Modeling of catalytic fixed-bed reactors: comparison of 1D and 3D particle-resolved simulations

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Highlights

- Calculations of packed bed reactors with detailed surface chemistry (catalytic partial oxidation, dry reforming).
- Comparison of particle resolved 3D CFD and 1D models for different tube-to-particle diameter ratio (N).
- Results show that 1D model agrees well with 3D results for different thermal condition for N down to 2.
- Distinct best-fit correlations identified for endothermic (DMR) and exothermic (CPOX) reaction.

1. Introduction

In the dynamic field of chemical engineering, modeling fixed bed reactors, particularly for heterogeneous catalysis, stands as a crucial challenge, intertwining the needs for efficiency and accuracy. This study embarks on a comparative analysis of packed/fixed bed reactor models including detailed heterogeneous chemical kinetics, targeting a vital issue: comparing time-consuming 3D Particle Resolved Computational Fluid Dynamics (PRCFD) models with the computational efficiency of 1D models. Through simulations of Catalytic Partial Oxidation (CPOX) and Dry Methane Reforming (DMR) processes under various conditions, including different tube-to-particle diameter ratios (N = 1.1, 2, and 7) and Reynolds numbers (Re = 29, 145, 290 and 1450), this study assesses the capability of 1D models to replicate the complex chemical processes (with and without chemical reactions) typically modeled in 3D packed bed reactor. This comparative analysis not only seeks to determine under which conditions 1D models can effectively match the fidelity of 3D models but also explores the factors influencing the performance and accuracy of 1D models. Ultimately, this research aims to identify scenarios where 1D models can be efficient alternatives to 3D models, enhancing the approach to reactor modeling and simulation in chemical engineering.

2. Methods

This study details the development of a 1D heterogeneous model utilizing the DETCHEM software package [2]. The model accounts for detailed gas-phase and surface chemistry and solves equations for mass, species, and heat balance while assuming constant radial fluid properties. The model incorporates over 60 empirical correlations for heat and mass transfer, aiming to enhance its predictive accuracy. The study also employs Computational Fluid Dynamics (CFD) simulations, which are executed through an integration of DETCHEM and OpenFOAM, referred to as the DUO code [3]. This combination allows for in-depth analysis of surface chemistry and precise species property modeling.

3. Results and discussion

Figure 1 presents a comparison of results for N = 2 (86 particles) and a Reynolds number (Re) = 362 (superficial velocity = 2.5 m/s), the simulations incorporate detailed surface kinetics for Dry Methane Reforming (DMR) and Catalytic Partial Oxidation (CPOX) under both adiabatic and non-isothermal conditions. The study's focus on N=2 is significant in this context as it poses a challenge for 1D models. This is due to the fact that empirical correlations are typically validated for higher N values. In the adiabatic DMR scenario (a), both models exhibit uniform temperature profiles, indicative of a stable thermal environment. Conversely, the non-isothermal DMR (b) shows an increase in temperature along

the bed (axial coordinated from 0 to 0.5 m), demonstrating the PBR model's ability to predict heat exchange with the tube wall. Scenarios (c) and (d) for CPOX reveal a rapid decrease in methane concentration at the inlet and a corresponding rise in hydrogen production. The non-isothermal CPOX simulation (d) indicates a significant temperature rise, aligning with the exothermic reaction behavior.

The 1D model aligns closely with the 3D CFD outcomes, suggesting its potential as a computationally efficient alternative for modeling reactor behaviors. This agreement is particularly noteworthy, considering the model's dependence on carefully selected heat and mass transfer correlations for accurate simulations. The study also reveals that the optimal correlations for the endothermic DMR reaction differ from those for the exothermic CPOX reaction, emphasizing the importance of selecting specific correlations based on the thermal nature of the reaction. The need for precise correlation selection in 1D models is critical to their success in emulating the complex behaviors of 3D reactors, as evidenced by the PBR's ability to replicate temperature increments in non-isothermal conditions and capture initial reaction hot spots in CPOX processes with fidelity comparable to that of the detailed CFD models.

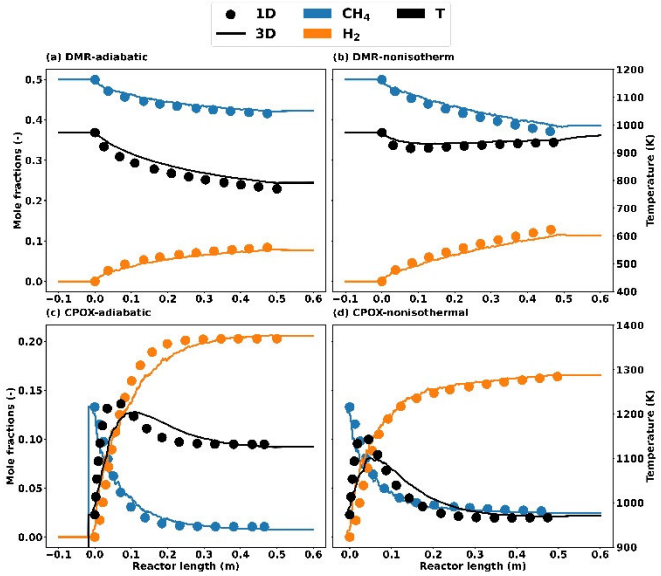

Figure 1. Comparison of 1D vs. 3D axially resolved gas-phase species (CH_4 and H_2) (primary y-axis)and temperature profiles (secondary y-axis) for (a) DMR adiabatic (b) DMR non-isothermal (c) CPOX adiabatic and (d) CPOX non-isothermal conditions.

4. Conclusions

In conclusion, this study has substantiated that 1D simulations, when equipped with appropriate empirical correlations for heat and mass transfer, can closely approximate the intricate chemical behaviors traditionally analyzed with 3D CFD models also for small values of N. The efficacy of 1D models is particularly pronounced in non-isothermal conditions, capturing the dynamics of heat and mass transfer with high fidelity. By carefully selecting correlations tailored to specific reaction types, such as CPOX and DMR, 1D models have been validated as effective and efficient alternatives to 3D simulations for industrial use.

References

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Keywords

Packed bed reactor, Heterogeneous catalysis, Heat and mass transfer.