Simulation of catalytic reactions in open-cell foam structures

Sebastian Muehlbauer[1], Severin Strobl[1], Matthew Coleman[2], and Thorsten Poeschel[1]

[1]Friedrich-Alexander-Universitat Erlangen-Nurnberg
[2]University of Notre Dame College of Engineering

October 18, 2020

Abstract

We describe a technique for particle-based simulations of heterogeneous catalysis in open-cell foam structures, which is based on isotropic Stochastic Rotation Dynamics (iSRD) together with Constructive Solid Geometry (CSG). The approach is validated by means of experimental results for the low-temperature water-gas shift reaction in an open-cell foam structure modeled as inverse sphere packing. Considering the relation between Sherwood and Reynolds number, we find two distinct regimes meeting approximately at the strut size Reynolds number 10. For typical parameters from the literature, we find that the catalyst density in the washcoat can be reduced considerably without a notable loss of conversion efficiency. We vary the porosity to determine optimum open-cell foam structures, which combine low flow resistance with high conversion efficiency and find large porosity values to be favorable not only in the mass transfer limited regime but also in the intermediate regime.

Hosted file

`SimulationOfCalalyticReactionInPourousStructures.pdf` available at https://authorea.com/users/368172/articles/487405-simulation-of-catalytic-reactions-in-open-cell-foam-structures