

# Optimization of bifunctional catalysts in the presence of diffusion limitations, by using a single particle model and a fixed bed model

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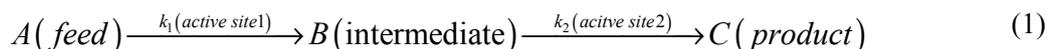
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Bifunctional catalysts are of great importance in multi-step syntheses, where two active sites catalyze different reaction steps. Because bifunctional catalysts may be more efficient than using two separate catalysts, especially when diffusional limitations in the catalysts are strong [1, 2], there is a significant need to develop better bifunctional catalysts for a great variety of refinery, bulk and fine chemical processes (e.g., catalytic reforming, benzene alkylation, isomerization, selective hydrogenations and oxidations). These catalysts can be synthesized by mechanical mixing, coprecipitation, impregnation and other techniques. However, there are still very few studies optimizing the architecture of bifunctional catalysts, let alone comparing the optimization results between different models involving several length scales, from the catalyst intra-particle structure to the reactor.

We built a single particle model as well as a fixed bed model, which couples the component continuity equations at particle scale and reactor scale, to optimize diffusion-limited reactions in bifunctional catalysts. A consecutive reaction scheme is chosen as the model reaction system for investigation, because this scheme can represent many reactions catalyzed by bifunctional catalysts:



Diffusivity and spatial distribution of active sites in bifunctional catalysts are optimized to either maximize the production rate of C for a single catalyst particle exposed to pure A, or to minimize the fixed bed catalytic reactor length for achieving 100% yield of C.

When using the single particle model, there is an optimal diffusivity in the porous catalyst; when employing the fixed bed model, the higher component diffusivities, however, could result in shorter bed lengths used to obtain 100% yield of C. In other words, the optimal structure at the single particle level does not necessarily translate to optimality at the reactor level, and a full reactor scale optimization is required to draw conclusions on what the catalyst structure should be to achieve the highest yields. Contradictory results between single-particle and reactor-level optimization results are also found when optimizing the spatial distribution of active sites. Three archetypical spatial distributions, i.e., uniform (D1), descending (D2, similar to egg-shell type) and ascending (D3, similar to egg-yolk type) toward the center of the catalyst particles, are studied in detail [3]. When using the particle model, D2 is best when there are strong diffusion limitations, and D3 is best in the presence of weak diffusion limitations. When employing the fixed bed model, D2 is always the best one. The inconsistency between the results is attributed to the changes in boundary conditions on the external surface of bifunctional catalyst particles, from the fixed bed reactor inlet to the outlet.

## References

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