World Academy of Science, Engineering and Technology
International Journal of Chemical and Materials Engineering
Vol:12, No:04, 2018

Simulation of Multistage Extraction Process of Co-Ni Separation Using Ionic Liquids

Authors : Hongyan Chen, Megan Jobson, Andrew J. Masters, Maria Gonzalez-Miquel, Simon Halstead, Mayri Diaz de Rienzo

Abstract : Ionic liquids offer excellent advantages over conventional solvents for industrial extraction of metals from aqueous solutions, where such extraction processes bring opportunities for recovery, reuse, and recycling of valuable resources and more sustainable production pathways. Recent research on the use of ionic liquids for extraction confirms their high selectivity and low volatility, but there is relatively little focus on how their properties can be best exploited in practice. This work addresses gaps in research on process modelling and simulation, to support development, design, and optimisation of these processes, focusing on the separation of the highly similar transition metals, cobalt, and nickel. The study exploits published experimental results, as well as new experimental results, relating to the separation of Co and Ni using trihexyl (tetradecyl) phosphonium chloride. This extraction agent is attractive because it is cheaper, more stable and less toxic than fluorinated hydrophobic ionic liquids. This process modelling work concerns selection and/or development of suitable models for the physical properties, distribution coefficients, for mass transfer phenomena, of the extractor unit and of the multi-stage extraction flowsheet. The distribution coefficient model for cobalt and HCl represents an anion exchange mechanism, supported by the literature and COSMO-RS calculations. Parameters of the distribution coefficient models are estimated by fitting the model to published experimental extraction equilibrium results. The mass transfer model applies Newman's hard sphere model. Diffusion coefficients in the aqueous phase are obtained from the literature, while diffusion coefficients in the ionic liquid phase are fitted to dynamic experimental results. The mass transfer area is calculated from the surface to mean diameter of liquid droplets of the dispersed phase, estimated from the Weber number inside the extractor. New experiments measure the interfacial tension between the aqueous and ionic phases. The empirical models for predicting the density and viscosity of solutions under different metal loadings are also fitted to new experimental data. The extractor is modelled as a continuous stirred tank reactor with mass transfer between the two phases and perfect phase separation of the outlet flows. A multistage separation flowsheet simulation is set up to replicate a published experiment and compare model predictions with the experimental results. This simulation model is implemented in gPROMS software for dynamic process simulation. The results of single stage and multi-stage flowsheet simulations are shown to be in good agreement with the published experimental results. The estimated diffusion coefficient of cobalt in the ionic liquid phase is in reasonable agreement with published data for the diffusion coefficients of various metals in this ionic liquid. A sensitivity study with this simulation model demonstrates the usefulness of the models for process design. The simulation approach has potential to be extended to account for other metals, acids, and solvents for process development, design, and optimisation of extraction processes applying ionic liquids for metals separations, although a lack of experimental data is currently limiting the accuracy of models within the whole framework. Future work will focus on process development more generally and on extractive separation of rare earths using ionic liquids.

Keywords : distribution coefficient, mass transfer, COSMO-RS, flowsheet simulation, phosphonium
Conference Title : ICAIL 2018 : International Conference on Advances in Ionic Liquids
Conference Location : Venice, Italy
Conference Dates : April 12-13, 2018