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Computational modeling of methanol synthesis in millireactors

Daulet Izbassarov[†], Judit Nyári[†], Arto Laari[*], Annukka Santasalo-Aarnio[†], Ville Vuorinen[†]

[†] Department of Mechanical Engineering
Aalto University
FI-00076, Espoo, Finland
e-mail: daulet.izbassarov@aalto.fi, judit.nyari@aalto.fi, annukka.santasalo@aalto.fi, ville.vuorinen@aalto.fi

[*] LUT School of Engineering Science
LUT University
FI-53851, Lappeenranta, Finland
e-mail: arto.laari@lut.fi

ABSTRACT

Methanol production via CO_2 hydrogenation is currently under a great deal of attention due to its CO_2 mitigation and excess electricity storage potential. Moreover, methanol is also a versatile product that can serve as a raw material for the chemical and petrochemical industries. Methanol synthesis from CO_2 and H_2 works similar to natural gas-based synthesis and is usually carried out in the fixed bed reactor. The performance of the process is governed by the fluid flow and its interaction with the catalyst material. One of the approaches for studying the fixed bed phenomenon is to use the one-dimensional approach, i.e., the plug flow reactor model. This approach predicts the overall global performance of the chemical reactor. Another more comprehensive approach is to use computational fluid dynamics (CFD) simulations. In the CFD, the fixed-bed can be modeled using two approaches the porous-media model and particle-resolved methodology. In the first method, the full-size reactor can be taken into account, while the latter one enables only partial reactor simulations. However, the latter approach provides more detailed information regarding local transport phenomena inside the bed. In the present work, both the plug flow reactor model and CFD methodology are considered. The formal approach is modeled using the Aspen Plus, while the latter one is considered within OpenFOAM framework. A catalytic solver is developed within OpenFOAM for numerical simulation of methanol synthesis over Cu/Zn/Al/Zr catalyst in a porous media. The solver allows solving the heterogeneous reacting, multi-component, compressible fluid flow with heat transfer in complex geometries. A global surface reaction model based on the Langmuir-Hinshelwood (LHHW) kinetic model is utilized. The same LHHW kinetic model is implemented in both the Aspen Plus and the OpenFOAM. The computational approach is first validated against standard benchmark problems for non-reacting and reacting cases from the literature. Finally, the method is applied to find optimal conditions for methanol production in a conventional packed bed reactor and a newly designed modular millireactor. The results obtained in this work are believed to enhance the process of methanol production from CO_2.

Keywords: CFD, OpenFOAM, Aspen Plus, Catalysis, CO_2 hydrogenation.