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Screening of ionic liquids as green oilfield solvents for the potential removal of asphaltene from simulated oil: COSMO-RS model approach.

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Abstract

Petroleum industry encounters a challenge to search prospective solvents for asphaltene species which is the main cause of arterial blockage in oil pipelines that results in flow assurance problem. Recently, Ionic liquids (ILs) have received significant attention as green oilfield solvents due to their tunable physicochemical properties. In this study, COSMO-RS (Conductor Like Screening Model for Real Solvents) was used to screen ILs to be used as the potential extractant for asphaltene. For benchmarking and validation purpose, the estimated activity coefficient at infinite dilution (AC^{id}) of 3 ILs with various organic solvents (125 data points) at different temperatures were used and the Root Mean Square Deviation (RMSD) value was found to be 0.14 which indicated the good reliability and the prediction capability of COSMO-RS. Henceforth, 240 ILs of different combinations, containing 6 types of cations namely: 1-butyl-3-methyl imidazolium [BMIM], 3-methyl-1-propyl pyridinium [MPPy], n-butyl-iso-quinolinium [C₄isoQ], 1-butyl-1-methyl-pyrrolidinium [BMPYRO], 1-butyl-1-methyl piperidinium [BMPIP] and Tetra methyl ammonium [TMAM] combined with 40 anions were investigated. AC^{id} data of all cation and anion combinations were used for selectivity, capacity and performance index

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