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Editorial

Special Issue: Applied Computational Fluid Dynamics (CFD)

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Many industrial and manufacturing processes exhibit complex and coupled fluid flow phenomena. Understanding these phenomena is a key factor in energy efficiency, reduced emissions and product quality, as well as other performance parameters. Compared to prototype-based design and development, Computational Fluid Dynamics (CFD) can allow for a more efficient and cost-effective evaluation of design alternatives. Since its early applications in the aerospace industry in the 1960s, CFD has made a significant impact in many other applications, e.g., biomedicine, mineral processing, metallurgy, and the process industry in general. This extended range of applications led to the considerable development of models and multiphysics concepts, which have been realized in various simulation platforms. However, owing to the different platforms and practices for dissemination across different applications, concepts that could be utilized and beneficial in other industries may not be well-known or easily accessible.

To address this, a cross-disciplinary, cross-industrial Special Issue on Applied Computational Fluid Dynamics was proposed, in which best practices, new methods, results, and frameworks could be presented, aiming for the mutual advancement of the field as a whole.

A total of seven contributions were made to this Special Issue, as summarized in the following section. The Special Issue is available online at https://www.mdpi.com/journal/processes/special_issues/applied_CFD (accessed on 30 January 2023).

An important contribution of applied CFD is related to the optimization of separators and reactors. A common feature for such optimization studies is that the design space can be relatively large, considering both flow rates and geometry for the various constituents of the in- and outflow. Detailed simulations of all possible configurations are not a viable approach, due to their high computational costs; nor are they necessary, as the design of experiment principles can be utilized to map out the main effects, combined with interpolation to determine a (local) optimum. With the introduction of machine learning, this process can be automated to a large degree, thereby increasing the efficiency and throughput of the design stage. A demonstration of such a workflow is given by Park and Go [1], as applied to the design of cyclone separators, in which simulations based on the 3D Reynolds Averaged Navier Stokes equations with a Lagrangian particle phase are realized in the commercial CFD code Ansys FLUENT. The simulation results describe the separation efficiency for the selected designs. These were were used to establish both a multi-linear regression (MLR) model and a deep neural network, concluding that the neural network outperformed that of the MLR.

The design and optimization of reactors and separators relies upon accurate and quantitative models that can reproduce actual flow phenomena, which is particularly challenging when considering multiphase flow, as encountered in, for instance, gas–liquid reactors. The transfer of mass, momentum and heat between phases relies on accurate predictions of their shape. This has led to the development of several numerical approaches, such as the classical Volume of Fluid (VOF) method of Hirt and Nichols [2], the Level Set (LS) method of Sussman et al. [3], the Coupled Level Set-VOF (CLSVOF) method of Sussmann

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and Puckett [4], and the more recent Conservative Level Set Method (CLSM) by Olsson and Kreiss [5]. Rivera-Salinas et al. [6] evaluated the applicability of CLSM for gas injection in a liquid by comparison to numerical results obtained with VOF, as well as experimental observations, with simulations realized in the commercial code COMSOL Multiphysics. The simulations indicate that the CLSM is accurate, robust and conservative for the most important features in gas injection processes, even under conditions in which capillary forces do not dominate. Reactor design will necessarily also involve a modeling of the reactions taking place and how the kinetics are influenced by fluid flow. In the Special issue, this is exemplified in the work of Loomba et al. [7], aiming to describe how operational and design parameters affect the productivity of biomass a photo-bioreactor. Simulations are realized using COMSOL Multiphysics (referanse), using a Eulerian–Lagrangian strategy to simulate gas injection at the bottom of the reactor, with a growth rate that depends on the instantaneous (local) light intensity, owing to photosynthesis. The biomass growth rate in the specific reactor was found to depend more on design parameters such as light intensity than operational conditions, which only significantly influenced the growth rate if this varied in orders of magnitude.

CFD is widely adopted within heat transfer, with applications in, for instance, heat exchangers, power generation and combustion, exemplified in the current Issue through the work of Ammar Ali et al. [8] and Keser et al. [9]. In the work of Ammar Ali et al. [8], the commercial code ANSYS Fluent is used to study the heat transfer and pressure drop in helically micro-finned tubes, aiming to improve the efficiency of heat exchangers. Helically finned tubes with alternating fin hights are identified to have a better performance than fins with a constant height. The second contribution regarding heat transfer, presented by Keser et al. [9], describes the development of an advanced simulation framework for the dynamic behavior of dense evaporating liquid fuel sprays, based on an Eulerian multi-fluid approach developed in the open source software OpenFOAM, with special attention being paid to thermal phenomena occurring within the moving droplets. The proposed model accurately predicts atomization and secondary breakup in the spray, as well as evaporation and mixing phenomena, thus representing a good foundation for further development.

Another important application of CFD in industry relates to the ventilation and optimization of fans, as exemplified by Hurtado et al. [10,11], using the commercial code ANSYS Fluent to optimize guide vanes for the fan intakes [10] and study the effect of parallel stations for primary fans [11]. Close to 220 studies were conducted for the guide vanes to span the design space, ultimately identifying that only elbows with relative curvatures of less than 1.0 benefit from guide vanes, reducing turbulence levels and vorticity by more than 50%. For the parallel fans, three different configurations were considered, namely, symmetrical- and overlap branches, and run-around bypass. These were assessed techno-economically, highlighting how CFD can be used in a wider context.

Evidently, Computational Fluid Dynamics has a broad range of applications, exemplified in the current Special Issue through cyclones, reactors, heat exchangers, fuel sprays and ventilation systems. The studies presented in the Special Issue utilize a wide range of tools and methods, allowing for optimization, the development of new approaches and economical assessments of different applications. A common challenge is that the design space can be large and consist of many interdependent variables, potentially resulting in the need for a large amount of computationally expensive simulations. The combination of CFD and machine learning algorithms, as exemplified by Park and Go [1], can effectively reduce the overall computational requirements and will most likely see extensive usage in the future.

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