

Self-Assembly of Ternary Mixture of Water-Vanillin-Ethanol via Dissipative Particle Dynamics

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We investigated phase behaviors of a mixture solution involved in the vanillin extraction via Dissipative Particle Dynamics (DPD). The ternary mixture, which consists of water, vanillin, and ethanol, is chosen and four phases depending on compositions have been formed; micellar, lamellar, transitional, and columnar. Ternary phase diagrams have been constructed at 298 and 333K, from which we identified an optimal range of extract compositions satisfying the solubility of vanillin into ethanol and the US FDA regulation for the ethanol usage for its extraction. The optimal volume percent ratios are 40:20:40 and 50:20:30 for water, vanillin, and ethanol, respectively, and the systems mostly show lamellar phases. It is also interesting to notice that those compositions are well met with an economic perspective.