Special Issue "CFD Modeling of Complex Chemical Processes: Multiscale and Multiphysics Challenges"

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Editorial

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After decades of development, computational fluid dynamics (CFD), which solves fluid mechanics and, more generally, transport phenomena problems using numerical analysis, has become a main-stream tool in many areas of engineering practice. In chemical processes, CFD is widely used not only in predicting fluid flow and mixing patterns in chemical reactors, but also in the simulation and modeling of various unit operations where complex flow and transport processes make process outcomes hard to predict and control. Although CFD models typically still require experimental validation, their application brings many advantages in process research and development. First, numerical solutions from CFD contain fully detailed information about the flow field and distribution profiles of other quantities of interest (temperature, pressure, chemical species concentration, etc.), which are often hard to measure directly from experiments, especially in situ. The availability of such detailed data on the fluid dynamics is often critical to process analysis and improvement. Second, a carefully validated CFD model can be used to predict process outcomes in new operating conditions and process design, with which untested process parameters can be prescreened. As such, the number of experiments and trials and errors can be greatly reduced. This not only reduces the cost in, e.g., process design, adaption, and scale-up, but also reduces the risk of potential safety, environmental, and health hazards associated with many chemical processes.

With the increasing power of high-performance computing (HPC) facilities and continued development of numerical techniques, the accuracy and sophistication of CFD models have improved. Obtaining reliable and practically useful predictions, however, is far from a simple click of a button, owing to the intrinsic complexities in many chemical processes. Most chemical processes involve complex coupling of fluid flow with other physicochemical processes, such as heat and mass transfer, chemical reactions, and particle/bubble/droplet dynamics. In addition, dynamics over vastly different length and time scales also interact in nontrivial ways. For one thing, many chemical processes involve flow turbulence, which is intrinsically multiscale. For another, multiphase flow processes where phase separation and fluid flow occur at different scales are also common. Overcoming multiscale and multiphysics challenges is thus often a central theme and requires innovative modeling approaches that best suit the particular systems.

This special issue "CFD Modeling of Complex Chemical Processes: Multiscale and Multiphysics Challenges" highlights some recent advances in the application of CFD in chemical processes. We take a very liberal approach and define chemical processes as those where principles of chemical engineering, such as transport phenomena, are important, even though the direct application may not fall within the traditional scope of the chemical industry. A total of 16 papers are collected, including one review, 14 original research articles, and one correction. The topics range from pure methodology development to the application of existing CFD tools in practical systems, and everything in between.

The review paper by Nakhaei et al. [1] offered a comprehensive and in-depth account of CFD application in gas–solid cyclone separators. It covered the fundamentals of gas–solid cyclone separator systems including their key performance metrics and how they are influenced by operating conditions. This was followed by an extensive review of available approaches for the numerical modeling of such systems and a summary of existing CFD studies at both ambient and elevated temperatures. Capabilities and limitations of existing approaches were also discussed.

Among the original research articles, Vachaparambil and Einarsrud [2] had a focus on modeling methodology. Based on simple benchmark problems, the study compared different surface tension models used in the volume of fluids method for gas–liquid two-phase flows. Special attention was given to the occurrence of spurious currents due to model inaccuracies.

Other studies all targeted more complex and practical engineering systems. Several studies applied CFD to different types of chemical and biochemical reactors. Ebrahimi et al. [3] studied the flow and mixing performance of double impellers in a stirred-tank reactor. Effects of impeller configuration and speed were reported. Han et al. [4] studied the combustion performance in a pulverized coal furnace with burners installed on the front wall by coupling the momentum balance (with turbulence model), species transport, and energy balance equations. The goal was to optimize the process for reduced nitrogen emission and air pollution. Reactors with multiphase flow were also represented. Khezri et al. [5] studied a bubbling fluidized-bed reactor for biomass gasification. The gas–solid flow was modeled with an Eulerian–Eulerian approach and various turbulence and drag models were compared. Effects of air distributors with different pore sizes were also examined. Tao et al. [6] again used an Eulerian–Eulerian two-fluid model to study a large-scale high-pressure gas–liquid bubble column reactor, with a focus on the effects of operating parameters on the gas holdup of bubbles of different sizes. An Eulerian–Eulerian two-fluid model was also used in Sarkizi Shams Hajian et al. [7] for the gas–liquid two-phase system in the production process of baker's yeast at the industrial scale. The study combined turbulence modeling with species transport and bio-kinetic models to analyze species distribution in the reactor.

CFD studies of other unit operations are also included. Wang, Z. et al. [8] studied a rotating packed bed process for gas desulfurization, where a liquid solution was dispersed in the gas phase for the selective absorption of H_2S. An Eulerian–Lagrangian approach was used where the dynamics of liquid droplets were described by coupling force balance with kinetic models for their coalescence and breakup, with which characteristics of droplets were studied. Qadir et al. [9] numerically simulated the gas separation process in membrane modules and studied the effects of membrane configuration and operating parameters. Landauer and Foerst [10] experimentally studied the triboelectric separation of starch and protein particles. After passing through a charging tube, particles carrying different triboelectric charges settled to different distances in a separation chamber under an electrical field. Effects of particle size and material on the settling distance were studied. The gas flow field in the chamber was modeled with CFD, and simulated particle trajectories in the flow and electrical fields were used to estimate the minimum charge for particle separation. Along the lines of particle processes, Yang et al. [11] used an Eulerian–Lagrangian discrete particle model to simulate the pneumatic conveying of coal particles, studied the effects of operating conditions on the pressure drop, and identified the range of model applicability by comparison with experiments.

Applications in transport processes not in the traditionally-defined scope of chemical engineering, which nonetheless were built on the same principles, are also represented in this special issue. Gao et al. [12] used CFD to model the hydrodynamics in the lateral inlet/outlet part of a pumped hydroelectric storage system. Surrogate models were then built based on CFD results and used for the geometric optimization of the device. Wang, W. et al. [13] measured the air flow, temperature, and relative humidity in the blind heading of an underground mine in situ to study the heat emission by equipment. CFD was conducted to obtain the detailed flow and temperature fields and to optimize the design of the ventilation system. Also in mining, Zhou et al. [14] numerically solved the air flow and species transport equations in a typical stone-coal mine laneway to study the effects of forced ventilation on the radon concentration. Numerical analysis of coupled fluid flow and transport processes was also the theme of Mousavi et al. [15], where the air flow and heat transfer in a novel sustainable farming compartment (SFC) was modeled. This SFC was designed with an evaporative cooling system where the vaporization of treated wastewater was used to absorb heat and the cooling effect was distributed across the domain by forced convection. An experimental prototype was also set up to demonstrate the concept, and CFD was used to optimize the system design and operating conditions.

Finally, we would like to express our sincere gratitude towards all authors for contributing to this special issue. We look forward to the continued development of CFD methodology and its application in chemical process engineering in years to come.

Conflicts of Interest: The authors declare no conflict of interest.

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