Reaction-diffusion study for non-linear reaction systems using Stochastic Rotation Dynamics

A. Sengar*, J. A. M. Kuipers*, R. A. van Santen† and J. T. Padding‡

* Department of Chemical engineering and Chemistry (STW)
  Eindhoven University of Technology (TUe)
  P. O. Box 513, 5600 MB, Eindhoven, Netherlands
  e-mail: info-ST@tue.nl, web page: https://www.tue.nl/en/university/departments/chemical-engineering-and-chemistry/

† Institute for Complex Molecular Systems (ICMS)
  Eindhoven University of Technology (TUe)
  P. O. Box 513, 5600 MB, Eindhoven, Netherlands
  e-mail: icms@tue.nl, web page: https://www.tue.nl/en/research/research-institutes/top-research-groups/institute-for-complex-molecular-systems/

‡Process & Energy Department (3ME)
  Delft University of Technology
  Leeghwaterstraat 39, 2628 CB, Delft, Netherlands
  e-mail: j.t.padding@tudelft.nl, web page: http://delftpe.nl/

ABSTRACT

Combining fluid mechanics with reactive systems at a mesoscale level is important to study coupled reaction-diffusion-convection problems where any of the processes can play a part in determining yield of the product. When reaction is in the non-linear regime, analytical solution to the differential equations becomes impossible. In this study, we aim to study a coupled reaction-diffusion system involving reactions that respond to the local concentration of reactant over a reactive surface both linearly and non-linearly. It is integral for the model development that the coupled fluid interactions in the bulk with the reactions occurring at the surface satisfy the mean-field approximation for both these phenomena so that the model follows rules from continuum mechanics even when the particle treatment is discrete. Stochastic rotation dynamics (SRD), a mesoscale coarse grained technique has been used to study the particle-particle interaction in the bulk and connection to the surface reactive system is achieved by expanding upon Langmuir Hinselwood reaction model kinetics. Evolution of the reaction leads to a multi-component mixture inside the bulk of the system, where hydrodynamic interactions of participating species lead to Maxwell-Stefan-like diffusion in the bulk. We look at the spatial and temporal concentration profiles of reactant across the model reactor developed and study them as a function of Damkohler number, Da. Da gives a qualitative and quantitative comparison between the reaction rate and the diffusive rate, using which we construct model systems with different physical parameters sharing the same Da. We end the discussion by commenting on the yield of product species generated and looking at the future prospective of including a flow to complete the reaction-diffusion-convection system.

REFERENCES