For the last decade ionic liquids have been regarded as compounds of interest by the academic and industrial communities. These compounds present several advantages when compared to other typical solvents. However, because of their novelty, a deep understanding of their phase behaviour and their interactions with other components is still needed. In this work, we made a review of literature studies on modelling systems with ionic liquids using equation of state models. Furthermore, we applied the Cubic Plus Association (CPA) equation of state to describe the phase behaviour of two ionic liquids, 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([C2mim][NTf2]) and 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide([C4mim][NTf2]). The first step was to study an adequate approach for the determination of pure component parameters for the ionic liquids. The parameters were obtained by fitting the predictions of the model to experimental vapour pressure and liquid density data. The parameters provide a good description of both experimental vapour pressures and liquid density, with maximum percentage deviations of respectively 8.9 and 1.3% for [C2mim][NTf2] and 5.7 and 0.5% for [C4mim][NTf2]. Different sets of pure component parameters for each ionic liquid were considered and their suitability to describe the behaviour of ionic liquids was evaluated by modelling the vapour–liquid equilibria (VLE) of mixtures with CO2 and the liquid–liquid equilibria (LLE) with water. The results for VLE proved to be very good in the range of pressures studied when using one temperature-independent binary interaction parameter, with percentage deviations in pressure between 8 and 13% for [C2mim][NTf2] and around 12% for [C4mim][NTf2]. For the LLE of ionic liquids with water a temperature-independent binary interaction parameter was also used, but the results do not describe the experimental data as well as with the VLE, with percentage deviations ranging from 4 to 100%. However, for some of the sets of pure component parameters a good description of the experimental data is obtained and work is in progress for improving the modelling of LLE with the CPA equation of state.

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