Abstract

[Petroleum industry](https://www.sciencedirect.com/topics/chemistry/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](https://www.sciencedirect.com/topics/chemistry/ionic-liquid) (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](https://www.sciencedirect.com/topics/physics-and-astronomy/activity-coefficient) at infinite dilution (ACid) of 3 ILs with various [organic solvents](https://www.sciencedirect.com/topics/chemistry/organic-solvent) (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](https://www.sciencedirect.com/topics/chemistry/piperidinium) [BMPIP] and Tetra methyl ammonium [TMAm] combined with 40 anions were investigated. ACid data of all cation and anion combinations were used for [selectivity](https://www.sciencedirect.com/topics/physics-and-astronomy/selectivity), capacity and performance index calculations to evaluate the effectiveness of ILs. Results showed that among the investigated combinations, ILs containing hetero-atomic aromatic cations combined with sterically hindered anion e.g. [C6F18P] is favorable for asphaltene removal at ambient temperature and atmospheric pressure.

