Application of CFD in chemical reaction engineering

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Highlights

- Computational models complement traditional experimental methods.
- Computer simulation models provide deeper process insights at different scales.
- CFD enables expanding exploratory analysis in harsh laboratory conditions.

1. Introduction

Computational Fluid Dynamics (CFD) serves as a valuable complementary tool in chemical reaction and reactors engineering, offering detailed insights that enhance traditional experimental approaches. This keynote explores how CFD integrates with experimental methods to optimize and understand diverse catalytic systems, providing a comprehensive view of its applications and benefits. CFD involves the use of advanced numerical methods to simulate fluid flow, heat transfer, and chemical reactions within reactors and process equipment in general. By solving the governing equations for fluid dynamics and chemical kinetics, CFD models can predict the behavior of complex systems under a range of operating conditions. This capability is particularly useful in situations where experimental studies are challenging due to harsh conditions or intricate geometries.

2. Application examples

As application example, the work reported by Reinao and Cornejo [1], exemplifies the use of CFD to explore novel geometric configurations of catalytic substrates (see Figure 1a). The study focuses on dual cell density monoliths, which consist of two concentric regions with different cell densities, to analyze and optimize flow distribution. By employing CFD models validated against classical data, is demonstrates that flow distribution in these substrates depends primarily on geometrical features rather than flow rate. Conducting a large series of experiments to measure flow distribution in such geometries is challenging and resource-intensive. It requires extensive setups, precise control of experimental conditions, and data collection, which can be time-consuming and costly. In contrast, CFD allows for comprehensive parametric studies, enabling researchers to simulate numerous scenarios and configurations quickly. Once the CFD models are validated with a few key experimental data points, they can be used to predict the behavior of the system under various conditions. This approach not only saves time and resources but also provides deeper insights into the underlying physics of the flow distribution. This highlights the utility of CFD in investigating and designing innovative substrate shapes, enhancing efficiency and performance under challenging experimental conditions.

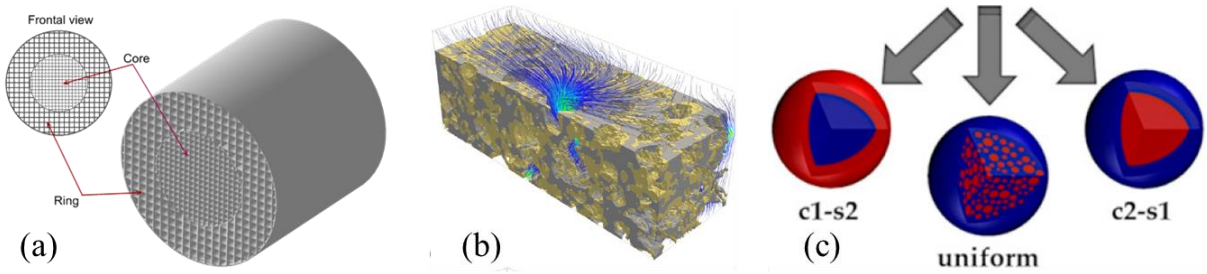

Figure 1. Example of systems studied aided by computational models. (a) Dual cell density catalytic monolith substrate [1]. (b) Coated porous wall-flow catalytic particle filter. (c) Core-shell pellet for the direct production of DME from CO2 hydrogenation

Another example demonstrating the utility of computational models is presented in the paper Plachá et al. [2]. This study introduces a pore-scale model to predict particle deposit formation within a catalytic filter wall. The model effectively captures the dynamics of particle growth, transition from deep to cake filtration, and the impacts on flow field, pressure drop, and filtration efficiency. Validated against time-resolved X-ray tomography (XRT) data, this CFD model provides detailed visualization and investigation of phenomena at a microscopic scale. Such investigations are challenging and expensive to achieve through physical experiments alone, particularly given the small pore sizes and the difficulty of tracking flow through them. The CFD approach allows for extensive parametric studies to be conducted efficiently and inexpensively, with only a few necessary validation points through experimental data. This enables researchers to optimize the design and performance of catalytic filters, addressing both current and future needs in automotive exhaust gas aftertreatment systems and serves as an additional example of the utility of CFD in chemical reactors engineering solutions.

Bizon et al [3] shows a different perspective. This study uses CFD to investigate the performance of bifunctional catalyst pellets with different spatial distributions of catalytic active centers (see Figure 1c). The CFD models allow for detailed exploratory analysis of several configurations, which is valuable given the complexity and cost of conducting extensive physical experiments to measure performance metrics like product yield and selectivity. By simulating numerous configurations computationally, researchers can identify optimal designs before transitioning to physical experiments. This approach enhances the understanding of catalyst behavior at a microscale, providing insights that are difficult to achieve through laboratory experiments, especially when dealing with intricate pore structures and interactions within the pellet. In this case, CFD enables the testing of a wide range of scenarios efficiently and inexpensively, thereby guiding experimental designs to focus on the most promising configurations only. This not only improves the efficiency and effectiveness of experimental work but also may significantly reduce associated costs and time.

3. Concluding Remarks

While experiments remain the cornerstone of chemical reaction engineering, CFD provides a powerful complementary perspective. By integrating CFD with experimental methods, researchers can achieve more efficient and sustainable chemical processes. This combined approach enhances understanding, helps optimize designs, and addresses complex challenges in catalytic systems, saving time and resources. The continued development and validation of CFD models will drive further advancements, supporting the industry's push towards research and development, optimization, and innovation.

References

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Keywords

Computational Fluid Dynamics; Chemical Engineering; Numerical Models; Multiscale Modeling.