Enhancing Polymer Blends Compatibility: From Bulk Thermodynamics to Compatibilizer Chemical Architecture

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Polymer blends can play a key role in the transition towards more sustainable material and production processes. The technological relevance of these materials is clear, but a deep understanding of their chemical physics is still lacking; phase separation and immiscibility are the rule not the exception and, gaining the ability to predict why and when this would happen opens the possibility of designing novel materials (and processes) with the most desired properties. Knowing the phase diagram before processing would allow precise control of the microstructure (which determines the macroscopic behaviour) of polymer blends. Phase diagrams can be determined from bulk thermodynamics, which allows to predict system miscibility conditions. In this work, the pressure-volume-temperature properties of different polymers are experimentally investigated and used to model their miscibility and interfacial properties. The composition and sequences distribution of a compatibilizer (copolymer) can significantly alter the thermodynamic stability conditions for a successful compatibilization; for a polymer A, polymer B, copolymer A-B system this is investigated both theoretically (thermodynamic models) and experimentally (Differential Scanning Calorimetry, Dielectric Spectroscopy, Rheology). The aim is to improve our understanding of the physical and chemical processes and properties underlying polymer compatibilization, and to pave the way for predicting the features a compatibilizer should have to achieve the desired performance in industrial applications.

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$$\frac{\Delta G_{mix}}{RT} = \left(\frac{\phi_1}{N_1}\right)\ln\phi_1 + \left(\frac{\phi_2}{N_2}\right)\ln\phi_2 + \left(\frac{\phi_3}{N_3}\right)\ln\phi_3 + \phi_1\phi_2\chi_{AB} + \phi_3(1-\phi_3)\chi_{blend}$$