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.

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