Fluid-fluid phase behaviour in the explicit hard spherocylinder solvent ionic model confined in a disordered porous medium

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We report our recent theoretical results on a study of the fluid-fluid phase transition of the explicit solvent model represented as a mixture of the restricted primitive model (RPM) of ionic fluid and neutral hard spherocylinders (HSC). We consider this model both in the bulk and in a disordered porous medium. To describe thermodynamic properties of such systems we combine two theoretical approaches, i.e., the scale particle theory (SPT) and the associative mean spherical approximation (AMSA) [1]. It is shown that the SPT is sufficient to provide a rather good description of a reference system taking into account hard-core interactions, and the AMSA is known to be efficient in treating the Coulomb interactions between the ions. Using the conditions of thermodynamic equilibrium, a phase coexistence for a RPM-HSC mixture is found at different temperatures, and the corresponding phase diagrams are built in the temperature-density and temperature-concentration planes. It is observed that the high-density phase mostly consists of the ions. On the other hand, the low-density phase is formed by a high concentration of solvent, thus the orientational order of HSC particles becomes possible in this phase. We have noticed that the orientation order strongly depends on the aspect ratio of HSC particles L_2/σ_2 and on the total pressure in the considered system. For instance, for $L_2/\sigma_2 = 5$ the low-density phase remains isotropic up to high pressures, while for $L_2/\sigma_2 = 10$ the formation of nematic phase of HSC particles is found at rather low pressures. In our study we discuss how a presence of disordered porous medium affects coexisting phases formed in RPM-HSC mixtures and establish conditions at which the nematic phase can occur in them.

1. M. Hvozd, T. Patsahan, O. Patsahan, M. Holovko, *J. Mol. Liq.*, **285** (2019) 244–251, doi: 10.1016/j.molliq.2019.03.171.