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Computational Fluid Dynamics

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PREFACE

This issue attempts to give a feeling of the state-of-the-art of the application of computational fluid dynamics (CFD) in chemical engineering. It is, however, not limited to a snap-shot but is aimed at providing a perspective: how did we arrive at the present status and where do we go from here? To do so, contributions from five complementary contributions are brought together. From the definition of CFD as the ensemble "of all computational approaches that solve for the spatial distribution of the velocity, concentration, and temperature fields" recalled by Fox, it is clear that a selection had to be made as to the topics covered. In the wake of volume 30 on "Multiscale Analysis" the present volume is organized from "small" to "large": from "bubbles and droplets" in the first contribution, to a "fixed catalyst bed" in the last one. The application of direct numerical simulations (DNS) clearly is still limited to the small scale. Today subgrid-scale (SGS) models are required to cover the full spectrum.

The reader will be confronted with some redundancy but this allows each contribution to stand on its own. Also, a good balance is maintained between the style of a tutorial and that of a research paper. Those who will read the complete volume will realize that opinions can vary from looking at CFD as an alternative for experimentation to emphasizing the need of experimental validation. Some contributions are entirely limited to velocity and temperature fields. Others, on the contrary, emphasize the difficulties associated with the combination of transport and reaction. The latter can introduce stiffness even for laminar flow. Averaging (e.g. Reynolds-averaged Navier–Stokes, RANS) or filtering (e.g. large eddy simulations, LES), performed to model velocity fields, does not alleviate this difficulty. Clearly, this is still quite a challenge.

The contribution from the Ohio State University by Ge and Fan is dealing with the simulation of gas–liquid bubble columns and gas–liquid–solid fluidized beds. A scientist of a major engineering company told me a few years ago that when he wanted to know how serious an academic group was about CFD, he would ask whether they could simulate bubble columns. He would only engage into further conversation if the answer was negative. The group from Columbus is wise enough to focus on a single air bubble rising in water, and bubble formation from a single nozzle. In a second part the hydrodynamics and heat transfer phenomena of a liquid droplet in motion and during the impact process with a hot flat surface, as well as with a particle are studied. The applied numerical techniques, such as the level set and immersed boundary method, are outlined and important contributions are highlighted. Next, detailed implementations for particular problems are presented. Finally, numerous simulation results are shown and compared with experimental data.

The second contribution addresses the different levels of modeling that are required in order to cover the full spectrum of length scales that are important for industrial applications. It is a joint paper from Twente and Princeton University and claims to put "Emphasis on technical details." The latter is a too modest description of what is really offered to the reader. The recent developments in two leading research groups on the modeling of gas-fluidized beds are presented. The holy grail for those interested in the design of industrial units being the closure of the model equations in general and SGS modeling in particular. The latest developments of both the "filtering" approach pursued at Princeton University by Sundaresan and coworkers and the "discrete bubble model" developed in Twente by the team of Kuipers are presented. The authors realize fully that there is still a long way to go, as evidenced by their last sentence: "Finally, the adapted model should be augmented with a thermal energy balance, and associated closures for the thermo-physical properties, to study heat transport in large scale fluidized beds, such as FCC-regenerators and PE and PP gas-phase polymerization reactors." This is even more so because inclusion of reaction kinetics remains beyond the scope of the contribution!

Chemical reactions come into the picture in the context of stirred turbulent vessels in Chapter 3. Van den Akker from Delft strongly emphasizes the potential of LES and DNS for reproducing not only the hydrodynamics of turbulent stirred vessels but also for providing a basis for simulating a wide variety of physical and chemical processes in this equipment. The author advocates the use of the lattice–Boltzmann (LB) technique to this purpose. Van den Akker certainly belongs to those who believe that one can and should be much more positive about the merits of CFD so far and about the term at which CFD will replace and improve existing mixing correlations. To quote him: "It may be easier to 'measure' the local and transient details of the turbulent flows in stirred vessels and the spatial distributions in e.g. mixing rates and bubble, drop and crystal sizes computationally than by means of experimental techniques!" When it comes to the design of chemical reactors the authors admit that CFD is certainly not a panacea. "Scale-up of many chemical reactors, in particular the multi-phase types, is still surrounded by a fame of mystery indeed."

The importance of chemical-reaction kinetics and the interaction of the latter with transport phenomena is the central theme of the contribution of Fox from Iowa State University. The chapter combines the clarity of a tutorial with the presentation of very recent results. Starting from simple chemistry and single-phase flow the reader is lead towards complex chemistry and two-phase flow. The issue of SGS modeling discussed already in Chapter 2 is now discussed with respect to the concentration fields. A detailed presentation of the joint Probability Density Function (PDF) method is given. The latter allows to account for the interaction between chemistry and physics. Results on impinging jet reactors are shown. When dealing with particulate systems a particle size distribution (PSD) and corresponding population balance equations are intro-

duced. The author emphasizes that a balance between the degree of detail or complexity of the chemistry and that of the physics should be maintained.

The last contribution comes from Dixon (Worcester Polytechnic Institute), and Nijemeisland and Stitt (Johnson Matthey). The subject is another classic of reactor engineering: the catalytic fixed-bed reactor. Heat transfer issues on both reactor scale and catalyst pellet scale are addressed. Steam reforming is used as a typical example of a strongly endothermic reaction requiring high-heat fluxes through the reactor walls. The presence of the tube wall causes changes in bed structure, flow patterns, transport rates and the amount of catalyst per unit volume, and is usually the location of the limiting heat-transfer resistance. Special attention is given to the modeling of the "structure" of a packed bed. The importance of wall functions, to be applied not only at the reactor wall but also at the external pellet surface, is stressed. The authors show ample results of their own work without neglecting the contributions of others. At the end of this chapter the reader will be convinced of the importance of the local nonuniformities in the temperature field not only within a catalyst pellet but also from one pellet to the other.

Let me conclude by thanking the authors for their willingness to contribute, despite health problems for some of them, and for their flexibility with respect to timing.

Guy B. Marin
Ghent, Belgium
April 2006

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3-D DIRECT NUMERICAL SIMULATION OF GAS–LIQUID AND GAS–LIQUID–SOLID FLOW SYSTEMS USING THE LEVEL-SET AND IMMERSED-BOUNDARY METHODS

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Abstract

The recent advances in level-set and Immersed Boundary methods (IBM) as applied to the simulation of complex multiphase flow systems are described. Two systems are considered. For system 1, a computational scheme is conceived to describe the three-dimensional (3-D) bubble

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dynamics in gas–liquid bubble columns and gas–liquid–solid fluidized beds. This scheme is utilized to simulate the motion of the gas, liquid, and solid phases, respectively, based on the level-set interface tracking method, the locally averaged time-dependent Navier–Stokes equations coupled with the Smagorinsky subgrid scale stress model, and the Lagrangian particle motion equations. For system 2, the hydrodynamics and heat-transfer phenomena of a liquid droplet in motion and during the impact process with a hot flat surface, as well as with a particle, are illustrated. The 3-D level-set method is used to portray the droplet surface deformation whilst in motion and during the impact process. The IBM is employed so that the particle–fluid boundary conditions are satisfied. The governing equations for the droplet and the surrounding gas phase are solved utilizing the finite volume method with the Arbitrary Lagrangian Eulerian (ALE) technique. To account for the multiscale effect due to lubrication-resistance induced by the vapor layer between the droplet and solid surface or solid particle formed by the film-boiling evaporation, a vapor-flow model is developed to calculate the pressure and velocity distributions along the vapor layer. The temperature fields in all phases and the local evaporation rate on the droplet surface are illustrated using a full-field heat-transfer model.

I. Introduction

Gas–liquid–solid (three-phase) flow systems involve a variety of operating modes of gas, liquid, and solid phases, including those with solid particles and/or liquid droplets in suspended states. Commercial or large-scale operations using three-phase flow systems are prevalent in physical, chemical, petrochemical, electrochemical, and biological processes (Fan, 1989). In the gas–liquid–solid fluidization systems with liquid as the continuous phase, the systems are characterized by the presence of gas bubbles, which induce significant liquid mixing and mass transfer. The flow structure in the systems is complex due to intricate coalescence and breakup phenomena of bubbles. The fundamental dynamics of solids suspensions in the systems is closely associated with the particle–particle collision and particle–bubble interactive behavior. For three-phase flows that occur in the feed nozzle area of a fluid catalytic cracking (FCC) riser in gas oil cracking, on the other hand, the gas phase is continuous where oil is injected from the nozzle with the mist droplets formed from the spray in contact with high-temperature catalyst particles (Fan *et al.*, 2001). The droplets may splash, rebound, or remain on the catalyst particle surface after the impact, and the oil is evaporated and cracked into lighter hydrocarbons. Such contact phenomena are also prevalent in the condensed mode operation of the Unipol process for

polypropylene or polyethylene production, where droplet–particle collisions in the feed nozzle are also accompanied by intense liquid evaporation. In this study, both systems involving three-phase fluidization and evaporative droplet and particle collisions are simulated using CFD based on the 3-D level-set and immersed boundary method (IBM).

CFD is a viable means for describing the fluid dynamic and transport behavior of gas–liquid–solid flow systems. There are three basic approaches commonly employed in the CFD for study of multiphase flows (Feng and Michaelides, 2005): the Eulerian–Eulerian (E-E) method, the Eulerian–Lagrangian (E-L) method, and direct numerical simulation (DNS) method. In the E-E method (Anderson and Jackson, 1967; Joseph and Lundgren, 1990; Sokolichin and Eigenberger, 1994, 1999; Zhang and Prosperetti, 1994, 2003; Mudde and Simonin, 1999), both the continuous phase and the dispersed phase, such as particles, bubbles, and droplets, are treated as interpenetrating continuous media, occupying the same space as does the continuous phase with different velocities and volume fractions for each phase. In this method, the closure relationships such as the stress and viscosity of the particle phase need to be formulated. In the E-L method, or discrete particle method (e.g., Tsuji *et al.*, 1993; Lapin and Lübbert, 1994; Hoomans *et al.*, 1996; Delnoij *et al.*, 1997), the continuous fluid phase is formulated in the Eulerian mode, while the position and the velocity of the dispersed phase, particles, or bubbles, is traced in the Lagrangian mode by solving Lagrangian motion equations. The grid size used in the computation for the continuous-phase equations is typically much larger than the object size of the dispersed phase, and the object in the dispersed phase is treated as a point source in the computational cell. With this method, the coupling of the continuous phase and the dispersion phase can be made using the Particle-Source-In-Cell method (Crowe *et al.*, 1977). The closure relationship for the interaction forces between phases requires to be provided in the E-L method.

In the DNS (Unverdi and Tryggvason, 1992a,b; Feng *et al.*, 1994a,b; Sethian and Smereka, 2003), the grid size is commonly much smaller than the object size of the dispersed phase, and the moving interface can be represented by implicit or explicit schemes in the computational domain. The velocity fields of the fluid phase are obtained by solving the Navier–Stokes equation considering the interfacial forces, such as surface tension force or solid–fluid interaction force. The motion of the object of the dispersed phase is represented in terms of a time-dependent initial-value problem. With the rapid advances in the speed and memory capacity of the computer, the DNS approach has became important in characterizing details of the complex multiphase flow field.

This paper is intended to describe recent progress on the development of the level-set method and IBM in the context of the advanced front-capturing and front-tracking methods. The paper is also intended to discuss the application of them for the 3-D DNS of two complex three-phase flow systems as described earlier.

II. Front-Capturing and Front-Tracking Methods

In the DNS of multiphase flow problems, there are various methods available for predicting interface position and movement, such as the moving-grid method, the grid-free method (Scardovelli and Zeleski, 1999) and the fixed-grid front-tracking/front-capturing method. In the moving-grid method, which is also known as the discontinuous-interface method, the interface is a boundary between two subdomains of the grid (Dandy and Leal, 1989). The grid may be structured or unstructured and even near-orthogonal, moving with the interface (Hirt *et al.*, 1974). It treats the system as two distinct flows separated by a surface. When the interface moves or undergoes deformation, new, geometrically adapted grids need to be generated or remeshed (McHyman, 1984). The remeshing can be a very complicated, time-consuming process, especially when it involves a significant topology change, and/or a 3-D flow. Methods in which grids are not required include the marker particle method (Harlow and Welch, 1965) and the smoothed particle hydrodynamics method (Monaghan, 1994).

The fixed-grid method, which is also known as the continuous-interface method, employs structured or unstructured grids with the interface cutting across the fixed grids. It treats the system as a single flow with the density and viscosity varying smoothly across a finite-thickness of the interface. The numerical techniques used to solve the moving interface problem with fixed, regular grids can be categorized by two basic approaches: the front-tracking method (e.g., Harlow and Welch, 1965; Peskin, 1977; Unverdi and Tryggvason 1992a, b; Fukai *et al.*, 1995) and the front-capturing method (e.g., Osher and Sethian, 1988; Sussman *et al.*, 1994; Kothe and Rider, 1995; Bussmann *et al.*, 1999). For a 3-D multiphase flow problem, the fixed-grid method is the most frequently used due to its efficiency and relative ease in programming.

The front-tracking method explicitly tracks the location of the interface by the advection of the Lagrangian markers on a fixed, regular grid. The marker-and-cell (MAC) method developed by Harlow and Welch (1965) was the first front-tracking technique applied in DNS, e.g., it was used by Harlow and Shannon (1967) to simulate the droplet impact on a flat surface without considering the viscosity and the surface-tension forces in the momentum-conservation equation. Fujimoto and Hatta (1996) simulated the impingement process of a water droplet on a high-temperature surface by using a single-phase 2-D MAC type solution method. The no-slip and free-slip boundary conditions are iteratively adopted on the liquid–solid interface for the spreading and recoiling process, respectively. Fukai *et al.* (1995) developed the adaptive-grid, finite-element method to track the droplet free surface in collision with a surface while considering the wettability on the contact line. The front-tracking method developed by Unverdi and Tryggvason (1992a, b) and Tryggvason *et al.* (2001) leads to many applications in the simulation of droplet or bubble flow. In this method, the location of the interface is expressed by discrete surface-marker

particles. High-order interpolation polynomials are employed to ensure a high degree of accuracy in the representation of the interface. An unstructured surface grid connecting the surface-marker particles is introduced within a volumetric grid to track the bubble front within the computational domain. Thus, discretization of the field equations is carried out on two sets of embedded meshes: (a) the Eulerian fluid grid, which is 3-D, cubical, staggered structured, and nonadaptive; and (b) the Largrangian front grid, which is 2-D, triangular, unstructured, and adaptive (Unverdi and Tryggvason 1992a, b). The infinitely thin boundary can be approximated by a smooth distribution function of a finite thickness of about three to four grid spacing. The variable density Navier–Stokes equations can then be solved by conventional Eulerian techniques (Unverdi and Tryggvason 1992a, b). This method can be numerically stiff as the density ratio of the two fluids increases, and may pose difficulties when the appearance, the connection, the detachment, and the disappearance of the gas–liquid interface are encountered. Such interface behavior occurs in the coalescence, breakup, or formation of bubbles and droplets in an unsteady flow. The front-tracking method is therefore computationally intensive. Agresar *et al.* (1998) extended the front-tracking method with adaptive refined grids near the interface to simulate the deformable circulation cell. Sato and Richardson (1994) developed a finite-element method to simulate the moving free surface of a polymeric liquid. The IBM proposed by Peskin (1977) in studying the blood flow through heart valves and the cardiac mechanics also belongs to the class of front-tracking techniques. In the IBM method, the simulation of the fluid flow with complex geometry was carried out using a Cartesian grid, and a novel procedure was formulated to impose the boundary condition at the interface. Some variants and modifications of this method were proposed in simulating various multiphase flow problems (Mittal and Iaccarino, 2005). An introduction to the IBM method is given in Section II.B.

The front-capturing method, on the other hand, is the Eulerian treatment of the interface, in which the moving interface is implicitly represented by a scalar-indicator function defined on a fixed, regular mesh point. The movement of the interface is captured by solving the advection equation of the scalar-indicator function. At every time step, the interface is generated by piecewise segments (2-D) or patches (3-D) reconstructed by this scalar function. In this method, the interfacial force, such as the surface-tension force, is incorporated into the flow-momentum equation as a source term using the continuum surface force (CSF) method (Brackbill *et al.*, 1992). This technique includes the volume of fluid (VOF) method (Hirt and Nichols, 1981; Kothe and Rider, 1995), the marker density function (MDF) (Kanai and Mtyata, 1998), and the level-set method (Osher and Sethian, 1988; Sussman *et al.*, 1994).

In the VOF method, an indicator function is defined as: 0 for a cell with pure gas, 1 for a cell with pure liquid, and 0 to 1 for a cell with a mixture of gas and liquid. An interface exists in those cells that give a VOF value of neither 0 nor 1. Since the indicator function is not explicitly associated with a particular front

grid, an algorithm is needed to reconstruct the interface. This is not an easy task, especially for a complex dynamic interface requiring 3-D calculation. Pasandideh-Ford *et al.* (1998) used a modified SOLA-VOF method to solve the momentum and heat-transfer equations for droplet deposition on a steel surface. Bussmann *et al.* (1999, 2000) developed a 3-D model to simulate the droplet collision onto an incline surface and its splash on the surface, utilizing a volume-tracking methodology. Mehdi-Nejad *et al.* (2003) also used the VOF method to simulate the bubble-entrapment behavior in a droplet when it impacts a solid surface. Karl *et al.* (1996) simulated small droplet (100–200 μm) impact onto the wall in the Leidenfrost regime using a VOF method. A free-slip boundary condition and a 180° contact angle were applied on the solid surface. Harvie and Fletcher (2001a,b) developed an axisymmetric, 2-D VOF algorithm to simulate the volatile liquid droplet impacting on a hot solid surface. The vapor flow between the droplet and solid surface was solved by a 1-D, creeping flow model, which neglects the inertial force of the flow. This model, despite being accurate at a lower *We*, failed to reproduce the droplet dynamics at a higher Weber number. Other front-capturing methods include the constrained interpolation profile (CIP) method (Yabe, 1997), and the phase-field method (Jamet *et al.*, 2001).

In the level-set method, the moving interface is implicitly represented by a smooth level-set function (Sethian and Smereka, 2003). The level-set method has proved capable of handling problems in which the interface moving speed is sensitive to the front curvature and normal direction. A significant advantage of the level-set method is that it is effective in 3-D simulation of the conditions with large topological changes, such as bubble breaking and merging, droplet–surface collisions with evaporation. In this study, the level-set technique (Sussman *et al.*, 1994) is employed to describe the motion of 3-D gas–liquid interfaces. In the following section a description of this technique is given.

A. Level-Set Method

The level-set method, which was first derived by Osher and Sethian (1988), is a versatile method for capturing the motion of a free surface in 2-D or 3-D on a fixed Eulerian grid. While similar to the VOF method, the level-set method also uses an indicator function to track the gas–liquid interface on the Eulerian grid. Instead of using the marker particles or points to describe the interface, a smooth level-set function is defined in the flow field (Sussman *et al.*, 1994). Consider a nonbody conformal Cartesian grid which is used to simulate the flow with a deformable interface Γ, as shown in Fig. 1. The whole computational domain is separated by the interface into two regions: Ω_- and Ω_+. The value of the level-set function is negative in the Ω_- region and positive in the Ω_+ region, while the interface Γ is simply described as the zero level set of