ALTA 2024 28
27 - 31 May | Perth, Australia

THERMODYNAMIC MODELLING OF RARE EARTH SOLVENT EXTRACTION

By

Brett Schug, Kevin L. Heppner

SysCAD, Canada

Presenter and Corresponding Author

Brett Schug

ABSTRACT

Rare Earth Elements (REEs) are becoming increasingly important due to their critical role in energy transition. In recent times, there has been significant activity and investment in production from mining and recycling. A key area of difficulty for metallurgical production of REEs is their separation, largely due to their similar electron structures which makes them chemically similar.

In this work, a thermodynamic model of solvent extraction (SX) is presented based solely upon experimental data in the open literature using the PHREEQC (USGS, 2021) interface with SysCAD. In previous work, Heppner (2021) calculated reaction equilibrium constants for the extraction of Nd and Pr based upon fitting to experimental data of Lyon et al. (2017). Here, that model is extended using separation factors published by Zhang et al. (2020) and references therein to estimate the equilibrium constants for all 15 REEs. Pitzer parameters and their temperature dependence are calculated for each cation-anion interaction in the REE chloride system from correlations published by Simoes et al. (2016, 2017). It is noteworthy that aqueous/organic exchange reactions are written in terms of free acid, not hydrochloric acid, and thus, are suitable for use in any acidic medium (e.g. chloride, sulphate, nitrate).

A test of the model was performed where a solution containing REE chlorides was fed to an extraction, scrubbing, and stripping circuit with conditions typical for initial separation of light, medium, and heavy REE elements. Results of the test model show typical trends in the SX separation of REEs, confirming the validity of the approach. This fundamental approach enables a wider range of applicability for the model compared to the use of plant isotherms.

This work focuses on the modelling methodology of the REE SX process, rather than the modelling of a specific processing plant. For this reason, the presented model requires validation against relevant plant data prior to use for plant design or optimisation.

Keywords: Rare earth elements, solvent extraction, equilibrium