerospace engineers so far. However, there is enormous potential of using it for many other manufacturing sectors including chemical, automobile, steel and cement. CFD deals with the solution of fluid dynamic equations on digital computers.

Computational modelling of industrial flow processes allows detailed analysis, at an earlier stage in the design cycle, for less money, with lower risk and in less time than experimental testing. Simulations have added advantage in that, diagnostic 'probing' of a computer simulation does not disturb the flow and usual operation! Various alternative configurations can be screened quickly using the validated CFD model. The detailed predicted flow field gives an insight into fluid behaviour and can sometimes give information which cannot be obtained from experiments. Therefore computational fluid dynamics (CFD) models are proving to be powerful aids in design and analysis of industrial flow processes. A critical review of CFD techniques and their potential and use for realizing performance enhancement will be useful at this stage. In this article, we discuss various aspects of modelling of industrial flow processes and its potential for enhancing performance of existing

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and new process equipment. Some examples of applications of flow modelling from our own research and consulting experience are described to illustrate the methodology. Challenges and opportunities with reference to the Indian context are discussed.

Computational fluid dynamics (CFD) framework

Computational fluid dynamics framework here means a complete tool for predicting the flow characteristics of the desired equipment. Various aspects of CFD framework along with key references are shown in Box 1. Several reviews describing the details of these aspects have been published (for example, refs. 2, 3). Here, we discuss some of the major issues without describing the mathematical details of specific formulations.

Transport equations

The closeness of predictions of the CFD model with the real flow behaviour depends on how well the user has represented the underlying physics in the mathematical formulations. Most of the industrial flow processes relevant to the process engineers, are complex and cannot be represented rigorously. The user, therefore, must appreciate the implications of the assumptions on which the formulation of the transport equations is based. Here we restrict ourselves to discussing major issues in the formulation of transport equations relevant for turbulent, dispersed multiphase flows, which are often encountered in chemical processing equipment.

Turbulence is often employed in industrial equipment to enhance the rates of transport processes. Turbulence is a three-dimensional, time-dependent, nonlinear phenomenon. The instantaneous velocity field in a turbulent flow is described by the Navier–Stokes equations. However because of the existence of extremely wide range of space and time scales in turbulent flow, direct numerical simulation of turbulent flows is possible only at relatively low Reynolds number and that too if the geometry is simple. For most engineering applications it is still necessary to use turbulence models along with time averaged Navier–Stokes equations. It must be realized that most of the available turbulence models obscure the actual physical processes like eddies, high vorticity regions, large structures which stretch and engulf and so on. However, the cautious application and interpretation of turbulence models have proved to be a valuable tool in engineering research and design, despite their physical deficiencies.

A turbulence model is a set of equations which express relations between the unknown terms appearing in the time averaged Navier–Stokes equations and the known quantities. Two equation turbulence models are the simplest ones that promise success for flows in which length scales cannot be prescribed empirically. The k-ε model is the most widely tested model for a variety of complex flows. Many modifications such as multiple scale k-ε models or extra terms to compensate the shortcomings of standard k-ε model have been developed. At present, the two-equation model forms the basis for most engineering simulations of complex flows. More advanced models which do not use the assumption of isotropic turbulent viscosity or the concept of turbulent viscosity itself have been developed (algebraic stress models and Reynolds stress models). Recently, renormalization group theory based (RNG) models of turbulence have been developed[4,5]. In RNG based k-ε model, the values of model parameters are evaluated by the theory. Moreover, the modifications of standard k-ε model like low Reynolds number modification, extra term of rate of strain are given by the RNG theory. While these models have not yet been sufficiently tested for engineering flow simulations, the initial results are promising. Considering that the framework of the standard k-ε model can be readily extended to RNG based k-ε models, the standard k-ε model is recommended for initiating simulations of industrial flow processes.

Multiphase flows are encountered in a variety of important industrial processes. For example, dispersed two phase flows are involved in steel making, cement manufacturing, polyethylene and polyvinyl chloride manufacturing, the fertilizer industry and in thermal power stations. It is indeed necessary to adequately represent the underlying physics of interaction of multiple phases in their mathematical models. An extensive literature exists on the modelling of dispersed two phase systems (reviewed recently by Ranade[3] and Sommerfeld[6] among others). There are two principally different approaches to simulate dispersed two phase flows, namely, the Eulerian/Lagrangian and the Eulerian/Eulerian approach. When dispersed phase hold-up is not very small and dispersed phase is introduced through a distributed inlet

Box 1. Computational Fluid Dynamics Framework

- **Transport equations**
  - + Modelling of turbulence (Refs. 5, 30, 31)
  - + Modelling of multiphase flows (Refs. 3, 6, 9, 32)
  - + Modelling of rheologically complex fluids (Ref. 11)
- **Numerical solution of transport equations**
  - + Discretization schemes (Refs. 12–14)
  - + Solution algorithm (Refs. 14, 15, 33)
  - + Solution of algebraic equations (Ref. 34)
- **Computer codes for CFD simulations**
  - + In-house codes (Refs. 16, 17)
  - + Commercial codes (Ref. 18)

rather than a single nozzle, it is easier and more efficient to use Eulerian/Eulerian approach in which both the phases are treated as continua.

Interphase coupling terms make two phase flows fundamentally different from single phase flows. In addition to the standard drag force, there are several other forces like virtual mass force (arising from the inertia effect) and Basset force (due to the development of a boundary layer around a bubble) which appear in the interphase coupling terms. An order of magnitude analysis presented by Hunt *et al.*[7] suggests that for large vessels ($D > 0.15$ m), where the square of the terminal rise velocity of bubble would be smaller than the product of the gravitational constant and characteristics length scale, the interphase coupling term will be dominated by the drag force term. Various correlations are available to estimate the value of drag coefficient appearing in the interphase drag force term[8].

For turbulent two phase flows, one can either use a standard Reynolds averaging procedure or one can use a practice similar to 'Favre' averaging in compressible flows. The time averaging of interphase interaction terms is tedious and involves several correlations. Johansen[9] has derived an approximation for the low dispersed phase holdup case with the particles following Stokes law considering all contributions (drag, virtual mass, history term and lift force). The assumption of gradient transport can be used to model the correlation between fluctuating velocity and dispersed phase holdup. The gradient transport is strictly valid only when the size of the energy containing eddies is much smaller than the distance over which dispersed phase hold-up varies significantly. It should be noted that in principle, the value of turbulent Schmidt number used in such gradient transport will depend on the size of dispersed phase particles and integral scale of turbulence. Turbulent eddies smaller than dispersed phase will not contribute to the dispersion of dispersed phase particles. At present, however, there is no systematic data or theory available to estimate the values of Schmidt number for turbulent, two phase flows. The user, therefore, has to exercise his/her discretion is setting these values and interpreting the results.

There are a variety of different flow processes, not covered in the above discussion. For simulation of granular flows, additional modelling of stress in moving assembly of solid particles, viscosity of solid phase and effective pressure for solid phase need to be incorporated in the flow model. There is also a large class of industrial flow processes which involves laminar flows of rheologically complex fluids like polymer melt, inks, pains and detergents. Several studies and reviews on modelling of different classes of flows (for example, Gidaspaw[10] for granular flows and Crochet *et al.*[11] for non-Newtonian flows) are available. Without describing these issues in detail, we now discuss some aspects of numerical solution of transport equations.

Numerical solutions of transport equations

Numerical solution of transport equations mainly comprises the discretization of the governing equations and the solution of the resulting algebraic equations. Discretization of the governing partial differential equations can be done using finite difference, finite volume or finite element frameworks. The finite element methods have not yet been rigorously tested for multiphase flows in three-dimensional domains. The memory requirements of these methods are also much larger than the corresponding finite volume methods. For equipment engineering applications, conservative form of the governing equations discretized using finite volume methods is most appropriate (at least at present) from the point of view of accuracy and economy of computational resources.

The accuracy of a numerical solution depends on how close by the discretized equations represent the original partial differential equations. The desire to use higher order approximations for discretization must be balanced against the limitations imposed by the complexity of the problem being solved, the availability of the computing resources, stability and convergence of the solution algorithm and capacity to tolerate unphysical over and undershoots. Among the various schemes, QUICK (or in modified form of SHARP[12]) and second order upwind differencing schemes[13] look more attractive from the point of view of accuracy and ease of implementation. In complex multiphase flows, a hybrid or power law scheme[14] is recommended at least at the beginning.

The selection of algorithm for solving the transport equations requires consideration of the coupling and signal propagation among the equations (and boundary conditions). It must be realized that there is no single best algorithm for all types of problems. One has to make a choice by evaluating convergence performance and ease of implementation. For multiphase flows, additional coupling between two phases through interphase forces need to be handled. Spalding[15] has proposed an inter-phase slip algorithm (IPSA) for this. In most of the two phase flow cases, the choice of algorithm for pressure–velocity coupling is often dictated by transparency and ease of implementation. After selecting a suitable algorithm for treating velocity–pressure coupling, the task that remains is to devise a suitable method to solve finite difference equations to obtain values of variables at all grid nodes. Because of interconnectedness and non-linearity, the task must be performed by iterative methods. Various methods such as point by point iteration (Gauss–Siedel or successive over-relaxation), linear

Gauss–Siedel and strongly implicit procedure (SIP) have been used for solving single phase flows. Convergence of pressure correction equation is often a rate limiting step especially for single phase flows. The rate of convergence depends quite strongly on the choice of under-relaxation parameters. Various techniques including methods based on additive correction philosophy have been proposed to enhance the convergence rates. Recently multigrid techniques have been shown to be very efficient in enhancing the convergence rates. Existence of dispersed phase raises further hurdles in the convergence of the iteration procedure because of additional coupling through the interphase terms. Spalding[15] has proposed partial elimination algorithm (PEA) to treat the interphase coupling efficiently. PEA involves manipulation of finite difference equations of the velocities of both the phases at the grid node to eliminate the velocities of the second phase from the finite difference equations.

Computer codes for CFD simulations

It is necessary to translate the already described solution procedure into computer codes to generate useful simulations of engineering equipment. A CFD code needs to be designed to give appropriate importance to general applicability, ease of use and economy of computations. Recently Cross *et al.*[16] have discussed the trends in CFD software engineering which are useful for the few code developer.

Our group (iFMg) has developed a CFD code called *SPARE* (for *SPA*rged *RE*actors) based on a partial elimination algorithm (PEA) and an inter-phase slip algorithm (IPSA, ref. 15) along with the SIMPLER algorithm[14]. The sets of discretized equations for each variable are solved iteratively by means of an ADI technique. The non-linearities in the phase momentum and turbulence equations are handled by standard under-relaxation techniques. The core subroutines and problem specification routines have been organized in separate groups. The major routines are designed in such a way as to enable the user to construct various algorithms by modifying just one program. All the empirical information and boundary conditions can be specified through a single routine[17]. The performance of *SPARE* has been extensively tested both qualitatively as well as quantitatively[3].

Instead of expanding the capabilities of an in-house research purpose code to carry out complex engineering flow simulations, it might be more efficient to use a commercially available general purpose CFD code. The development of a suitable mathematical model can be done using an in-house CFD code. The validated model can then be incorporated within the commercially-available code to carry out real life simulations. A number of CFD codes are available commercially (recently reviewed and compared by Dombrowski *et al.*[18]), each with its own particular set of features. Most of these codes provide user-friendly facilities for modelling complex geometries and grid generation. The powerful postprocessing facilities developed by professional programmers also aid user interpretation of simulated results. It should be noted here that though a variety of ready-to-use commercial codes are available, the experience and insight gained through the use of in-house codes turns out to be very valuable. The most important feature of the CFD code from the point of view of industrial application is the ability to incorporate or extend the code via user-written modules. Because no matter how general the code is, it will be necessary to develop specific submodels to simulate specific processes. Many of these commercial codes provide the ability to incorporate user-defined physical property models, source terms and new numerical features.

Methodology of flow modelling

Steps in a typical flow modelling project are described in Box 2. The first step of any flow modelling project is to relate the fluid dynamics with the overall objectives of the project and its implications for the performance enhancement. The complexity of the flow modelling tool can then be decided to achieve the set objectives. It is also essential to understand and quantify various time and space scales and the geometric complexity of the

Box 2. Typical flow modelling project

- **Problem definition**
  + Identify key processes governing the overall performance
  + Relate these processes with fluid dynamics of the process equipment

  = **Interaction with design and operating teams**
- **Development of generic flow model**
  + Turbulence
  + Multi-phase flows
- **Development of specific sub-models**
  + Reaction source terms
  + Physical property models
  + Interphase transport models
- **Mapping these models onto CFD solver codes**
  + Grid generation
  + Solution parameters
  + Post-processing strategies
- **Validation of the CFD model**
- **Application for design and process optimization**

system. This will enable one to represent the problem at hand in a mathematical framework. After finalizing the objectives and mathematical model, the next step is to map this mathematical model onto the computer code. The mapping of flow model mainly consists of specifying the geometry of the equipment under study, generation of appropriate grids within the solution domain, setting terms in the transport equations included in the CFD code or supplying additional problem-specific submodels to the CFD code and specification of corresponding boundary conditions. Prior knowledge of the various scales and likely regions of steep gradients will help in generating a suitable grid for the problem at hand. While generating the grids, extremes of aspect ratios and skewness should be avoided. The grid orthogonality has relatively little impact on flow accuracy in general, provided the angle between grid lines is not too small.

Once the appropriate grid is generated, the user has to select/specify the necessary information about the properties of fluids like molecular viscosity, density, conductivity. The correct specification of boundary conditions on the edges/external surfaces of the solution domain is crucial for the correct mapping of the problem. Care must be taken to understand and eliminate the influence of the location of outflow and inflow boundaries on the predicted flow results. Wall functions are routinely used to provide boundary conditions near the wall for turbulent flows which avoid the necessity of using very fine grids near the walls. However, one must be careful about such usage especially when heat or mass transport from the wall is important or when the accuracy of calculation of forces exerted by fluid on walls is important.

Once the problem has been mapped onto the CFD code, a user is interested in knowing details of simulated results. However, it is extremely important to understand the sensitivity of the predicted results to a variety of parameters like grid spacing, time step, boundary conditions and so on. This will normally involve some preliminary simulations to arrive at desired values of a variety of parameters involved in the simulations. It is often convenient to use grid sequencing techniques to solve complex problems. Normally, converged results can be obtained rapidly for the small number grids even with zero initial guess for all over the solution domain. These results can then be interpolated and used as initial guesses for the finer grids. It is also often desirable to increase the complexity of the problem in steps after starting with the most simplified situation. Underrelaxation factors for the different variables need to be employed appropriately to enhance the overall convergence rates. Patankar[14] has listed many suggestions in this regard. The monitoring of convergence for each equation can also give clues about how to enhance the overall convergence rate of a CFD code.

Once the results are obtained on a sufficiently fine grid, it is necessary to formulate effective post-processing strategies to display these numerical solutions so that many aspects of the flow structure can be carefully studied. Appropriate validation exercise can then be carried out to verify whether the CFD model has captured the important flow characteristics of the problem at hand. The validated flow model can then be used to understand the various features of fluid dynamics and its relation to the process performance. The insight gained through such an exercise may lead to the evolution of better configurations or better operating protocols which will eventually lead to enhancements in process performance.

Flow modelling examples

Mixer design

Stirred mixers are among the most common process equipment in the chemical and allied industries. In such mixers, the contained fluids are circulated by the rotating impeller. The flow around the impeller interacts with stationary baffles and generates complex, three-dimensional, inherently unsteady flow. The fluid dynamics and therefore, the performance of the mixer depend on a variety of design and operating parameters such as size, number and shape of impeller blades, location of impeller(s), number of impellers, etc. Considering the

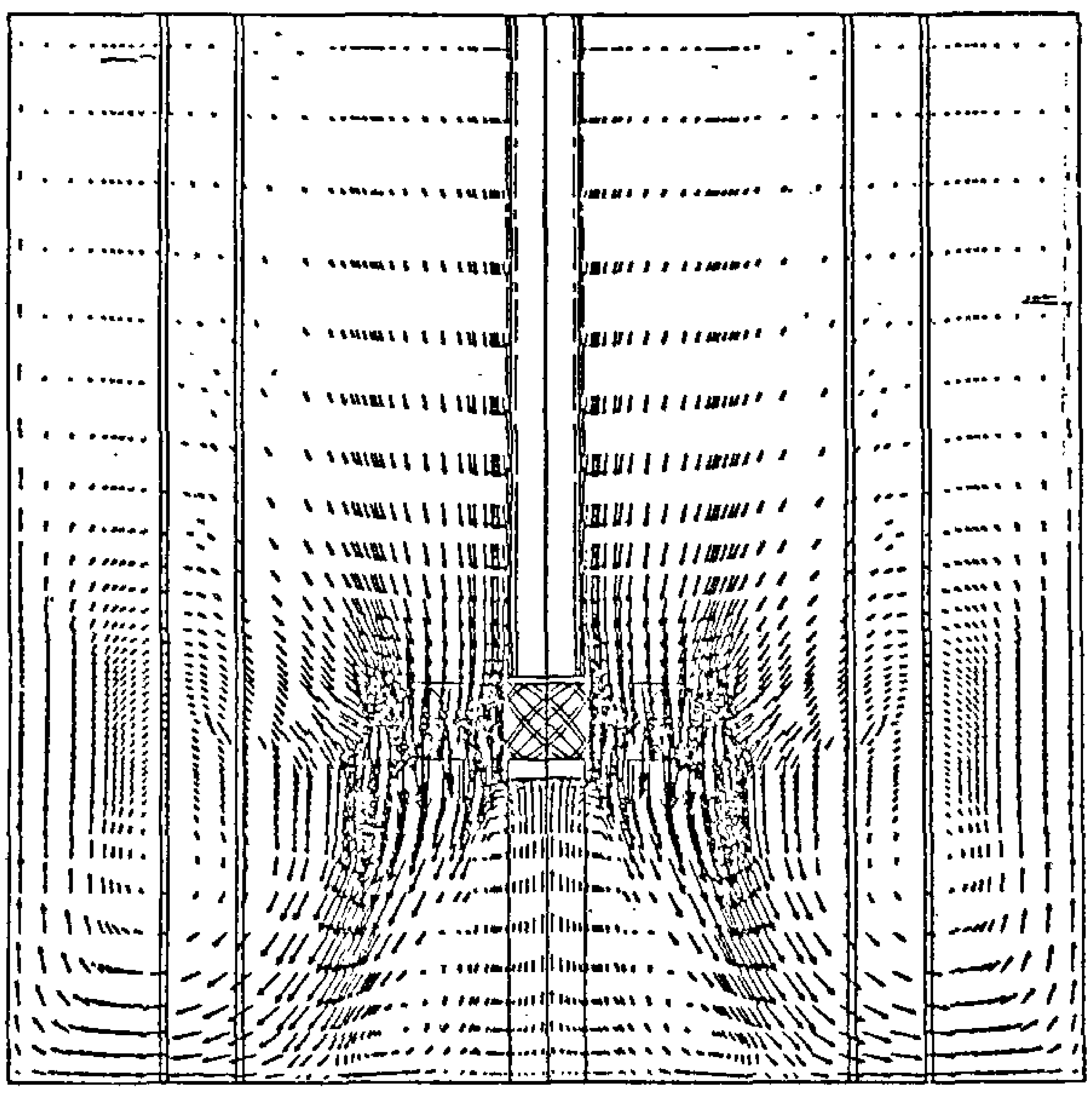


Figure 1. Stirred vessels (from ref. 19). Predicted vector plot at midplane between the baffles $D = H = 0.3$ m, downflow, pitched blade turbine, turbulent regime. D, vessel diameter, H, height of the reactor.

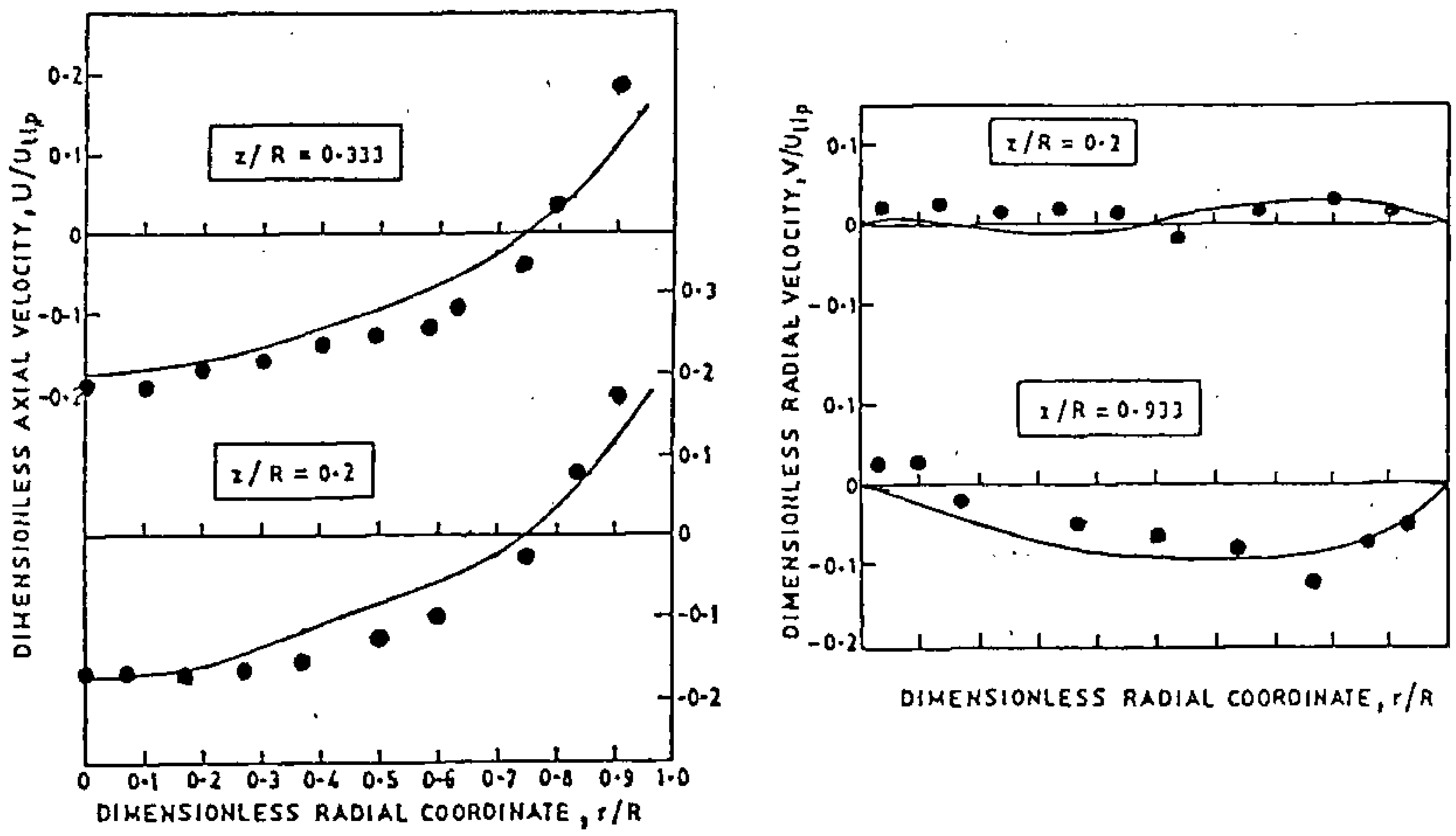


Figure 2. Stirred vessels (from ref. 20). Comparison of predicted mean velocity profiles with experimental data $D = H = 0.3$ m, disc turbine, turbulent regime.

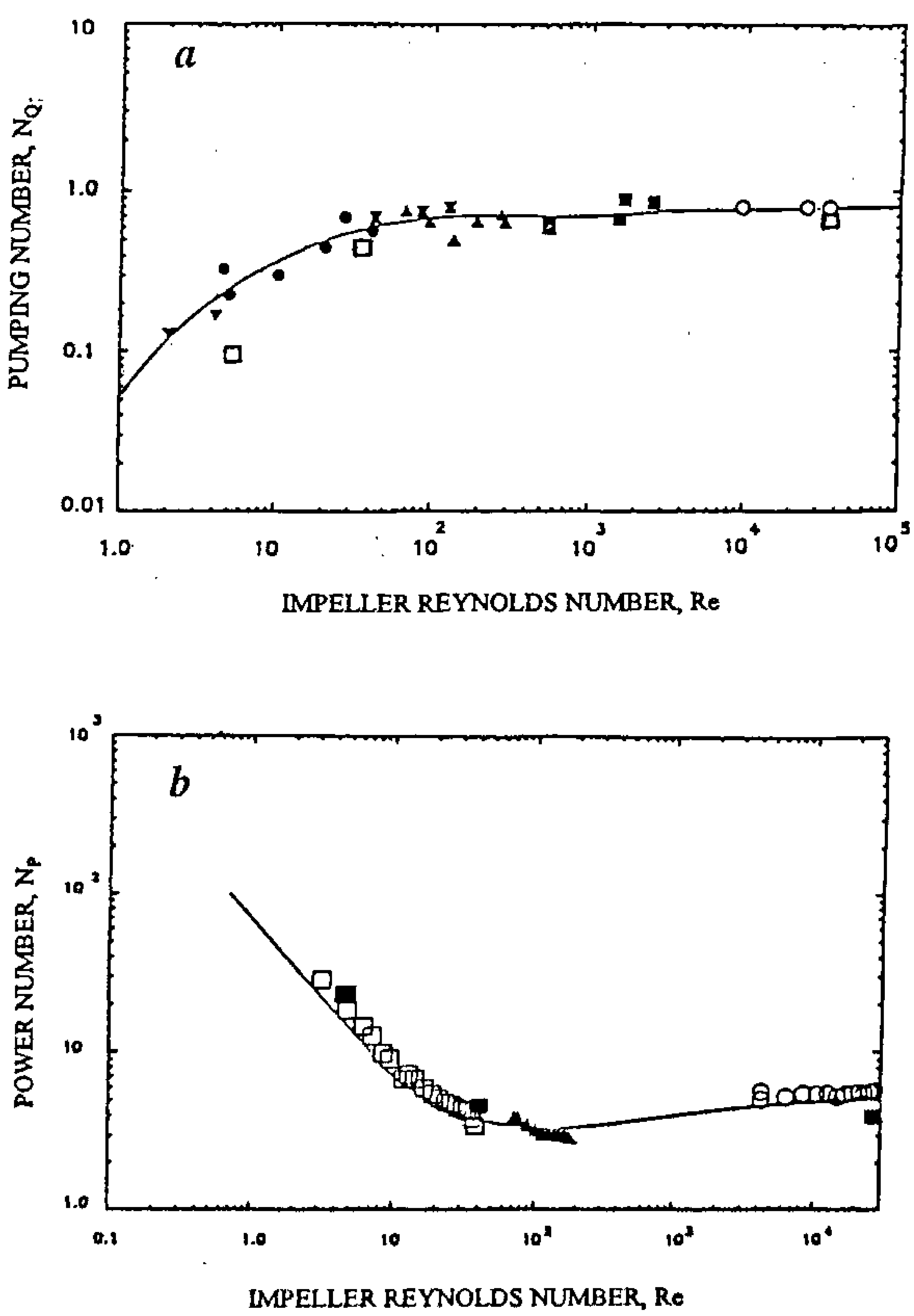
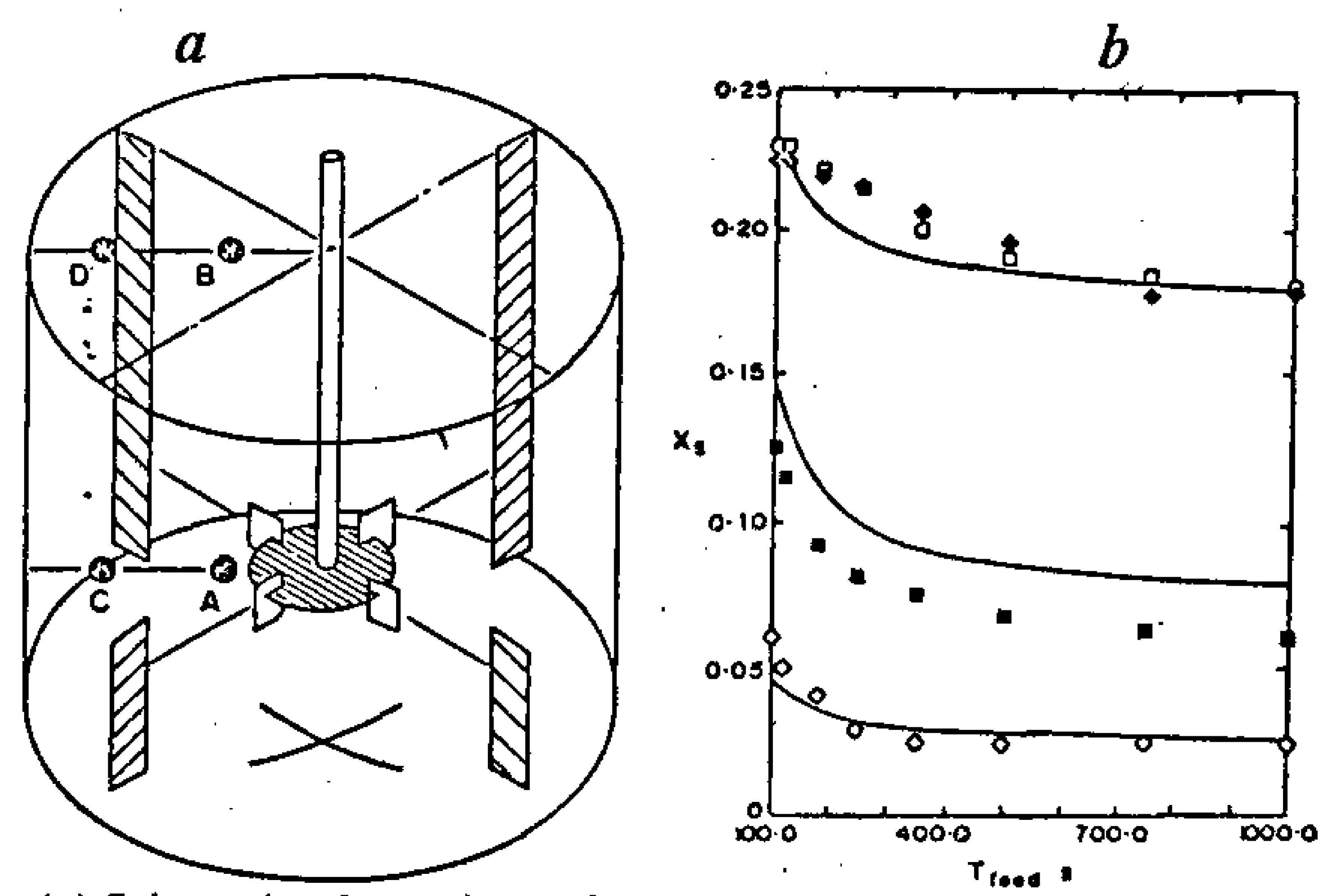


Figure 3. Stirred vessels (from ref. 20). Comparison of overall impeller characteristics with experimental data $D = H = 0.3$ m, disc turbine, turbulent regime.



(*a*) Schematic of experimental set-up

$T = 0.3$ m and 0.45 m
$H = T$, $H_C = T/3$, $D = T/3$ Impeller – Rushton turbine

Feed point	r/R	z/R
A	0.368	0.0
B	0.368	1.22
C	0.690	0.0
D	0.690	1.22

H_C, Clearance of the impeller from the vessel bottom

(*b*) Comparison of different feed locations

$V_A = 0.019$ m^3, $C_{B0} = 11.82$ mol/m^3, $N = 156$ r/s,
$N_{A0}/N_{B0} = 1.1$, $V_B/V_A = 0.01$

Symbol	Description
◇	Feed point A
■	Feed point B
◆	Feed point C
□	Feed point D
–	model

N, Impeller rotation speed.

Figure 4. Reactive mixing in stirred vessels (from ref. 22).

large parameter space, conventional design procedures rely on thumb rules and empirical correlations. New and innovative designs are often sidelined because of time and resource constraints on carrying out experimental studies. Flow modelling will prove to be an ideal tool to understand the fluid dynamics and performance of these mixers. The validated flow models can be used to screen the large parameter space to identify most promising configurations. The complex interactions of baffles, internals (like coils/spargers), shape of the vessel and impellers can be conveniently studied using the flow model.

We have developed a computational model, based on quasi-steady state approximation, to simulate flow generated by a variety of impellers in fully baffled stirred mixers[19,20]. The vector plot of the predicted flow field generated by a downflow pitched blade turbine (PTD) is shown in Figure 1 for a typical r-z plane. This figure shows the well documented flow pattern of PTD. It should be noted that these results were obtained without using any empirical impeller boundary conditions. The model predictions also show satisfactory quantitative agreement with the experimental data (Figures 2 and 3) over the wide range of impeller Reynold number. The computations also revealed a wealth of details about the flow structure around the rotating impeller blades which are hard to obtain experimentally. The flow model adequately captures the influence of impeller location, blade width, blade angle, etc. on the generated flow and mixing. Other important details like interaction of baffles and rotating impellers, fluid forces on the impeller blades can be analysed using the flow model. The predicted flow results will therefore be useful for analysing and improving the blending, solids suspension, residence time distribution and scale-up performance of the mixers.

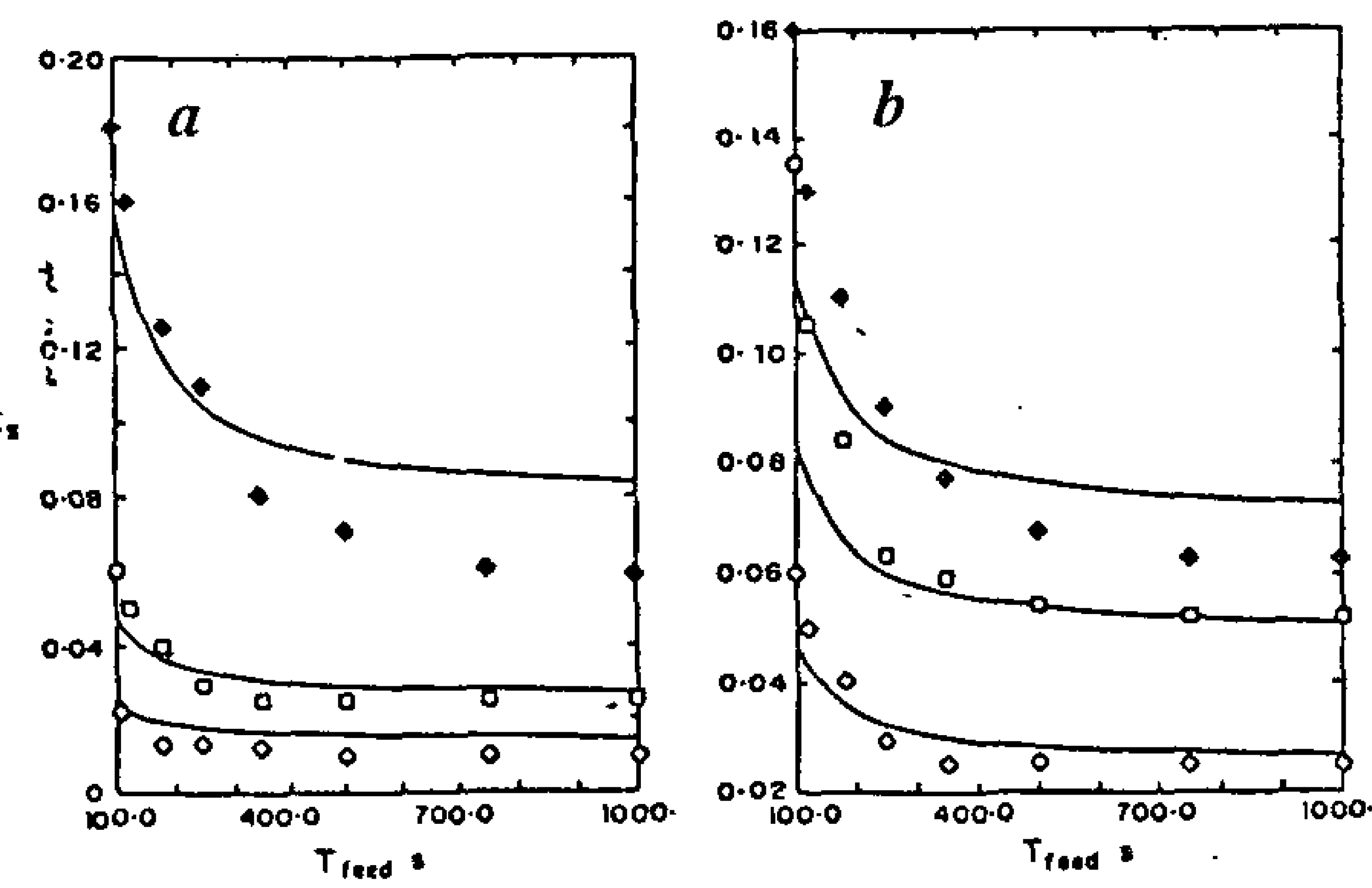
Enhancing selectivity of series–parallel reaction system in stirred reactor

Many high-value chemicals (pharmaceutical products) are manufactured in stirred semi-batch reactors, in which the limiting reactant is added continuously to maximize the yield of the desired product. If the chemical reactions are fast, the yield and selectivity is mainly a function of mixing[21]. A variety of design parameters such as feed pipe location, feed pipe, impeller type and location, etc. affect the overall performance of such reactors. A flow model including the reactive mixing will be a very effective tool to optimize these systems.

We have considered a series–parallel reaction scheme carried out in a semi-batch reactor (schematic diagram of the considered reactor set-up is shown in Figure 4 *a*). A model was developed to understand the interaction of turbulent mixing and fast chemical reactions[22]. This reactive mixing model was integrated with the flow model of the stirred reactor (as described earlier). The overall model was successfully applied to predict the yield and selectivity patterns of series–parallel reaction schemes under a wide range of parameters. The comparison of computed results with experimental data is shown in Figures 4 and 5. The model was used to evaluate the influence of feed pipe locations, stirrer speeds, reactant concentrations, reactor size and feed time, etc. on reactor performance. The study resulted in identification of optimum feed pipe location and feed rate of limiting reactants.

Bubble column reactors

A bubble column reactor (in which reactant gas itself provides the required stirring and mixing) offers an attractive way to carry out gas–liquid reactions because of its simple construction and easy operation. However, because of their simple constructions, bubble column reactors also have an inherent limitation of having fewer



a, Influence of stirrer speed on X_s for feed point A. Conditions are same as in Figure 4 except stirer speed.

Symbol	Impeller speed, r/s
◇	3.78
□	2.60
◆	1.26
–	model

X_s, Yield of undesired product.

b, Influence of reactant concentration on X_s for feed point A. Conditions are same as in Figure 4 except reactant concentration.

Symbol	Concentration of B, C_{B0}, mol/m^3
◆	35.46
□	23.64
◇	11.82
–	model

Figure 5. Reactive mixing in stirred vessels (from ref. 22).

degrees of freedom available to control their performance characteristics. In bubble columns, local flow, turbulence and gas hold-up distribution are interrelated in a complex way with the operating and design variables. A detailed flow model therefore becomes a necessity to understand these complex interactions and to interpret the experimental results. One of the major disadvantages of bubble column reactors is the high degree of backmixing prevailing in such reactors. Performance of these reactors can be substantially improved by appropriately tuning the degree of backmixing by employing suitable column internals like radial baffles. Flow models can be advantageously used to minimize the required experiments for identifying suitable internals and for confident scale-up with these internals.

We have developed[23] computational models to make quantitative predictions of turbulent fluid dynamics of bubble column reactors operated in a heterogeneous regime. Two submodels are proposed to account for the influence of bubble wakes and column walls on the motion of bubbles. Model predictions show satisfactory agreement with the published experimental data over the wide range of column diameter and superficial gas velocities. Figures 6 and 7 show the comparison of the predicted results with the experimental data obtained for bubble column of 0.29 m diameter for two different gas velocities. The influence of radial baffles on mixing in bubble columns was adequately represented by the computational model[24]. Detailed three-dimensional predictions along with the submodel for the sparger will provide invaluable information for scale-up and fine tuning of large bubble column reactors.

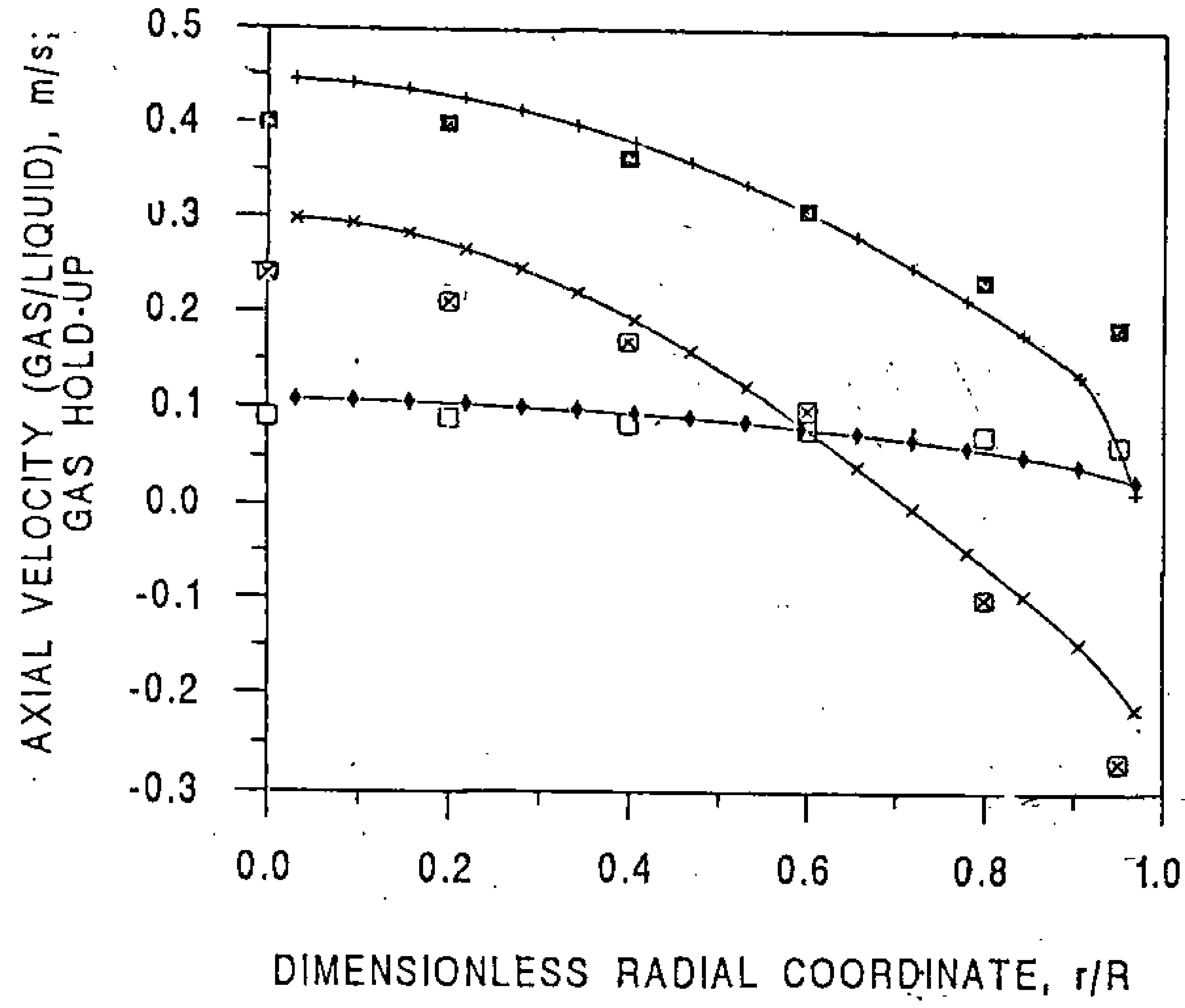


Figure 6. Bubble columns (from ref. 23). Comparison of predicted axial velocities of gas and liquid phase and gas hold-up with experimental data. $D = 0.29$ m, $H = 4.5$ m, gas velocity = 0.02 m/s.

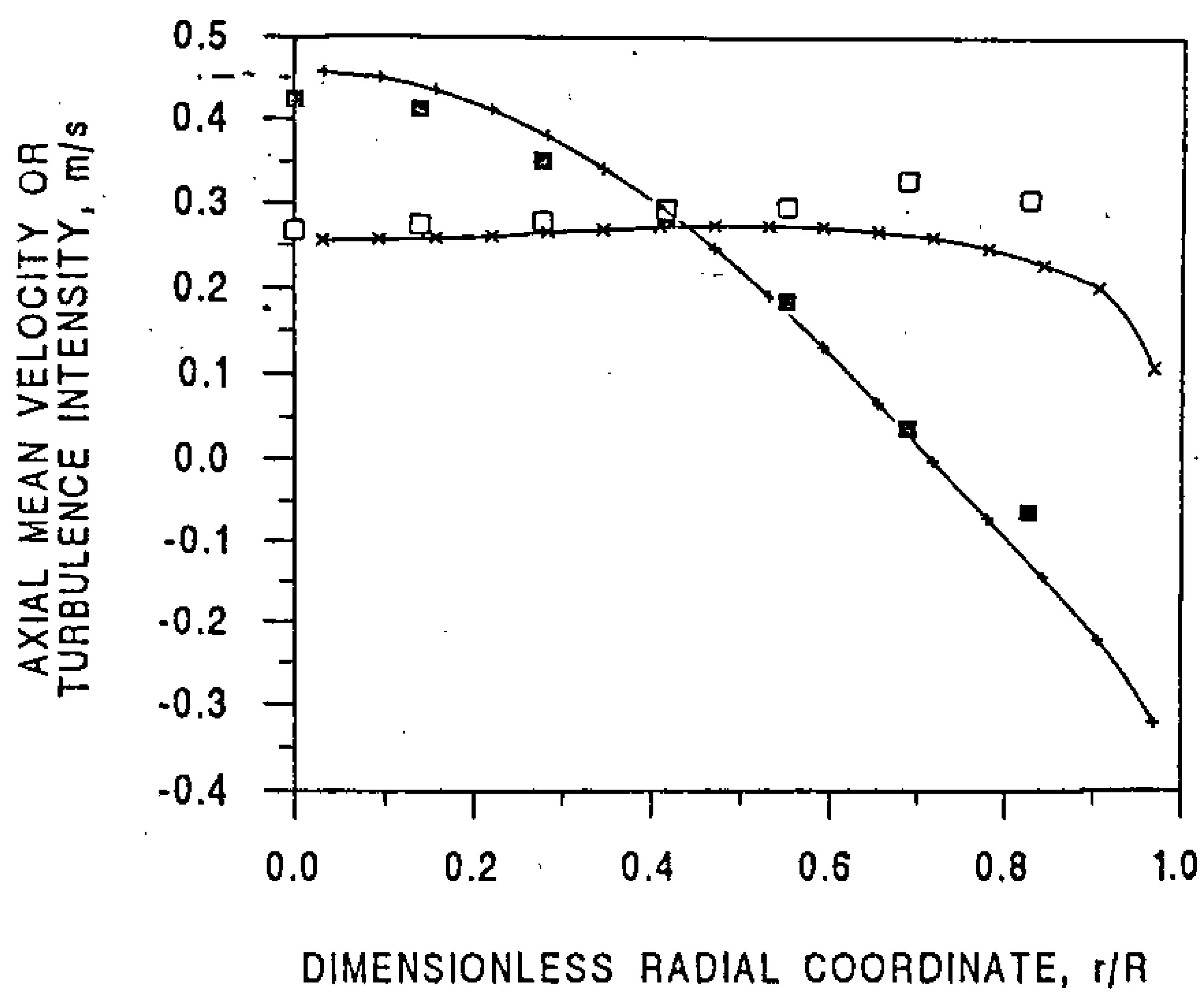


Figure 7. Bubble columns (from ref. 23). Comparison of predicted axial velocity and turbulence intensity with experimental data. $D = 0.29$ m, $H = 4.5$ m, gas velocity = 0.06 m/s.

Fixed bed reactors

Performance of fixed bed reactors crucially depends on the distribution of reactants. Deflection baffles are often employed to evenly distribute the feed vapours coming from the reactor inlet in the form of high velocity jets. A computational model was developed to optimize the design of deflection baffles for an industrial fixed bed reactor. Pressure losses can be accurately predicted. The reaction kinetics can be coupled with the flow model to predict the detailed temperature and concentration fields within the fixed bed reactors. Fixed bed reactors are also used in the radial flow mode for a variety of large scale processes (isomerization of *p*-xylene, ammonia synthesis, etc.). Fluid dynamics of radial flow fixed bed reactors (RFR) is very complex and involves abrupt changes in flow directions. Flow models can help to optimize the shroud and support screen design, to minimize the flow mal-distribution and to enhance the performance of the radial flow reactor. Such a study is recently reported by Ranade[25]. The predicted flow field for three different conditions is shown in Figure 8. The corresponding velocity profiles at the outlet of the catalyst bed are shown in Figure 9. It can be seen that, unless support screens are appropriately redesigned, loading more catalyst in the reactor (by filling zones B and C) may not lead to the desired increase in the throughput of the reactor (because of the severe mal-distribution evident from the profile *b* of Figure 9). Detailed flow modelling and simulations are therefore necessary to realize the full potential of the available catalyst (and to develop better understanding and insight).

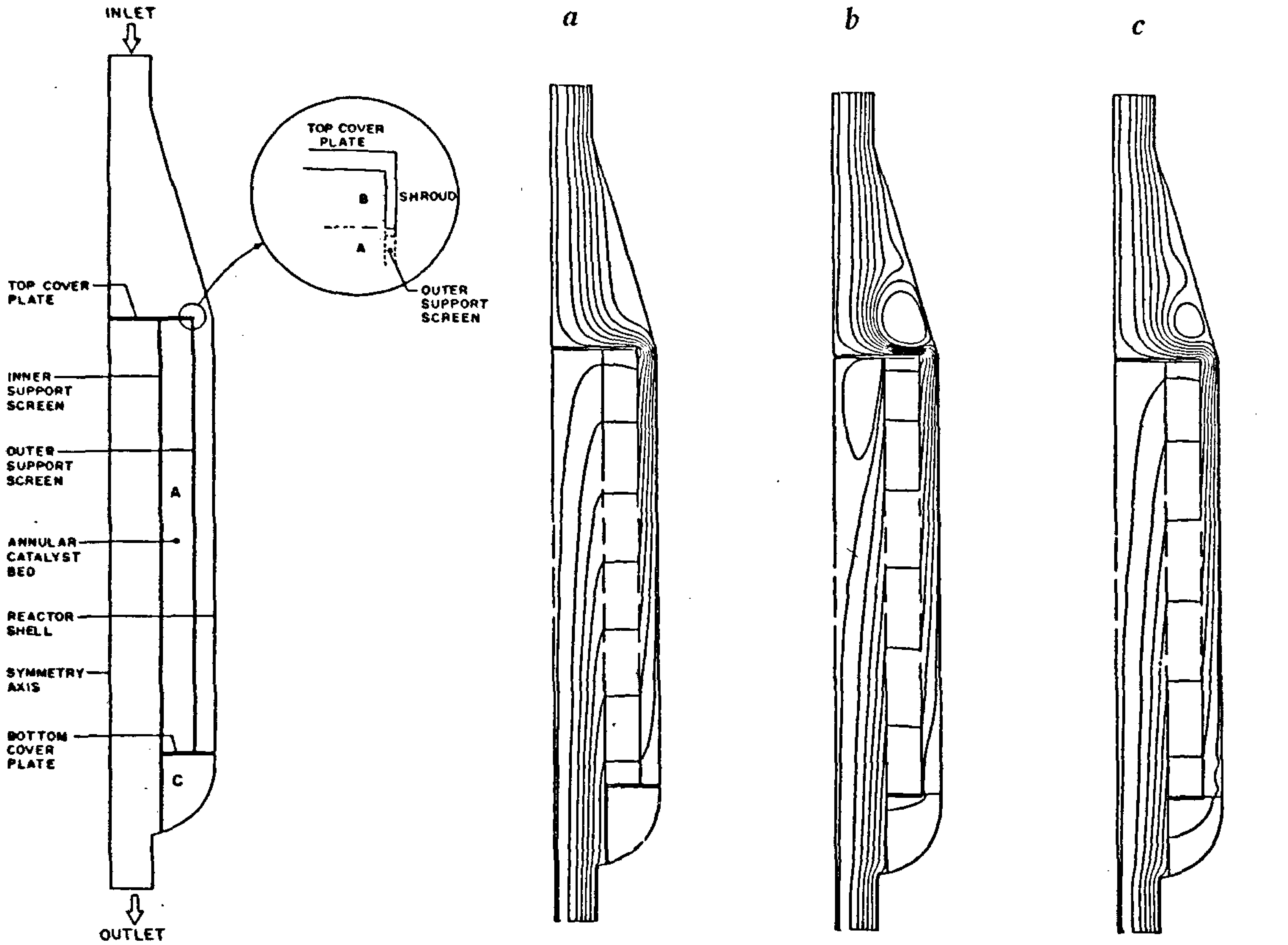


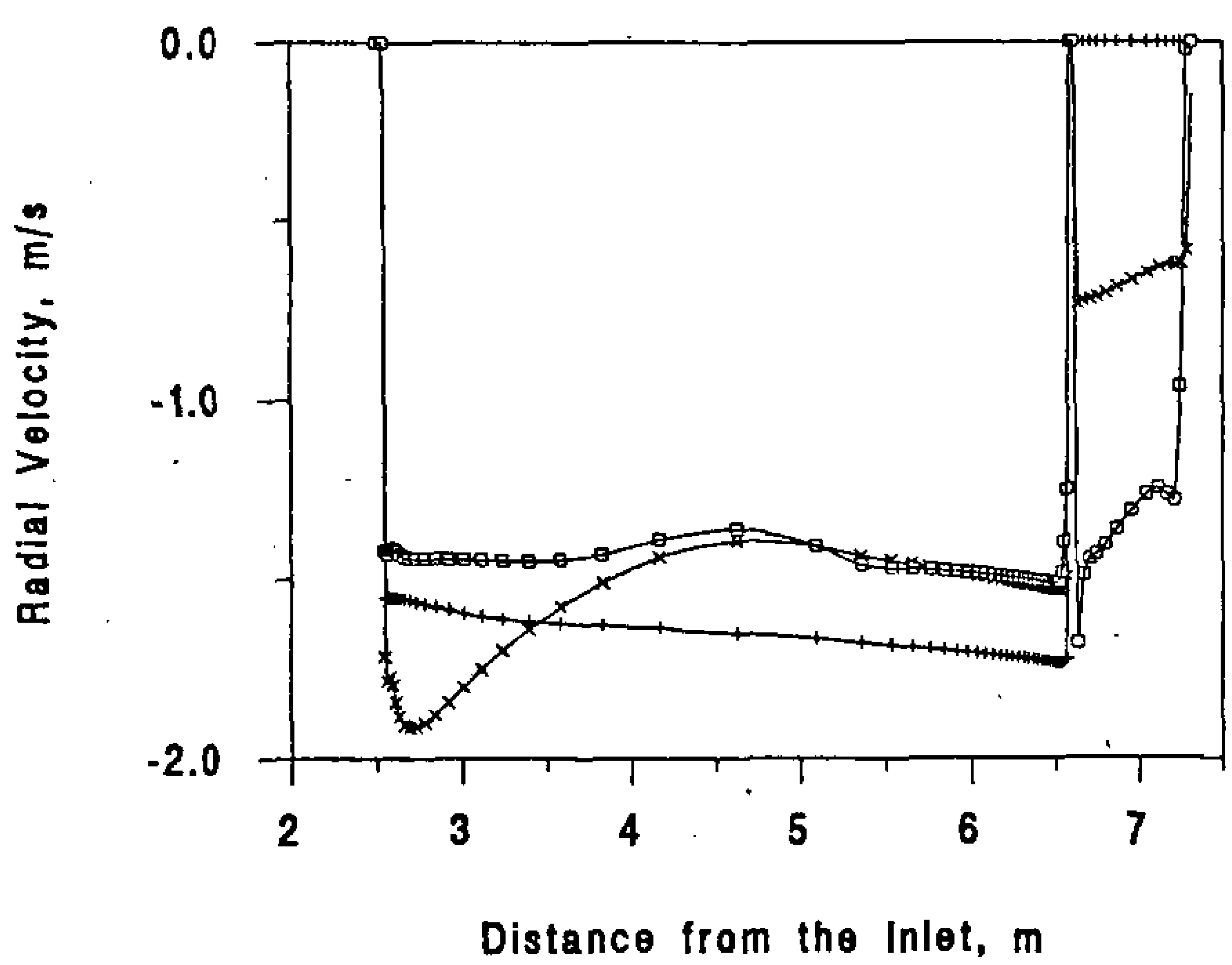
Figure 8. Radial Flow Reactor (RFR) (from ref. 25). Contour plots of stream function. Comparison of predicted flow field for three different configurations of RFR. ***a***, Catalyst in zone A, top cover plate with shroud; ***b***, Catalyst in zones A, B and C, no shroud, with screens same as in *a*; ***c***, Catalyst in zones A, B and C, no shroud, with adjusted screen resistances.

The list of applications of flow modelling may be enlarged to encompass almost all types of process equipments. We have carried out flow modelling of jet mixers[26], flow meters[27], polymerization reactors, etc.

Industrial flow modelling: The Indian scenario

The opportunities and potential for enhancing performance of the existing assets of Indian process industries are truly enormous. Apart from improving the utility of existing assets, flow modelling tools offer a unique opportunity to bridge the gap between technology suppliers and technology buyers. The expertise built over the years of experimentation can now be developed within short span with substantially less resources by judiciously using flow modelling tools and expertise. Successful realization of these potential improvements depends on several factors. Two of the most crucial factors are availability of flow modelling expertise to solve practical problems and willingness and commitment of Indian industries to upgrade their technologies by investing in indigenous flow modelling research.

Basic flow modelling requires expertise in fluid mechanics and numerical techniques. However successful modelling of industrial flow processes requires much more knowledge and expertise than just these two fields. More often than not, industrial flow problems cannot be modelled rigorously. Broad-based chemical and process engineering expertise along with the knowledge pool on different fields ranging from estimation of physical properties, rheology to kinetics and catalysis is therefore essential. New approaches of flow modelling need to be developed to make the complex industrial problems tractable without jeopardizing the objectives. We have made a small beginning at National Chemical Laboratory (NCL) by initiating an 'industrial flow modelling



Symbol	RFR configuration (as denoted in Figure 8)
+	(a)
×	(b)
□	(c)

Figure 9. Radial Flow Reactor (from ref. 25). Profiles of radial velocity at the bed outlet.

group (iFMg)'. We have an advantage of availability of a large chemical and process engineering knowledge pool at NCL. We are working on a variety of performance enhancement projects sponsored by Indian as well as multinational companies from abroad.

It is, however, essential to form a critical mass of industrial flow modellers (from research laboratories and industries) in order to derive the maximum benefits. Many industries in India have purchased commercial flow modelling codes. However, as far as we know, the use of these codes to solve real life industrial problems is very limited. In order to increase the level of confidence in the flow modelling approach, it is necessary to have more interaction between flow modellers and engineers working on practical problems. It may be necessary to form CFD user groups or to organize workshops to facilitate such interaction. (In October 1995, we had carried out one such workshop, along with the applications group of C-DAC, on industrial flow modelling.) This will help us to address the crucial question of availability of the required flow modelling expertise.

The other key factor of willingness of Indian industries to invest in flow modelling research also needs to be discussed here. Complex industrial flow problems cannot be solved in a few days. In the initial stages, it is indeed necessary to painstakingly build the required expertise to solve industrial flow problems either with indigenous or commercial CFD codes. Indian industry should, therefore, be willing to invest funds to develop such an expertise and computing facilities for realizing the potential performance enhancements. Considering the costs involved (of manpower, hardware, software and other facilities), it may be worthwhile to formulate a consortium of industries (private as well as public sector) to fund such research on flow modelling of industrial processes.

It must be added here that first rate work on modelling of industrial processes can be sustained only if it is backed up by basic research in complex flows. It is necessary to identify short and long term goals for further research on both computational as well as physical aspects of industrial flow modelling. The most important areas of computational character in which further work is needed are:

- ways of conducting fine-grid computations cheaply;
- minimizing numerical diffusion without jeopardizing the robustness;
- preserving order and flexibility in CFD codes as the complexity of their physical content increases.

Further research on problems of physical character primarily concerns the development of better turbulence models and formulation of tractable approaches for simulating industrial flows involving inherently unsteady large scale flow structures. Recent advances in applying renormalization group (RNG) theory need to be explored further. The consortium mentioned earlier should therefore also invest part of their funds for such basic research. Such investments on flow modelling research will help us to bridge the gap which separates us and technologically advanced nations.

Concluding remarks

In this review, we have described the overall methodology for modelling of industrial flow processes. The opportunities and potential of using flow modelling techniques for realizing performance enhancement were discussed. The basic framework of computational fluid dynamics was described. Application of the suggested methodology was illustrated with the help of case studies.

Predictions of CFD models can go wrong for two main reasons (other than human error and machine malfunction): they may be based on physically incorrect mathematical representations of basic physical phenomena or upon numerically deficient representation (incorrect discretization, inadequate resolution, incomplete convergence and so on). The inadequacies of the later kind are easier to quantify. The bounds of numerical accuracy of the specific code can be obtained by comparing results with the analytical solution of some simple but representative problem. Villasenor and

Spalding[28] have presented 14 flow problems which can be used for the benchmarking exercise. Recently Haworth *et al.*[29] proposed a useful approach to error estimation and physical diagnostics in multidimensional CFD simulations. Only a carefully planned validation and benchmarking exercise can transform the CFD model and code into a useful design tool. Inadequacies of the mathematical model are almost always present because the physics of complex, turbulent and multiphase flows is not yet properly understood. It is the duty of flow modeller to identify those aspects of flow, which are crucial to process performance and represent it with adequate accuracy in the mathematical model.

Despite their limitations, computational fluid dynamic models have been shown to be capable of predicting detailed flow fields within industrial process equipment. CFD models can also be used to study aspects of flow which are not easily amenable to experiments (e.g. high temperature). This unique capability of a computational tool may have most impact on equipment engineering practice. Detailed flow modelling of industrial processes offers new possibilities for performance enhancement and innovation in the design of process equipments. With the emergence of cheap, high speed computing platforms and availability of the commercial CFD codes and support, flow modelling needs to be properly exploited by the process industry to maximize the performance of the various processes and process equipment.

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