Modeling of Phase Behavior of Associating Polymer Blends

Sabine Enders^{1, C} and Richy Bergmann^{1, S}

¹Karlsruhe Institute of Technology, Karlsruhe, Germany sabine.enders@kit.edu

Recently, plant-based meat substitutes have generated considerable interest for their benefits in terms of environmental sustainability and personal health [1]. Extrusion is an important technology for preparing wholecut plant-based meat substitutes with meat-like fibrous structure and texture. However, it remains challenging on a more fundamental level to understand the interactions during extrusion processing related to the transition of the protein molecules or phase into fibrous structures, which is considered a "black box" with scarce information inside [1]. Additionally, an understanding of the extrusion process remains a major challenge, as the various protein-rich raw materials (e.g., from different plant origins) exhibit very different material properties [2]. From the thermodynamic point of view, the demixing behavior of the protein-rich raw materials is the most important key to a better understanding. The miscibility gap for polymer blends can be modeled using lattice theories, for instance, the Lattice Fluid Theory proposed by Sanchez and Lacombe [3]. However, this thermodynamic model does not consider the association interaction, which occurs in proteins and has a large impact on the phase behavior. Therefore, we incorporate the association interaction into the Lattice Fluid Theory using different approaches, like the extension suggested by Panaviotou and Sanchez [4] or the extended chemical association lattice model [5]. The contribution discusses the advantages and disadvantages of both models regarding the calculation of the demixing behavior of associating polymers. The calculations were performed using model polymers having associating functional groups, for instance, polymers produced from lactic acid. The calculated miscibility gaps were compared with experimental data taken from the literature.

References

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