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A Computational Approach for Selection of Optimal Catalyst Shape for Industrial Catalytic Reactions

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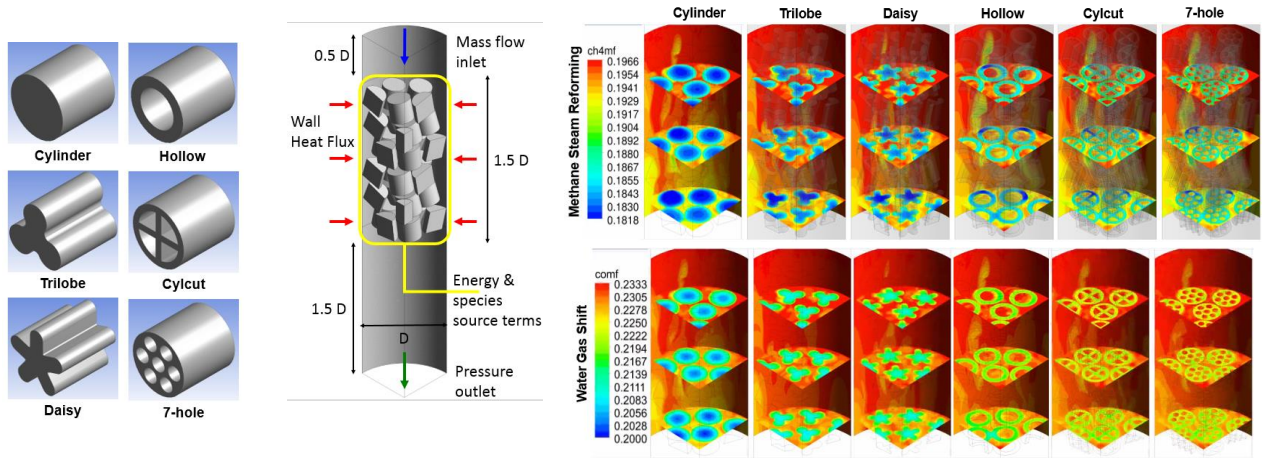
Highlights

- Resolved particle-scale CFD simulations to predict reactor performance with six different particle shapes (cylinder, trilobe, daisy, hollow, cylcut, 7-hole).
- Three different industrial catalytic reactions (methane steam reforming, water gas shift & methanol reactions) were investigated.
- Comparison of the differences in reactor performance for different particle shapes under different industrial conditions for selection of optimal catalyst shape for a particular reaction.

1. Introduction

Due to their high surface to volume ratio, random packed beds are widely used in chemical process industry to perform catalytic reactions. Different particle shapes (usually spherical or cylindrical, but also some complex shapes) are being used for various industrial catalytic reactions. The particle shape has a major impact on the local transport phenomena (flow, heat & mass) which influences the overall reactor performance with respect to pressure drop, reactant conversion etc. However, there is lack of information on choosing an optimal catalyst shape for a particular catalytic reaction in the open literature.

A lot of work has been done to develop empirical correlations and lower order models for the packed beds reactor design. But, these models do not sufficiently represent the effects of particle shapes which heavily influences the local transport phenomena and thereby reactor performance. This also points that the uniform temperature and species distribution on the particle surface is too simplified an assumption that ignores the local inhomogeneity. In recent years, particle-scale (mostly spheres or cylinders) CFD simulations are being used for prediction of reactor performance which alleviates the limitations mentioned earlier again, but their applications are limited mostly to flow and heat transfer studies, with a few incorporating reactions. Therefore, the main objective of this work is to use this computational approach to analyze the effect of particle shapes on various industrial reactions thereby choosing an optimal catalyst shape for a particular reaction.



(a) *(b)* *(c)*

Figure 1: *(a) Different particle shapes considered in the present work, (b) CFD model with boundary conditions and (c) reactant (CH_4 in MSR, CO in WGS) mass fraction distribution in different r-θ planes for MSR and WGS reactions at Re=50000.*

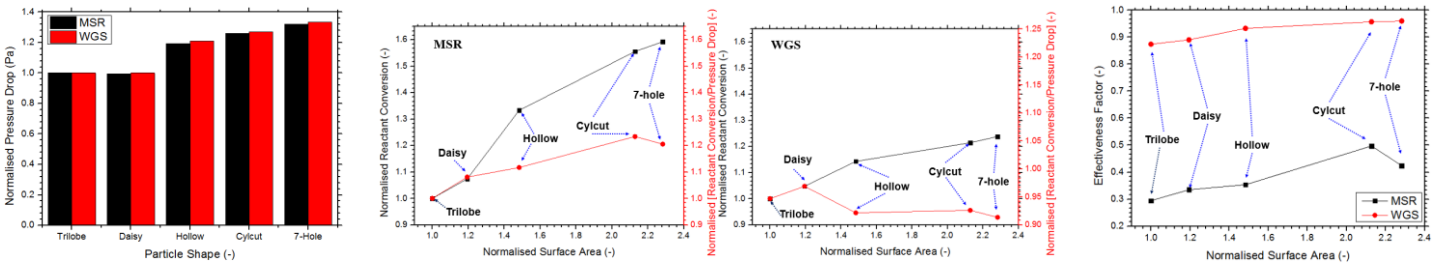
2. Methods

The CFD model consists of a cylindrical packed bed (d_t=100 [mm], h_t=150 [mm]) with 30 particles arranged in random manner was used. Six different particle shapes namely cylinder (d_p=10 [mm], h_p/d_p=1), trilobes, daisy, hollow cylinder, cylcut and 7-hole cylinder were considered (see Figure 1(a)). Despite all the particle

shapes, except cylinder, having equal particle volume (0.6*cylinder volume); the particle surface area differs due to the shape of individual particles. The mesh generated consists of 14.3-30.6 million elements depending on the particle shape. Three industrially important catalytic reactions namely methane steam reforming (MSR), water gas shift (WGS) and methanol (MeOH) reactions were investigated. The reaction and diffusion inside the particle were modelled using the user-defined scalars for species mass fraction defined in particle and fluid with conservative flux across the fluid-particle interface [1]. Alumina material properties were used for the particle. The fluid properties and the boundary conditions for the respective reactions were taken from the literature. The CFD model and generic boundary conditions for different reactions are shown in Figure 1(b). The main difference was in wall heat flux like influx for MSR, adiabatic for WGS and outflux for MeOH. The conservation equations were solved using ANSYS 18.0 with SST k-ω turbulence model for closure using 128 CPU-cores. Further details will be provided in the full length manuscript.

3. Results and discussion

Preliminary simulations were performed with cylinder particle shape to optimize the bed length with appropriate accounting for entrance effects and computational grid in order to reduce the computational cost (results not shown here). Later, the optimized model was extended to different particle shapes for MSR and WGS reactions. A comparison of the reactant (CH_4 in MSR, CO in WGS) mass fraction distribution in different r-θ planes is shown in Figure 1(c). For both the reactions, strong gradients existed inside the cylinder, trilobes and daisy particle shapes, whereas, they were relatively less for hollow, cylcut and 7-hole due to better access for the reactant to particle core. However, for a particular shape, the gradient are much smaller for WGS compared to MSR indicating relatively less diffusion limitations in WGS. In order to quantify the differences arising due to different shapes, ΔP (see Figure 2(a)), reactant conversion & reactant conversion per unit ΔP (see Figure 2(b)) and effectiveness factor (see Figure 2(c)), all values normalized with trilobe for better visualization, were compared. The ΔP was found to increase with increase in particle surface area due to high wall shear (for both the reactions). Similarly, the reactant conversion increased with particle surface area due to higher effectiveness factors, however the slopes were different due to difference in diffusion limitations between the reactions. In summary, 7-hole cylinder offered the best reactant conversion for both the reactions, whereas, cylcut and daisy gave the best reactant conversion per unit ΔP for MSR and WGS, respectively.



(a) *(b)* *(c)*

Figure 2: *Effect of (a) particle shape on ΔP, normalized surface area on (b) reactant conversion & reactant conversion per unit ΔP and (c) effectiveness factor for MSR and WGS reactions at Re=50000, all values normalized with trilobe for better visualisation.*

4. Conclusions

Preliminary investigations showed that particle shape has a significant influence on reactor performance. Also, differences in reactor performance were observed for a particular shape between the MSR and WGS reactions due to difference in diffusion limitations. The work will be extend to model the MeOH reactions. This work helps in selecting optimal catalyst shape for different industrial catalytic reactions. This approach can be extended to any particle shape and industrial catalytic reactions to optimize particle shapes for improved reactor performance.

5. References

[1] Dixon AG, Taskin ME, Nijemeisland M, Stitt EH. Ind. Eng. Chem. Res. 2010; 49(19):9012-25.

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