HEHEHP AND D2EHP DATABASE TO PREDICT RARE EARTH SOLVENT EXTRACTION

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ABSTRACT

We combined a semi-empirical extractant database, a rigorous electrolyte thermodynamic model, and a process simulator to predict solvent extraction of rare earth elements from an HNO3 solution to the hydrocarbon phase. We then predicted the extractant regeneration and metals separation using a caustic solution.

We created the extractant database using publicly available data for D2EHP and HEHEHP and for these extractants with fifteen rare earth elements. The data included extractant solubility in water, metal extraction isotherms, distribution ratios, dimerization constants, acidity constants and heats of saponification. We created several species for each extractant including the base acid, the ionized acid, and the dimerized acid. We also created several metal-extractant complexes for each of the rare earth elements. In total, over 100 individual species were created for the fifteen rare earth metals with the two extractants.

We combined the database with an electrolyte thermodynamic model to compute the liquid-liquid partitioning of the following systems: H_2O-extractant, H_2O-extractant-diluent, and H_2O-HNO_3-$RE(NO_3)_3$-extractant-diluent. We can match with reasonable accuracy the extractant solubility in water, the heats of saponification, and the partitioning isotherms for all fifteen rare earth elements. We also predicted with limited accuracy, the effects of pH, diluent:extractant ratio, total ion concentration, and temperature on metal partitioning. We present the partitioning isotherms for each element in the individual extractant/diluent mixtures and when both extractants are in a 50:50 mixture.

We then used the speciation model with a process simulator to calculate the mass, chemistry, and energy balance across a series of solvent extraction units. We simulated the process without and with mass transfer limiting parameters. We obtained a reasonable match between predicted and reported extraction efficiencies when we include mass-transfer parameters.

Lastly, we identified areas where we can improve existing chemical properties and partitioning mechanisms and where additional experimental data is needed to make a model more robust.

Keywords: Rare Earth, Solvent Extraction, process simulation