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 Hinshelwood 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

[1] T. M. Squires, R. J. Messinger, and S. R. Manalis, *Making it stick: Convection, reaction and diffusion in surface-based biosensors*, McGraw Hill, Nature Biotechnology **26**, 417 (2008)

[2] R. Krishna and J. Wesselingh, *The Maxwell-Stefan approach to mass transfer*, Chemical Engineering Science **52**, 861 (1997).

[3] T. Ihle, D. M. Kroll, *Stochastic rotation dynamics. I. Formalism, Galilean invariance, and Green-Kubo relations*, Phys. Rev. E **67**, 066705 (2003).