International Seminar
Stirring and Mixing
Applications of Modern Experimental and Numerical Methods

Erlangen, October 25th to 28th

Development of Mixing Technology – State of the Art and Unsolved Problems

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Abstract:

State of the art of mixing operations [1] reveals a remarkably high standard of this process operation and also discloses some deficiencies in the research and development of it. – In the past, R&D was carried on by 1. Universities; 2. Providers of mixing equipment (mixing firms); 3. Users of mixing equipment (large chemical companies, etc.). Each of them has specific incentives for and different possibilities in performing R&D which on the one hand favours the achievements and on the other hand gives reason for blunder and failure.

Universities stick to the basic research which often takes years to accomplish and therefore do not consider current needs of the industry (which is one of the major taxpayers!). As a result, their contributions to the solutions of ecological problems (waste management) and to the modern mixing tasks in biotechnology (shear damage on microorganisms, mixing of highly non-Newtonian fluid, etc.) have been marginal. – Due to the restrictions in laboratory space and lack of technical application their results often do not represent a reliable scale-up criteria and neglect the energetic aspects.

As a result, mixing firms and users of mixing equipment have to bridge the missing knowledge by their own research. Very often they have only a limited time left for it. This leads to solutions which are restricted to the considered process. This fact is often neglected and leads to applications in areas where solutions would be superior. A problem common to suppliers and users is the fact that they do not pass on their achievements to others. – It must also be stated that mixing firms still stick to mixers as mixing devices and neglect the advantages offered e.g. by nozzles, dispersers, etc.

The biggest problem common to all of the three institutions is the disregard and even the abuse of the methods provided by the dimensional analysis [2]. A further major disadvantage is caused by the unnoticed distinction between the micro- and macromixing and their influence on mixing operations.

[1] M. Zlokarnik: "Rührtechnik – Theorie und Praxis", Springer-Verlag 1999.
[2] M. Zlokarnik, Chem. Eng. Sci, 53 (1998) 17, 3023 – 3030: Problems in the application of dimensional analysis and scale up of mixing operations.

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An Introduction to Míxing Tasks

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Abstract:

This paper reviews the challenges and rewards presented by modern mixing technology. The aim is almost never fluid blending for its own sake, in practice the main objective more probably lies in the furtherance of a process. A lack of fundamental knowledge is shown to affect potential profitability because of the liklihood of a waste of material, financial and equipment resources, on a significant scale.

An initial consideration of a range of typical process objectives leads to a discussion of the problems that arise in various operations involving single and multiphase blending, dispersion and suspension. Most common process difficulties arise when there are conflicting requirements between the properties of the systems and the objectives. Equipment selection and operational protocols are often a compromise. For example, the rheology of the starting materials may suggest a suitable type of equipment for the mixing operation, but the choice of processing route determines the properties of the final product. Similar considerations arise for many mixing operations with multiphase systems, for example when there is a conflict between product fragility and a process need for rapid reaction or effective suspension.

Possible routes for investigation and analysis are suggested for various process areas. The potential benefits of reappraising some conventional aspects of process design and operation are also considered.

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Application of Dimensional Analysis and Scale-up in Mixing Operations; An Introduction

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Abstract:

The dimensional analysis is based upon the recognition that a mathematical formulation of a physico-technological problem can be of general validity only when the process equation is *dimensionally homogenous*. Therefore, the aim of the dimensional analysis is to check whether the physical content in examination can formulated in a dimensionally homogenous manner or not.

The transformation of a physical dependency from a dimensional into a dimensionless form is automatically accompanied by an essential *compression* of the statement: The set of the dimensionless numbers is smaller than the set of the quantities contained in them, but it describes the problem equally comprehensively. The *pi theorem* states: Every physical relationship between n physical quantities can be reduced to a relationship between m = n – r mutually independent dimensionless groups, whereby r stands for the rank of the dimensionless matrix, made up of the physical quantities in question and generally equal to the number of the basic quanitites in them.

The representation of a physical problem in a dimensionless form is *independent of scale* ("scale-invariant"), and this presents the basis for a *reliable* scale-up: According to the Theory of models, two processes may be considered completely similar if they take place in a geometrically similar space and if all the dimensionless numbers necessary to describe them have the same numerical value.

Clearly, the scale-up of a desired process condition from a model to industrial scale can be accomplished reliably only if the problem was formulated and dealt with according to the dimensional analysis!

What is Scale-Up in Industrial Mixing Processes?

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Abstract:

The content of the presentation deals with two important general topics related to scale-up: Economical and technical views. Also a comment on the future development trend is given.

The economical view illuminates the impact of successful product launching on business economy. The main factors having direct influence on the new product economy are *development time* and *the pilot investments* during development phase. By using intelligent approach and methodology a chemical company can minimise both of those. This can boost the renewal of product portfolio and still keep the costs in control. This methodology has as an essential element process modelling combined with economical evaluations.

The technical view illuminates what scale-up is all about and why understanding flow of fluid is important. The traditional scale-up way has been to compare or fit certain characterising numbers in different scale. This still is practical in simple scale-up cases. However, in scaling-up fast chemical reactions understanding of basic phenomena like chemical kinetics, mass transfer and particle size formation mechanisms (if two phases) are of crucial importance. These are not independent but all of them are affected by the flow environment. Thus the product quality depend on how well flow can be predicted and controlled in a new or existing reactor. The assumption of ideal mixing should not to be used in case of fast chemicals reactions.

CFD is one of the most interesting near future scale-up tools just because the CFD analysis can *combine the chemicals reactions, particle populations, mass transfer, heat transfer and fluid flow* and thus gives the relevant information on the most important phenomena in a given geometry. This is exactly what makes it powerful. There is still a lot of work to be done in the CFD software development area, but already until today very promising results have been achieved in the recent European Union-funded research programmes.

Methods of Fluid Mechanic for Stirring and Mixing

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Abstract:

In the introductory part of the presentation, the development of fluid mechanics is indicated and it is stressed what methods were available for fluid mechanics investigations during the various phases of stirrer and mixing investigations. Up to recently, investigations had to concentrate on experimental studies which were carried out for pre-determined stirrer and mixed vessels geometries. Results obtained in laboratory investigations needed to be transferred to large scale stirred vessels, and similarity considerations were used for this purpose. As the presentation shows, the reason for going this way was enforced on stirrer and stirred vessel research by the state of the development of methods of fluid mechanics and their applications to practically relevant flows. Developments in the field of high-performance technical and scientific computing has let two methods that permit these days fluid flow investigations in stirred vessels to be carried out numerically. Direct numerical simulations are possible for the Reynolds number range Re = 20.000. In the Reynolds number range: 20.000 = 200.000, the application of large eddy simulations is feasible. For Re > 200.000 it is recommendable to utilise numerical predictions based on the Reynolds equations. This requires the application of turbulence models and the *k-epsilon*-model is usually employed for stirred vessel predictions. New turbulence models are presently being developed for more complex flow investigations. Present and future developments are indicated in the presentation.

The lecture proposes the combined application of experimental and numerical methods to advance the development of stirrer-vessel-combination. The suggested combined application helps to yield improved stirrer designs. An example is indicated and its advantages are outlined.

Advanced Measuring Techniques for Stirred Processes

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Abstract:

The design of stirred processes depends critically on the availability of accurate power consumption, mixing time, circulation time and mean flow and turbulence data. Recently-developed and state-of-the-art techniques for the measurement of these quantities will be described and their methodology, principles of application, advantages and limitations will be assessed. The importance of having precise information and the significance of accurate experimental data for impeller and vessel design will be demonstrated through examples of the effects of impeller blade design and thickness, vessel scale-up and impeller positioning.

Telemetric shaft torque measurement, mixing time measurement through both conductivity probes and liquid crystal thermography, circulation time measurements with miniature flow followers and ensemble-averaged and time-resolved laser-Doppler anemometry techniques will be analysed and characteristic results will be presented.

A case study of impeller development for efficient homogenisation of miscible fluids in stirred vessels will be described and the implications of impeller selection for different mixing tasks will be discussed. The significance of the control of trailing vortices through appropriate blade design will be demonstrated, together with the effect of blade shape on the achievable levels of mean flow and turbulence generation in a stirred vessel.

Application of the Laser-Doppler-Anemometry to Examine Singlephase Flow Fields in Stirred Reactors

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Abstract:

Stirring and mixing processes depend significantly on the flow field that is generated by the employed stirrer element. Beside the large scale flow field throughout the entire stirred tank the flow in the vicinity of the impeller influence considerably the desired process result. The trailing vortex system -near impeller blades has been identified as the major flow mechanism responsible for mixing and dispersion in stirred vessels, and high turbulence levels in the vortices have an important impact on such phenomena as drop breakup and cell damage in stirred reactors. Therefore, flow fields generated in stirred reactors need to be investigated in detail to better understand such flow phenomena and to provide useful indications for the optimization of mixing processes. In addition, detailed quantitative experimental data is essentially required for an accurate validation of numerical simulations.

Laser Doppler anemometry has proven to be more accurate in the measurement of flow fields in stirred tank reactors than any other technique (e.g. Pitot probes, hot-wire anemometers), since (a) it provides flow information even in unsteady and highly turbulent flow regions as well as in the return flow areas of the tank and (b) it operates without fluid contact.

The presentation aims at introducing the laser-Doppler anemometry and to demonstrate how this technique is applied for investigations of stirred vessel flows.

At the LSTM-Erlangen a fully automated, refractive-index-matched stirrer test rig was developed that allows detailed measurements of the flow field to be made angle-resolved laser Doppler anemometry. The large scale flow fields can be investigated as well as the complex flow characteristics in the vicinity of the impellers.

If the LDV-measurements are processed as 360° ensemble-averaged measurements, the fluctuating quantities contain both periodic and turbulence contributions, which can lead to significant overestimation of turbulence quantities in the impeller stream. Such measurements are not suited for validation of numerical simulations; therefore, angle-resolved LDV measurements are required in which the flow information is assigned to the corresponding angle of the impeller.

The flow field within the impeller region (i.e., between the blades) is an important flow region because trailing vortices are generated there. Through exact matching of the refractive index of the stirred medium to the refractive index of the measuring section, it was possible to gain optical access to the inner part of the impeller without any distortion of the laser beams. For this purpose, the vessel walls, the baffles and the impeller blades were constructed from transparent Duran glass with the same refractive index as the working fluid (n = 1.468), a mixture of silicone oils. A high-resolution measuring grid was realized in the entire flow field by automation of the data acquisition, whereby the optical probe was mounted on a 3-D traversing unit controlled by a PC via a CNC-controller.

The results of such LDA-measurements will be demonstrated for two test cases, a pitched blade turbine and a Rushton turbine. The mean flow field throughout the entire reactor will be shown in form of velocity vector plots and the distribution of turbulence kinetic energy in form of contour plots. The flow within and in the immediate vicinity of the impellers will be presented in the form of an animation in which planes at each degree between two impeller blades are shown step-by-step, leading to a rotating impeller movie. With the help of such animations, the generation, development and break-down of trailing vortices can be characterized exactly.

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Examinations of the Flow in Multiphase Stirred Vessels

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Abstract:

In stirred tank reactors exist different multiphase operations. For crystallisation or solid catalysed liquid reactions it is necessary to achieve solid-liquid mixing by suspending solid particles. Liquid-liquid mixing of two immiscible liquids is required to produce a huge interfacial area for extraction processes. Absorption of gas in a liquid, often combined with a chemical reaction, is done by gas-liquid mixing in stirred tank reactors. There exist also operations where a three phase mixture has to be obtained.

This brief introduction makes clear that this topic is very extensive because of the various mixing tasks and the adapted measurement techniques used to describe the process. Therefore this talk focuses on the phase Doppler method which could in principle be applied to all these mixing operations. It is an optical measurement technique and accordingly there exist some limitations of its application. But with this measurement technique it is possible to provide local information on the flow variables (mean and fluctuating velocities) and additionally on the size distribution of a solid or dispersed phase without disturbing the flow.

As an example flow investigations are demonstrated on gas-liquid dispersion and mixing in stirred vessels. Basic principles of this operation are shown. The physical background of the phase Doppler method is explained. Based on this the design of a phase Doppler set-up is illustrated.
Results of an investigation with an aerated Rushton turbine obtained by the mentioned phase Doppler test rig are presented. The flow field of the bubbles and there local distribution over the tank are shown and discussed.

Determination of Flow Fields in Production Size Reactors

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Abstract:

For the optimum design and operation of stirred tank reactors it is imperative to know about the flow fields inside the reactor. In past times it was not possible to measure the flow field within a large scale reactor with sufficient accuracy or without disturbing the flow fields with the probes. Ultrasonic Doppler Velocimetry (UDV), which takes a measurement of the local velocity based on determining the Doppler deflection caused by a particle in the fluid, allows for the collection of sufficient data about the flow field even in large scale reactors.

The presentation will present the basics of the measurement principle and will show the results gathered on a technical scale and on a production size reactor. It gives special interest to the flow around the collection of heating coils inside the reactors. The stirred tank was equipped with a double pitched-blade turbine.
The results of the Ultrasonic Doppler Measurements have been described with graphical presentations focusing on the relative speed u/u_{tip} and turbulence values.

Main objective of the presentation is to demonstrate that UDV can be used for large scale measurements and therefore is the ideal instrument for the validation of numerical simulations or the optimization of stirred tank reactors. The results from comparisons of the executed measurements with CFD simulations and the results from reactor optimizations derived from the valuable information which was collected will be presented in separate papers.

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Systematic Investigations of Micromixing Phenomena in Stirred Tank Reactors

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Abstract:

The stirred tank reactor is one of the most commonly used reactor-type in the chemical and process industry. It is used for a vast number of processes, which all have different characteristics and demands, many of which are mixing sensitive. For the correct design of the reactor it is important to exactly understand the fluid mechanical behaviour of the system mixer/reactor and the mixing times according to a macro and micro scale, otherwise the process cannot run properly. Poor yield and waste of material can be the consequence.

The presentation gives some basic considerations for the design of mixers for micromixing sensitive processes and experimental results collected on a lab scale. The considerations apply turbulence theory towards a basic approach for the mixer design.

For the experimental studies of the mixing phenomena a standard de-colorization method was used to characterise the macro-mixing behaviour of four different mixers. An extensive investigation of the micro-mixing behaviour followed by the use of a jodide/jodade reaction to determine micro-mixedness and segregation. The following stirrers were used in the experiments; two Rushton-turbines with different blade thicknesses, a Pitched-blade turbine, and a Hyperboloid-impeller with different blade heights. Feed time, impeller speed and feed location were varied.

Introduction into Numerical Computation of Flows in Stirrer Configurations

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Abstract:

The talk will give a general introduction into the field of numerical simulations of flows in stirrer configurations, a subject that, due to recent improvements in simulation performance, appears to be of increasing importance in the various industrial sectors where stirring techniques play an important role. The following items will be covered in the lecture:

- Motivation, problems and properties related to stirrers, capabilities of numerical simulations as against experiments
- Examples of practical stirrer geometries
- Problems and methodologies related to grid generation
- Governing equations for laminar and turbulent stirrers, coordinate systems, turbulence modelling aspects
- Discretization techniques and solution methods, moving grids, clicking-mesh, sliding-mesh
- Exemplary computations with FASTEST-3D and STAR-CD of different laminar and turbulent stirrer configurations
- Aspects of numerical accuracy and computational efficiency depending on physical and numerical parameters, comparisons with experiments, comparisons of turbulence models
- Conclusions and future developments

All aspects will be presented in an overviewing character without going into details. However, concrete results of simulations carried out at our department will be presented in order to illustrate the actual possibilities and limitations of numerical simulations in predicting the complex three-dimensional flow fields related to practical applications in stirrer technology.

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Modelling and numerical calculation of multiphase flows in stirred vessels

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Abstract:

Stirred vessels are used for numerous operations in process industries. The design of the process mainly relies on experience accumulated over the years and hence is mainly of empirical nature. However, even for quite simple mixing operations the scale-up from a laboratory vessel to industrial-scale equipment constitutes a large problem. This scale-up problem becomes more severe when two-phase mixing processes are considered, such as the mixing of two immiscible fluids, particle suspensions, and dispersion of gas. Due to the additional parameters and scales being involved a reliable scale-up of these operations is almost impossible.

During the last 10 years computational fluid dynamics (CFD) is increasingly used by industry for supporting the design and optimisation of mixing processes in stirred vessels. The modelling of two-phase flows however, requires the incorporation of many physical phenomena which lack of a theoretical description, such as coalescence and break-up of bubbles and droplets.

The two approaches for describing the behaviour of the dispersed phase in a stirred vessel will be introduced, namely a representation of the dispersed phase by a continuum model (also called two-fluid model) and by a discrete particle model. The latter know as Euler/Lagrange approach has numerous advantages over the continuum model as long as dispersed two phase flows are considered and therefore, the lecture will focus on this approach. The resent developments in modelling the basic physical phenomena as for example particle turbulence interaction, turbulence modification by the dispersed phase, and inter-particle collisions will be introduced and their importance will be emphasised.

Results on the dispersion of solid particles in a stirred vessel using the multiple-frame of reference method will be presented in order to demonstrate the dispersion characteristics for different boundary conditions and to reveal the effect of the particle phase on the flow structure and the turbulence. The reliability of the numerical predictions will be demonstrated based on comparisons of calculated integral parameters with available experimental data.

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Detailed Calculations in Singlephase Stirred Tank Reactors

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Abstract:

The presentation will give the approach and results of CFD-simulations at LSTM-Erlangen of the single-phase flow in baffled stirred tanks equipped with a Rushton turbine (first case) and a pitched-blade turbine (second case). The numerical results are compared to experimental LDA data also obtained at LSTM-Erlangen.

In the first part of the presentation, the numerical approach of the simulations will be reviewed. The simulations were performed with an approximate steady state method which models the relative motion of impeller blades and baffles.

Emphasis will be put on the second part of the presentation which gives the results obtained for the flow field near the impeller blades and in the discharge region of the impellers. For both types of stirrers, the trailing vortices were predicted in the simulations, and very good agreement between experimental and computational results concerning the turbulence kinetic energy in the discharge region was achieved.

The results showed in this presentation were obtained by the LSTM-Erlangen during the Brite EuRam project "Chemical reactor modeling for fast exothermic and mixing sensitive reactions" (BE96-2172, contract number BRPR-CT-0185).

Chances for High-Performance Supercomputers in CFD

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Abstract:

Computers have experienced a remarkable increase in computer power through the past three decades. This is most obvious for personal computers and workstations. However, it remains often unnoticed that the computational speed of contemporary supercomputers has been increased by the same order of magnitude as for PCs and workstations. The increase in computational speed has triggered wide spread interest in computational fluid dynamics (CFD) since it was for the first time possible to solve 'real-world' problems numerically (time-dependent, with complex geometries, additional scalar equations, etc.). With the advent of computers that are one order of magnitude faster approximately every five years, the problems that are being investigated have continued to get more and more complex and demanding in the recent years.

The numerical simulation of the fluid flow in contemporary stirring devices is computationally very demanding even for single-phase flow due to the inherently time-dependent geometry of the device. If multi-phase flows and/or chemical reactions are considered, the requirements become even higher. Therefore, supercomputers are nowadays often the platform of choice to attack the challenging problems of stirring devices with sufficient accuracy.

To show what supercomputers can do for demanding CFD calculations and in particular for the simulation of stirring devices, we first describe the state-of-the-art for recent supercomputers and workstations in terms of computer power and roughly estimate the requirements for the different modelling approaches of the time-dependent flow in a stirring device. Next the cost-effectiveness of computations performed on workstations and supercomputers is analysed. Then the key technologies that contribute to the speed of todays workstations and supercomputers are highlighted and coding strategies for software to fully exploit the architectural details of contemporary CPUs are discussed. Finally, we will try to predict future directions for the development of computer hardware and outline consequences.

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Multiphase Flow Simulation in Stirred Reactors Using Population Balance Methods

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Abstract:

In most of today's CFD calculations of dispersed two-phase flows, the particles are assumed to have the same size and shape, i.e. the mono-disperse assumption. In reality a wide spectrum of particle sizes and shapes exist at every point. Particularly, in gas-liquid of liquid-liquid flows it is impossible to control the sizes and shapes of the bubbles and droplets when break-up and coalescence occur.

Population balance is a well-established method used to analyse the size distribution of the dispersed phase. Models for break-up and coalescence are available within the population balance frame work. In this paper we will present the implementation of the population balance method into the CFX-4 computer software via the MUSIG (MUltiple-SIze-Group) model of Lo (1996).

The MUSIG model was applied to analyse flows in the liquid-liquid mixing vessel of Neste Chemicals and the gas-liquid mixing vessel of LSTM Erlangen University. The two-fluid model in CFX-4 was used to simulate the flows. The dispersed phase was divided into 10 groups to represent droplets and bubbles of different sizes. The break-up model of Luo and Svendsen (1996) and the coalescence model of Prince and Blanch (1990) were applied so that droplets and bubbles were allowed to transfer between these size groups according to the break-up and coalescence rules. Comparisons between the computed and measured size distributions of the dispersed phase have shown encouraging results.

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The Importance of Micromixing Phenomena in the Simulation of Chemical Reactions in Stirred Reactors

(Advanced closure model for reactions of any speed in liquids and gases)

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Abstract:

Inclusion of reaction kinetics in CFD simulations has the power to make CFD results truly useful. Many flow fields are designed to promote reactions. Inclusion of chemical effects enables the interactions between the flow and chemistry to be determined and the actual process result to be predicted.

However, conventional closure models in CFD programs are found to have major deficiencies in describing turbulence-chemistry interactions, especially where multi-scale mixing (macro-, meso- and micromixing) and multi-step competing reactions are concerned.

An advanced closure model has been developed by PFD, primarily for reactions in liquids, but now also extended to reactions in gases. This enables reactions such as polymerisation, combustion, neutralisation, hydrolysis and many others to be modelled accurately using a single consistent procedure, irrespective of reaction speed or order. The model is applicable to non-isothermal and non-adiabatic systems, including catalysed reactions.

Example calculations will be presented from tubular reactors, combustors and stirred tanks.

International Seminar
Stirring and Mixing
Applications of Modern Experimental and Numerical Methods

Erlangen, October 25th to 28th

Thermodynamical Modelling for Mixing Processes

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Abstract:

This paper describes some ambitious CFD development work carried out as part of a European industrial research consortium project to develop and improve chemical reactor simulation tools.

The CFX computational fluid dynamics program was adapted by the project partners to include special models for mass and heat transfer, thermodynamics, chemical kinetics and micromixing and applied to calculate reactor performance in nonideally mixed chemical reactor.

The effect of thermodynamics on fluid flow simulations is discussed. In the CFD simulation of chemical mixing processes the thermodynamics has to be correct to be able to predict the fluid flows in mixed reactor correctly. The thermodynamics models comprise, the models for density, viscosity, enthalpy and specific heats of the fluid mixture. The most important thermodynamic properties of the fluid flows are the density and viscosity. Density and viscosity depend on the chemical composition of the reacting fluid flows and the temperature.

Viscosity of the fluid depends often also on the shear force of the fluid, called non newtonian fluids. The non newtonian behavior has big influence of the fluid flow, since in the effectively mixed regions the viscosity may be order of magnitude lower than in the poorly mixed regions.

The temperature of the fluid is affected by the thermal conductivity and the heats of reactions.

The concentration of the fluid flow depend on the reaction rates of the different chemical components and the convective fluid flows.

The basic models for the thermodynamic properties are introduced. The effect of density and viscosity of newtonian and non newtonian fluid flows in mixed tank are illustrated.

International Seminar
Stirring and Mixing
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Erlangen, October 25th to 28th

Software Solutions with Scalable Rigor for Mixing Problems

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Abstract:

The presentation describes the "scalable rigor" approach of AEA Technology Engineering Software to simulate and solve mixing problems in chemical and process engineering. Scalable rigor characterises software tools which allow a suitable level of analysis of design and optimisation problems within given resource and time constraints. The scalable rigor approach is particularly suitable for mixing problems as the design engineer will typically face a spectrum of challenges ranging from simple parametric studies to development of innovative mixing concepts.

The scalable rigor approach will be demonstrated for batch and static mixers. The concept is realised through a series of software products, starting with the HYSYS process simulation tool, where mixing is treated in a lumped parameter fashion, and continuing through to the CFX software where three-dimensional fluid flow and mixing processes are simulated and analysed. The software chain is completed by the BASYS suite of products and services which cover issues such as batch recipes, and hazard analysis for stirred tanks. The link from HYSYS and BASYS to CFD is provided by the CFX-ProMixus software which allows design engineers to harness the capabilities of three-dimensional CFD simulation software with a minimum of specialised CFD training.

The highest level of the scalable rigor approach is the development and validation of new mixing techniques. By participating in several European and national research projects in this area, AEA Technology Engineering Software has advanced the predictive capabilities of the software. Extensive validation work, which is was conducted as part of the projects, has increased the confidence level in mixing simulations. Key results of this research will be shown in the presentation.

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The Application of FLUENT in Stirring and Mixing Technology

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Abstract:

International Seminar
Stirring and Mixing
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Erlangen, October 25th to 28th

FASTEST: The powerful CFD-Tool for Mixing and Stirring Processes

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Abstract:

FASTEST is the CFD tool of first choice, whenever the customer demands high accuracy of results and short turnaround times in the optimisation and development process.

FASTEST is especially developed for highest CFD-power, necessary for challenging tasks in the field of computational fluid dynamics. The most modern techniques used in FASTEST, like multi-grid method, parallelisation and vectorisation enables the user to reach the claims of the market, using computer platforms from single PC, PC-or workstation cluster, or form parallel computers up to the very powerful vector-parallel computers. The power of 1 GFlop on an NEC-SX4 and approximately 4.5 GFlops on a NEC-SX5 gives the user the benefits he is searching for: High-quality CFD results used for the development of high quality, and well optimised products.

The stirring and mixing process is calculated using clicking grids for simulating the stirrer movement relative to the stationary buffles, the method with highest accuracy possible. The method of multiple reference frame is entirely implemented, too.

A powerful grid generating system can be used to generate the grid on the basis of 3d-CAD data, with highest flexibility guaranteed. This tool is fast and easy to use, and allows flexible changing of geometries during the optimisation process.

The results of the CFD-calculations with FASTEST in stirring and mixing have been evaluated by many experiments. FASTEST has proved its capabilities in many demanding fluid flow and complex stirring situations.

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STAR-CD in the Stirring and Mixing Technology

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Abstract:

STAR-CD is extensively used in the chemical industry to model the mixing processes of single and multiphase stirred vessel flows. The capabilities of STAR-CD for such applications are listed.

A fully automatic mesh generator, developed by Aventis Research & Technologies GmbH & Co KG now allows a quick and easy analysis of 3-D impeller geometries. This meshing tool was developed to accelerate CFD analysis of commonly used technical mixing systems. Examples of meshes of arbitrary geometry combining impellers, baffles, and vessels are shown.

The impeller motion can be predicted using a range of multiple reference frame or sliding mesh models available in STAR-CD. The flow field can simultaneously be predicted using free-surface and multiphase flow models. Typical applications of such models are presented.

The automatic mesh generator developed by Aventis Research & Technologies GmbH & Co KG, in combination with the advanced modelling capabilities of STAR-CD provide engineers with an effective tool to better understand and improve mixing processes.

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New Developments in Mixing Technology

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Abstract:

The applicable criteria for the design of agitators are depending on the process engineering and the economical conditions of each application field. While in the chemical industry mixing vessel reactors with increased productivity and safety standards or mono-product-lines with increased reactor volume are of central importance, environmental protection industries consider energy costs and availability of installation when choosing a design for the agitators. An agitator manufacturer has to consider these specific facts of each branch in his R&D work. The new and further development of impellers and mixing systems for special applications must focus on complex process procedures as well as the agitator being a single component in the process environment.

In the last years the significantly improved possibilities in the field of computational fluid dynamics (CFD) as well as the mechanical FEM-based calculations led to the application of these methods in the optimization of process and mixing equipment. In some applications such as single phase mixing or heat transfer, reliable results can be expected from CFD calculations. Contrary to two-phase applications physical models are required for the preduction of integral process parameters such as mass transfer rates since reliable mathematical models are not availabe in commercial CFD-codes.

In the lecture two practical examples are presented showing that numerical calculations and conventional experimental investigations can be used to optimize impellers and mixing systems as well as to present process solutions:

- Fluid mechanical optimization of impellers (FGD, Mineral Processing, Biogas)
- Combined vortex gassing system for hydrogenation reactors.

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Erlangen, October 25th to 28th

New Methods for the Development and Optimisation of Stirred Vessels

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Abstract:

Stirred tank reactors are used for a vast number of fields of application. A variety of stirrer- and reactor-types (and the combination of both) exists. Furtheron there are diverse methods of investigations on flowfields induced by these mixers.

The work carried out in the field of mixing aims at a first stage towards the improvement of the methods which are applicated for the investigation of fluidmechanical characteristics of stirred vessels. The next step is the application of these methods in order to gain detailed information on a mixing sensitive process. What follows is the usage of these information for the development and optimisation of stirred vessels. Finally these newly designed stirred vessels will be implemented and practically tested.

To illustratte the above mentioned, the presentation will show and characterise a novel stirrer. On the base of theoretical considerations rules for the design of stirred vessels will be derived. It will be shown how the needed information on the turbulent flowfield can be detected experimentally. It will be presented that by a combination of experimental and numerical fluidmechanical methods the design of mixer/vessel combinations can be done more properly.

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Status and Latest Developments in Glasslined Mixing Systems

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Abstract:

For decades, the classical one-piece impeller had been the one and only standard for mixing in glasslined reactors. Introducing one-piece glasslined reactors type BE according to DIN 28136 required agitators that can be fitted to and removed from a glasslined shaft. This was first implemented by Pfaudler with the known Cryo-lock-technology and copied by other manufacturers since then.

The Cryo-Lock technology first gave the flexibility to design glasslined turbines and mixers with a shape optimized for several mixing processes. Since the late eighties, a wide variety of glasslined turbines for mixing purposes like blending, emulsification, gas dispersion, homogenization etc. have been developed and installed in a large number of glasslined reactors worldwide.

Utilizing the Cryo-Lock-technology, Pfaudler now invented up to date mixing systems. These incorporate transition regime turbines, gas dispersion turbines, high viscosity mixing turbines and a new type of baffle, known as the Concave baffle. All these mixing components have been developed for improving mixing performance in each of the mentioned mixing applications. Some of the technical features of this new mixing system and some relevant performance data will be presented.

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Contributions of CFD to Submersible Mixing – Examples from Wastewater Treatment

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Abstract:

Flygt submersible mixers, or agitators, have proven suitable in the agitation/mixing of paper pulp, digested sludge, drilling mud, ore slurry etc. where high densities, yield stresses, apparent viscosities, temperatures etc. provide difficult conditions for motors, seals and impellers. However, the most common application is still suspension of activated sludge, inflow mix-in, and current creation in waste water treatment plants-municipial and industrial.

Submersible mixers, make use of a jet mixing principle, by which large masses of liquid can be set in motion with a limited effort. The freedom in mixer positioning, paired with a physical basis for mixer sizing, ensures efficient solution of a variety of mixing applications.

Each application includes one or several mixing tasks, e.g. resuspension of settled solids and/or keeping a suspension homogeneous. The flow field required for these tasks is achieved by correct sizing and location of one or several momentum sources, i.e. mixer thrusts. Hence the mixer thrust is a basic performance parameter.

In order to define and meet quantitative mixing requirements, detailed knowledge of both the flow field generated by the mixers, and the effects of flow characteristics on mixing actions, such as resuspension of solids, is required. The complex physical properties of activated sludge form a challenge to model mixing mathematically. A semi-empirical approach to sludge resuspensioning will be sketched. A unified approach is now developed, much with the help of computational fluid dynamics.

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Design of Static Mixers by Means of Modern CFD-Tools

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Abstract:

Static mixers are tubular devices with fixed internals that cause a radial displacement of the flow. Thereby concentration and temperature differences are equalised over the cross section of the pipe. Axial deviations are not evened out which means that a constant feeding of components to be mixed is required. Static mixers are used also for other unit operations than mixing, e.g. dispersing, heat and mass transfer and chemical reactions. Static mixers are applied to continuous processes only.

The target of the design of static mixers is to achieve a certain quality of mixing with the lowest possible pressure drop (low operating costs) and the smallest possible volume/diameter/length of the mixer (low capital costs).

In the past experimental methods were applied for optimising static mixers. Today CFD has also become an important tool. However, for a successful application, the following prerequisites must be fulfilled:

- Correct prediction of the relevant results (e.g. homogeneity, pressure drop)
- Correct and efficient modelling of the (sometimes quite complicated) geometry of static mixers

The application of CFD has been successful in the following cases:

- Calculation of homogeneity in laminar and turbulent flow
- Calculation of pressure drop, also for non-newtonian products
- Investigation of residence time distribution
- Distribution of solid particles in gas flows
- Distribution and evaporation of droplets and gas flows
- Optimisation of the velocity distribution upstream of reactors
- Investigation of the effect of density and viscosity differences of the components to be mixed

The application of CFD will be shown by means of concrete examples. It is not the intention of the speech to show the theoretical background, but to clarify the benefit of CFD in the engineering practice, which essentially contributes to find good technical solutions in a fast and cost effective way.

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A Selection of Stirring Systems Used for Stirring and Mixing Tasks

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Abstract:

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High-Precise Stirrers in Processing Technology

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Abstract:

Todays markets demand the adaption of the delivery program to the continous change of conditions. Customers are expecting more than ever high quality, low prices, fast transactions, and custom made products and solutions especially for their demand. Strict security-, health- and environmental inspections as well as profitable energy balances put up higher standards on processes, the equipment, the management and last but not least the documentation. It is our business to support our customers in these fields and to offer optimum solutions:

Fast running agitators top mounted, side and bottom entry
Gear drive agitators top mounted, bottom entry
Coolable agitators
Fermenters
Coaxial drive agitators
Compact mixing units
Magnetic stirrers
Custom made constructions
Colloidal mills
Construction elements
Sealing technology
Tripods and lifting devices

The presentation shows some examples chosen from our delivery program for applied process technology. It will represent the possibilities of mixing technology in the scope of DIN, FDA, GMP and validation, as well as the creativity in realisation of new processes at our company PRG.

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Mixing in the Chemical Industry

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Abstract:

The selection and design of agitators and motionless mixers is critical for the successful operation of chemical plants. Success is measured in terms of meeting desired production rates, yields and purities and doing this safely - no injuries to personnel, environmental releases or damage to equipment. Ultimately, the successful design of mixing equipment is a major contributor to the profits made by the chemical industry around the world.

The DuPont corporation is one of the largest chemical manufacturers in the world with $ 24.8 billion in revenue and $ 4.7 billion in net income in 1998. A wide variety of products are made including high value / low volume fine chemicals (agricultural and pharmaceutical), fibers and their intermediates (nylon, Lycra®, Kevlar® among others), fluoro-chemicals and polymers (Suva®, Teflon®) and titanium dioxide (Ti-Pure®). There are very few DuPont processes that do not involve mixing to some degree.

The selection and design process (for all unit operations) is carried out by specialist consultants who work in a central engineering organization, DuPont Engineering Technology, with chemists and process and project engineers from the operating units. The ultimate responsibility for the process design lies with this consultant while the responsibility for the mechanical design lies with the equipment vendors. In many cases, the time allowed for studying a new process or looking for improvements in existing ones is short since getting product to market is often a critical project requirement.

This presentation will discuss some of the design techniques used by DuPont's mixing consultants for designing equipment for mixing:

1. Non-Newtonian fluids.
2. Competitive chemical reactions.
3. Gas-liquid and boiling reactors.
4. Blending of low viscosity, miscible liquids.
5. Solids suspension.

In conclusion, potential improvements, through techniques such as CFD, to the designs developed by DuPont's mixing consultants will be discussed.

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Applications of Computational Fluid Dynamics to Mixing in the Chemical Industry

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Abstract:

In chemical processes, mixing is often the crucial point in a process optimization. Along with more traditional methods such as dimensional analysis and experimental investigations Computational Fluid Dynamics (CFD) offers insight in flow phenomena and solves mixing problems among other applications.

At Bayer's CFD-group, mainly commercial CFD software is used. Thus, successfully applying CFD also means understanding the different physical models which the commercial codes offer. In order to calculate the flow field in a mixing vessel, two different CFD models for a Rushton turbine (a sliding-mesh-model and a multiple-reference-frame-model) are applied. Parallels and differences are shown and the correct sets of boundary conditions and grid requirements for the physical models are discussed. In addition, the convective and dispersive transport of a tracer is investigated and compared to experimental data. The simulation is based on a steady-state solution of the flow field which is achieved with the multiple-reference-frame model. All the simulations are performed with the parallel version of the commercial CFD software Fluent V5.0 on an SGI Origin.

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Virtual Mixing by CFD – Added Value?

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Abstract:

Mixing processes are of great importance in chemical engineering. For design and optimization purposes, it is necessary to know the potential and limitations of available design tools and methods. This is especially true in the case of the relatively new tool CFD, where the following questions have to be answered:

- What are the benefits of using CFD?
- When should CFD be used?
- When is it inappropriate to use CFD?

In this presentation, examples of successful applications of CFD will be given and its limitations will be demonstrated with examples from STR´s, CSTR´s, and mixing nozzles. The pure fluid dynamics in mixing vessels can be analyzed accurately using CFD. The required numerical resources depend mainly on the desired accuracy, which is determined by the spacial and temporal resolution and by the depth of the physical modeling. The modeling is often the limiting step especially in reacting and multi-phase systems.

Limitations of computing mixing processes occur due to different reasons. In the laminar flow regime, numerical diffusion can strongly affect the results, whereas in the turbulent flow regime, limitations of the applied mixing model influence the results. Therefore, improved methods and models for the description of mixing processes are required for all flow regimes.

Often these questions raised above confuse the CFD novice more than convince him of the benefits of applying CFD. If the geometry is complex in addition requiring therefore a considerable amount of grid generation work and thus, money, then most often the beaten path of experimentally oriented problem solving will be chosen. However, in the case of complex geometry and sophisticated physical models in particular, CFD offers the unique chance of observing local processes in detail and hence, also the chance to analyze their primary causes.

The same is true for parameter variation studies. Knowing the limitations, even qualitative results can provide valuable hints for process optimization. The demand for quantitative results must not be regarded too strong, especially when there are only integral experimental data available such as power consumption or total mixing time by de-coloring experiments. The knowledge obtained by the combination of flow analyses with physical models developed in other areas offers new possibilities for problem treatment and in depth research, e.g. micro-mixing models for incineration processes can be applied to reaction problems in chemical processes.

This know-how transfer from other established areas offers new chances in the design and understanding of chemical process using CFD.

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Possible Applications of CFD-Software in Wastewater Treatment

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Abstract:

- Simulation of sedimentation processes
  - Desired sedimentation:
    grit chambers, two-phase flow of water and sewage flocs in sedimentation tanks
  - Undesired sedimentation:
    in pipes, channels and tanks
- Simulation of mixing in anoxic and anaerobic zones for nitrogen and phosphorus removal
  - Mixers in long rectangular tanks
- Developing geometry of inlet- and outlet-structures
- Problems of flow equalisations in distributors
- Short-circuiting flow in aeration tanks
  –layout of aerators

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Software Aided Design of Stirred Vessels - the Bridge between Experience and CFD

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Abstract:

The stirred tank reactor is one of the most commonly used reactor-types in the chemical and process industry. It is used for a vast number of processes, which all have different characteristics and demands. Therefore for almost each reactor an individual design process becomes necessary. Within this process, a software package for the pre-design of stirred vessels prior CFD-simulations will be a great assistance. Such a tool will speed up the design process and ensure satisfying results in designing STRs and appears as a complementary tool to CFD-programs.

An application fulfilling the above criterions was developed by INVENT. It is based on the one hand on design algorithms found in literature. On the other hand the software comprises a database containing the results and experience of former STR designs which will be useful for future STR designs.

At this time the application calculates relevant parameters for the mixing tasks homogenisation, dispersing, heat transfer and suspending solids. The mixing equipment is limited to the following agitators: Rushton Turbines, (Double) Pitched Blade Turbines and Pfaudler Impellers. The bottom and top shapes taken into consideration are dished and flat.

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CFD as an Industrial Reactor Design Tool for Crystallisation

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Abstract:

A CFD package has been customised to model precipitation reactions for the production of fine chemicals in various reactor types. Unlike conventional calculations, a CFD approach allows prediction of the distributions of species concentrations, supersaturation, total crystal number and mass density. Visualisation of these distributions allows a rapid assessment of effects of flow patterns within the vessel, leading to improved insight into the system. Furthermore, the description of the development of the solid crystal phase by moment equations of the population balance allows for a much more rapid assessment of product quality (crystal size and its variation) and yield than the alternative multi-phase modelling approach. Parametric variation of principal design features, such as impeller speed and feed location can then provide a rapid optimisation of reactor design.

This paper illustrates the application of these techniques to the precipitation of barium sulphate in a continuous stirred tank reactor, and concentrates on the effect of feed location on product quality and yield.

International Seminar
Stirring and Mixing
Applications of Modern Experimental and Numerical Methods

Erlangen, October 25th to 28th

Numerical Simulations of Dynamic Mixers

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Abstract:

The numerical simulation of industrial processes is a very interesting field of Chemical Engineering and the simulation of macro- and micro-mixing is a very challenging topic. Models are basically made up of two different types: one is the eulerian approach, which shows what happens in any part of the reactor, as the software like CFX-4 does; the other one is the Lagrangian approach, which follows the history of vortexes and gives only information on the outlet of the reactor.
An industrial test case for the two models is Caprolactam (CPL) synthesis; CPL production involves a main, fast and exothermic reaction and different side reactions; tests performed in the laboratory reactor show the reactive system is mixing sensitive.
The reaction section of the plant under study is a loop reactor equipped with a Rotor Stator Mixer. This is the core of the plant and it is composed of a four blade rotor and a high shear screen with square holes, which is typically employed when very intensive mixing is required.

The knowledge of both kinetic and physical-chemistry is a fundamental requirement for successful simulation. Most information come from EniChem background; in order to obtain missing information appropriate experiment were performed; specific properties like kinetic laws and viscosity functions have been experimentally estimated .

Code validation were planned using a step by step procedure: at first the fluiddynamic simulation has been compared with LDA measurements (LSTM) to verify that flowfield is correct; then reactive simulation are compared with extended Bourne Reaction System data (BHR) in order to validate micromixing modules.
The last step is the simulation of the loop reactor for CPL production; CFX-4 performances were checked by comparison with laboratory loop reactor tests carried out at Enichem (Porto Marghera) in which the influence of mixing on product quality was important.
The results are reported and discussed.

The results here reported have been obtained within European project CRS («CHEMICAL REACTOR MODELLING FOR FAST EXOTHERMIC AND MIXING SENSITIVE REACTIONS»- BRITE PROJECT number BE95-2172); the partners involved with EniChem in European project are: AEA (GB), BHR (GB), INVENT-UV (DE), LSTM-Institute of Fluid Mechanics in Erlangen (DE), Neste oy (FI) and PFD (IE).
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Challenges for CFD in the Chemical Industry

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Abstract:

Computational Fluid Dynamics has become a valuable tool for analysis and design of petrochemical processes and, with the ever increasing capabilities of computers, the solution to larger problems are becoming more and more feasible. Two important applications of CFD in the chemical manufacturing industry include impeller stirred tank reactors and hydrocarbon pyrolysis furnaces. These applications involve significant challenges in modeling the isolated and combined effects of turbulence, chemical reaction/combustion, multi-phase flow phenomena and radiation heat transfer. Since CFD results alone do not offer any direct information about the mixing processes, a significant computational challenge of interest is to assess mixing performance.

Application of large eddy simulations (LES) to real problems in the chemical industry are still intractable. The continued pace of current computational improvements will eventually result in an increase in application of LES to some of these problems. For the near future however, Reynolds-Averaged Navier-Stokes (RANS) techniques will remain foremost in the design and analysis of large scale thermofluid problems involving complex geometries.

In this paper we discuss, using several computational examples, the current status and shortcomings of LES and RANS in complex geometries for both reacting and non-reacting flows. We also present some numerical results which illustrate a technique for computing mixing performance in impeller stirred tanks using a discrete time particle mapping procedure.

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Mixing in the Next Century

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