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Influence of particle shape on reaction and transport patterns in fixed beds for methanol partial oxidation to formaldehyde

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Formaldehyde is a very important chemical with a wide range of applications. Methanol partial oxidation on Fe-MoO3 catalyst is the most favorable method for formaldehyde production. The catalyst for this process is highly selective toward formaldehyde production (selectivity > 90%). Methanol conversion in the process is also high (conversion > 98%). The scholarly work on methanol partial oxidation has been mostly focused on the catalyst optimization, and very few studies have tried to evaluate the fixed bed performance and detailed interactions of fluid flow, reaction and transport in the system.
In this work we focused on the effects of the fixed bed configuration on the system performance, particularly, selectivity toward formaldehyde. To investigate the potential impact, a detailed computational method is developed to integrate the flow with the transport and reaction in both the fluid and solid phases. The catalytic particles with complex shapes are explicitly modeled using resolved-particle CFD simulations. Four different particle shapes are studied: sphere, cylinder, ring and tri-lobe. It is shown that the local selectivity is highly correlated with radial temperature gradient and particle shapes. Furthermore, the radial heat transfer is also affected by the particles shapes. The results suggest that particles with more area to volume ratio not only provide more surface for fresh feed to react but also due to shorter diffusion path prevent the formaldehyde from further oxidation. However, such particle shapes could negatively affect the radial heat transfer, and cause a higher radial temperature gradient. The results provide new insights for a better design and optimization of fixed bed processes.
Finally, the three-dimensional resolved-particle CFD results are compared with a standard 1-dimensional model. The limitations of the latter model are discussed and a resolution for their improvement is suggested.

References

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Primary authors: Mr PARTOPOUR, Behnam (Worcester Polytechnic Institute); Prof. DIXON, Anthony (Worcester Polytechnic Institute)

Presenter: Mr PARTOPOUR, Behnam (Worcester Polytechnic Institute)

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