Karlsruhe Institute of Technology

CoDiCo FRP

Seminar series of the Graduate School GRK 2078

Referee:	**Prof. Dr. habil. rer. nat. Sabine Enders** Institute of Technical Thermodynamics, (KIT)
Dates:	Thursday, January 12, 2023
Time:	15:45-16:45pm
Location:	Building 10.81, Emil Mosonyi-Hörsaal (HS 62) Please note that you can also participate in the event online
Title:	**Advanced Thermodynamics of Polymer Containing Systems**

Abstract

The thermodynamic properties, like phase behavior and interfacial properties, are complex because these depend on molecular weight, semicrystallinity, tacticity, and branching and in the case of copolymers additionally on the chemical composition. Additionally, all mentioned properties are polydisperse. On the other hand, currently, no thermodynamic model is available to model the thermodynamic properties as a function of all influence parameters.
One milestone in this direction is the Lattice-Cluster Theory (LCT), originally developed by Freed at. al. [1]. The special feature of the LCT is that the impact o molecular weight and arbitrary branching can be considered. The LCT will be applied for the modeling of liquid-liquid equilibria of solutions made from hyperbranched polymers [2]. This allows the study of the impact of the degree of branching on phase behavior. The combination of the LCT with the density gradient theory permits the calculation of the interfacial properties including the interfacial tension, the concentration profiles across the interface, and the interfacial thickness. The predicted interfacial tensions will be compared with experimental data [2].
Another practical- important thermodynamic property is gas solubility, where the semicrystallinity has a large impact. The incorporation of the Flory-approach for semicrystallinity in the LCT framework allows the prediction

Another practical-important thermodynamic property is solubility in solvents, where the semicrystallinity and the degree of branching has a large impact. The incorporation of the Flory approach for semicrystallinity in the LCT framework allows the prediction of solubility as a function of the molecular weight, degree of branching, and semicrystallinity [3]. Using this approach experimental crystalization fractionation could be predicted very close to experimental data [4].
In polymer processing, for instance, using an extruder, the gas solubility, the impact of shear rate on the phase equilibria, and the glass transition are required. These challenges can be solved by coupling the LCT framework with mechanical theories. In the case of gas solubility, the coupling was realized with the cavitation stress theory [5], and in the case of shear rate influence, the storage energy of a non-newtonian fluid must be included [6]. Finally, the LCT in combination with the Generalised Entropy Theory can also be used for the modeling of the glass transition and the impact of dissolved gases.

References

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[5] M. Fischlschweiger, A. Danzer, S. Enders, Fluid Phase Equilibria 506 (2020) 112379.
[6] R. Horst, B.A. Wolf, Macromolecules 24 (1991) 2236-2239.
[7] M. Fischlschweiger, S. Enders, Annual Review of Chemical and Biomolecular Engineering, 10 (2019) 1.

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You are cordially invited to take part in the event.

Prof. Dr.-Ing. Thomas Böhlke
(Spokesperson of GRK 2078)