Introduction To A Series Of Featured Articles: "Multiphase Computational Fluid Dynamics For Industrial Processes"

Dmitry Eskin[1]* and Jos Derksen[2]

1. Schlumberger DBR Technology Center, 9450-17 Avenue, Edmonton, AB, Canada T6N 1M9

2. Chemical & Materials Engineering, University of Alberta, ECERF 7-028, Edmonton, AB, Canada T6G 2V4

We are starting publication of a series of featured articles entitled "Multiphase Computational Fluid Dynamics for Industrial Processes." In this short Introduction we can only touch upon some of the important issues of industrial computational fluid dynamics (CFD) applications.

It is difficult to underestimate the importance of CFD for modern industries. Advanced technologies require powerful computational tools to avoid expensive large-scale experiments and speed-up process and equipment optimisation. CFD is a rapidly evolving discipline oriented on developing computational tools for solving problems related to transport processes: fluid mechanics, heat and mass transfer, reactive flow, multiphase flow.

In narrow terms CFD is the numerical solution of the mass, momentum, and energy conservation equations with properly defined boundary conditions. Those equations may be supplemented with (Newtonian or non-Newtonian) constitutive equations and equations of state for compressible fluids. In broader terms CFD also involves modelling (parameterisation) of phenomena at length and time scales that are too small to be fully resolved computationally; the three most prominent examples being turbulence, flows involving multiple phases, and reactive flows.

In strongly turbulent flows, the spectrum of length and time scales is simply too wide to be completely resolved in a single computation. Models for small-scale turbulence are used to alleviate the computational burden and make simulations of large-scale industrial turbulent flows possible. Multiphase flows usually take the form of a continuous phase that carries one or more dispersed phases. The solid particles, or droplets, or gas bubbles that constitute the dispersed phases are often too small to be fully resolved; their impact on the macroscopic flow patterns needs to be modelled. A similar multi-scale issue relates to chemically reacting flow where mixing at the micro (molecular)-scale defines the rate of chemical reactions.

The most important issue in predictive modelling of chemical industrial processes is how to deal with their multiphase character. Process equipment (chemical reactors, burners, mixers, crystallizers, hydro and pneumatic conveying pipe lines, fluidized beds, flotation cells) usually operates with multiple phases, modelling of which is much more complicated than that of a single phase flow. In dependence on the phases composing the flow system, the geometry of the flow domain and the process conditions (flow rates, agitation speeds), an abundance of flow regimes and flow phenomena can be distinguished. Resolving and predicting these in a numerical simulation is a clear and grand challenge.

Key in virtually any simulation effort is to distinguish between the relevant and irrelevant physics and model what is relevant. Though, general mathematical descriptions of multiphase processes are known, it is practically impossible to solve all the conservation equations numerically without simplifications.

There are the two major groups of approaches, which are currently used in engineering and science:

1. Methods based on a simplified model representation of some processes involved in a certain multiphase system.
2. Methods of direct numerical simulation.

The simplified model representation focuses on the macro-scale processes and global flow patterns, and uses simplifying assumptions and models to represent micro-scale effects. Direct simulations aim at fully resolving the micro-scale including the behaviour (motion, deformation, breakup, coalescence,

*Author to whom correspondence may be addressed.
Can. J. Chem. Eng. 89:203–205, 2011

DOI 10.1002/cjce.20520
Published online in Wiley Online Library (wileyonlinelibrary.com).

aggregation) of individual dispersed phase particles (solids, droplets, bubbles). Given the high resolution at the micro-scale, direct simulations are only able to simulate small volumes and thus need simplifying assumptions regarding the macro-scale, such as homogeneous turbulent conditions, or simple shear flow.

The first group of methods is usually employed when a computational domain is large and/or a number of different phenomena revealing themselves on different scales are involved. For example, a force interaction of dispersed and continuous phases is modelled through a drag force that is calculated based on empirical correlations. Heat and mass transfer in such a case are also described by empirical equations. The situation becomes even more complicated when concentration of a dispersed phase is high. Then dispersed phase components interact with each other. Those interactions lead to generation of additional stresses in a flow, causing a change in flow pattern. If particles are solid then kinetic theory of granular media can be employed for modelling dispersed phase dynamics. Models where both continuous and dispersed phases are represented as two interacting interpenetrating continua are classified as two-fluid models and often used in engineering practice. Such models are incorporated into commercial CFD codes (e.g., fluent and CFX) and widely used for computing of large-scale technological devices (e.g., fluidized bed chemical reactors, hydraulic or pneumatic conveying pipelines, etc.).

Alternatively, the equations of motion of the dispersed phase are solved in Lagrangian coordinates. In this case motion of each particle is tracked. Collisions of a tracked particle with others are accounted for assuming that it moves through a cloud formed by other particles. It is assumed that particle–particle collisions are binary and mutual orientations of colliding particles are random. Post-collision particle velocities are calculated based on momentum conservation for particle pair. This approach is more accurate than the two-fluid model, but limited to relatively low particle concentration and computationally expensive.

If the second phase is not dispersed down to small size particles or droplets the two-fluid approach cannot be used. If both phases are immiscible fluids then dynamics of each fluid is modelled by solving the corresponding conservation equations. The models for each fluid flow are coupled through no-slip conditions and equality of stress on the fluid/fluid boundary. That boundary is tracked by one of the known techniques (e.g., volume of fluid method). The option of computing immiscible fluid flows is provided by modern commercial CFD codes. Examples of successful application of such an approach are modelling a bubbly flow in a capillary channel, a liquid film flow on a surface, etc.

Direct Numerical Simulation (DNS) is a direction that is rapidly developing during the last 20 years. DNS methods suppose solving the conservation equations for all phases composing the system directly, without introducing simplifying assumptions. For example, in a case of a fluid–solids flow a dispersed phase is treated as a moving boundary of a complicated changing configuration.

There are a number of different DNS methods.

A DNS method is often considered as a technique for solving problems on the meso-scale that is assumed to be a minimum scale representing an important property of a flow system. An example of such a property is an apparent viscosity of a slurry or an emulsion. The meso-scale in this case is a characteristic size of a computational domain that is sufficient to calculate the apparent viscosity based on accurate modelling of dynamics of interacting carrying and dispersed phases. A DNS method should not require a model of turbulence, that is, such a method should allow resolving Navier–Stokes equation from a micro-scale (significantly smaller than the inner turbulence scale) to a relatively large-scale (e.g., a few percent of a tube radius for a pipe flow).

Some known DNS methods are based on direct solution of the conservation equations for all components of a given flow system. Unfortunately, these equations are strongly non-linear and characterised by poor convergence and numerical stability.

The other group of DNS methods is based on ideas borrowed from statistical mechanics. A fluid is represented as a system of particles, characterised by a probability density in a 6-dimensional space (3 coordinates in the geometrical space and 3 coordinates in the velocity space). Dynamics of such a system is described by a known Boltzmann equation. It was proven that the Boltzmann equation can be reduced to the Navier–Stokes equation, therefore the Boltzmann equation can be used for modelling fluid flows.

Examples of methods based on such an approach are: the Lattice Boltzmann Method (LBM), its predecessor Lattice Gas Automata (LGA), and Dissipative Particle Dynamics (DPD) approach. LBM and LGA methods employ a fixed grid. The velocity in each node is discretised to a number of fixed directions. The simplified kinetic equation formulated for such a grid allows obtaining an approximate solution of the Boltzmann equation and the Navier–Stokes equation, respectively.

The Lattice–Boltzmann technique can be applied to modelling flows in a domain with very complex boundary conditions. The LBM equations are free of drawbacks associated with strong non-linearity of Navier–Stokes equation. LBM has been successfully used for modelling multiphase flows, especially on a micro-scale.

The DPD is an off-lattice mesoscopic simulation method which involves a set of particles randomly moving in continuous space. Each particle moves under the action of three pairwise-additive forces: a conservative force, the dissipative force, and the random force. The DPD technique has an advantage over other methods when it is necessary to relate the macroscopic non-Newtonian flow properties of a fluid to its microscopic structure.

Though DNS methods are prospective for accurate modelling of flows on a meso-scopic level their applicability are often limited to small computational domains. Modern technological equipment is often characterised by enormous dimensions. DNS methods may serve as an excellent tool for deriving correlations or models used as sub-models for macro-scale CFD codes.

In an ideal world, micro, meso, and macro-scale simulations are tightly connected to provide a multi-scale approach for truly predictive modelling of large-scale industrial processes. The challenges in multi-scale modelling are the formulation of generic coarse and fine graining techniques to meaningfully connect simulations at vastly different length and time scales.

The topic of our article series on CFD of multiphase flow covers—given the above considerations—a broad spectrum of methods and applications. The articles presented can be considered as examples of developments and applications of CFD techniques. Their common theme is solution of engineering problems arising in process industries. We hope that the series will be interesting for scientists from industry and academia as well as for practicing engineers involved in simulations of multiphase systems.

Dmitry Eskin
Schlumberger DBR Technology Center, 9450-17 Avenue, Edmonton, AB, Canada T6N 1M9

Jos Derksen
Chemical & Materials Engineering, University of Alberta, ECERF 7-028, Edmonton, AB, Canada T6G 2V4