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A SURVEY ON MODELS FOR THE PREDICTION OF PHASE EQUILIBRIA IN POLYMER SOLUTIONS

G. A. Mannella*, V. La Carrubba and V. Brucato

DICGIM, (Dipartimento di Ingegneria Chimica, Gestionale, Informatica e Meccanica), Università di Palermo, Viale delle Scienze, Ed. 6, 90128, Palermo, Italy

**Corresponding author: g.mannella@unipa.it*

Various liquid-liquid phase separation techniques are currently involved in the production of polymeric porous structures for various applications, e.g. membranes for a wide range of applications and scaffolds for tissue engineering purposes. Binary and mainly ternary polymer solutions allow to obtain a vast latitude of pore sizes and morphologies. The final morphology of the membrane is strongly affected by the thermodynamic properties of the solution: the phase equilibria of the polymer solution play a key role in the structure formation, e.g. affecting the separation mechanism. Therefore, a deep characterization of phase equilibria in polymer solutions can be a valid support in the membrane production processes. However, the experimental derivation of phase diagram is time and cost consuming. A fully predictive tool based on thermodynamics of polymer solutions would provide a better control of membrane morphology, together with an easier exploration of a wide quantity of solvents. Many theories are available in literature to model polymer solution thermodynamics. Among the lattice fluid (LF) theories, the group contribution models and the compressible LF were chosen to test the applicability on a PLLA-dioxane-water ternary polymer solution, which is used for the preparation of scaffold for tissue engineering. As a general result, the inadequateness of group contribution models to predict the phase separation must be highlighted, together with a scarce sensitivity to temperature. Moreover, a major task stems about the free volume of water in relation to other components. The compressible LF model resulted more sensitive to temperature, suggesting its suitability for modeling polymer solutions containing water.