Contribution ID: **16**

Type: **Poster + 3 Minute Pitch**

Mesoscopic simulation and characterization of the morphological evolution in phase separating fluid mixtures

Wednesday, 16 May 2018 16:52 (2 minutes)

In several applications, morphology evolves over time, e.g. in the formation of pores in porous polymer membranes or in the formation of porous particles during spray polymerization of suspensions in a drying chamber. For example, during the preparation of porous polymer membranes by phase inversion process, a homogeneous polymer solution phase separates at contact with a coagulation bath due to a miscibility gap [1]. A polymer rich and a polymer lean phase, representing membrane matrix and pores, are formed. The shape of the morphology can be very different depending on the material properties and process conditions. A direct quantitative comparison of the morphology of porous polymer membranes in experiments and numerical simulations is not possible because of the stochastic nature of the origin of phase separation. A reasonable way to compare different morphology is to compare the characteristics of the morphology. In the context of phase separating fluids, Minkowski functions, Betti numbers, interfacial shape distributions and Doi-Ohta mapping [2] were used to characterize morphology. The latter approach was originally introduced in rheology by Doi & Ohta [3] to describe morphological dependent viscosity of polymer blends. We use Doi-Ohta mapping to characterize the morphology during phase separation because an advantage of the Doi-Ohta approach is that it offers a thermodynamic-consistent evolution equation of the characteristics of the morphology by reducing the Cahn-Hilliard level to a macroscopic level.
The aim is to extend the Cahn-Hilliard-SPH model proposed earlier by some of the authors [4] to account for thermal fluctuations in the concentration by adapting the form of thermal noise suggested in [5]. The result is a thermodynamically consistent model for diffusion controlled phase separating fluid mixtures for engineers, which can be used to investigate the evolution of anisotropic morphology from initially homogeneous fluid mixtures. We simulate different morphology, characterize the anisotropic nature by Doi-Ohta mapping and conclude that the characteristics of the anisotropy is well captured in the Doi-Ohta approach.

References

[1] H. Strathmann: Introduction to Membrane Science and Technology. 1 ed., Wiley-VCH, 2011.
[2] A. Jelic, P. Ilg, H.C. Öttinger. Bridging length and time scales in sheared demixing systems: From the Cahn-Hilliard to the Doi-Ohta model. Physical Review E, 81(2010), 011131.
[3] M. Doi, T. Ohta. Dynamics and rheology of complex interfaces. I. Journal of Chemical Physics, 85(1991), 1242.
[4] M. Hirschler, M. Huber, W. Säckel, P. Kunz, U. Nieken. An application of the Cahn-Hilliard approach to Smoothed Particle Hydrodynamics. Mathematical Problems in Engineering, 2014(2014), 694894.
[5] C. Thieulot, L. P. B. M. Janssen, P. Espanol. Smoothed Particle Hydrodynamics model for phase separating fluid mixtures. II. Diffusion in a binary mixture. Physical Review E, 72(2005), 016714.

Acceptance of Terms and Conditions

Click here to agree

Primary authors: HOPP-HIRSCHLER, Manuel (University of Stuttgart); ZANDER, Christian (University of Stuttgart); Prof. NIEKEN, Ulrich (University of Stuttgart)

Presenter: HOPP-HIRSCHLER, Manuel (University of Stuttgart)

Session Classification: Parallel 8-F

Track Classification: MS 4.22: Evolving porous media and coupled chemical and physical processes