Abstract Submitted
for the DFD20 Meeting of
The American Physical Society

Modeling polymer blend demixing: complications and simplifications in the Gibbs energy of mixing function[1] PIERRE WALKER, Imperial College London, PAVAN INGUVA, Massachusetts Institute of Technology MIT, KEZHENG ZHU, HON WA YEW, ANDREW HASLAM, OMAR MATAR, Imperial College London — The Cahn-Hilliard equation, which can be used to model polymer blend morphology at a continuum scale, tracks the decrease of the Gibbs energy of the system through changes in the homogenous free energy, which is given the Gibbs energy of mixing, and the interfacial energy. In most problems, the Gibbs energy of mixing function is typically set as a simple quartic polynomial or in the case of polymer blends, the Flory-Huggins equation. In certain cases, such as for mineral solutions or alloys, more suitable free energy functions have been employed. However, more accurate and complex equations of state (EoS) applicable to polymer blends such as Statistical Associating Fluid Theory (SAFT) based EoS have yet to be explored within a phase-field setting. In this work, we explore how these advanced EoS can be integrated to model binary polymer blends, looking at both thermophysical properties and blend morphology. At the other end of the complexity spectrum, we also investigate the impact of various simplifications to the free energy function and the Cahn-Hilliard equation on the numerical solution.

[1] This work is supported by the PREMIERE (EP/T000414/1) Programme Grant.

Pavan Inguva
Massachusetts Institute of Technology MIT

Date submitted: 29 Jul 2020

Electronic form version 1.4