

MODELLING OF MULTICOMPONENT ION EXCHANGE IN LITHIUM ION BATTERY RECYCLING

By

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ABSTRACT

Lithium ion batteries are applied in various mobile devices and utilized as power source in electronic vehicles (EVs) due to various advantages such as their high energy density, large operating temperature range and sensible discharge resistance [1]. Recycling of spent LIBs has been reviewed by various researchers and new processes for metal recovery from LIBs have been suggested to recover valuable materials.

Although ion exchange offers advantages and potential in metal recovery due to its high selectivity, ion exchange has only played a minor role in LIB recycling. Recently, our research group proposed a process to remove impurity metals via ion exchange while producing high purity Co/Li/Ni containing battery grade raffinate [2]. Aminomethyl phosphonic acid functional chelating resin (Lewatit TP 260) offers great potential for this process as it shows high affinities towards the impurity metals (Al, Cu, Fe and Mn) and low affinities towards the valuable target metals (Co, Li and Ni) [2].

As part of the process development towards a continuous ion exchange process for metal recovery from LIBWL, equilibrium data is required to model and optimize the process. To our knowledge, the available literature lacks LIB metal equilibrium data at higher concentrations and acidities. Additionally, the literature also lacks in thermodynamic data to describe nonidealities of resin and aqueous phase which makes modeling of ion exchange processes in LIB recycling challenging. In this research, single metal sorption curves have been measured at LIB metal concentration range and high acidity for the first time. Equilibrium data was obtained via batch equilibrium experiments in test tubes using chelating resin Lewatit TP 260 in protonated form at three adjusted pH values (0, 1 and 1.8) and two temperatures (22°C and 60°C). Ion exchange and metal uptake were enhanced with increased temperature and increased pH. Three equilibrium models have been tested to model the equilibrium data and to gain model parameters to predict ion exchange equilibria of multi metal solutions.

In ion exchange from concentrated solutions, the charges of the functional groups must be balanced by the mixture of counter-ions. Physical adsorption isotherm models cannot thus be applied. In principle, the stoichiometric equilibrium of an ion exchange reaction can be described using the mass action law (MAL). Here, MAL was used with the assumption of ideal behavior in the electrolyte and the resin phase. In addition, two explicit equilibrium models were used to describe the experimental data. The non-ideal competitive adsorption (NICA) model by Kinniburgh et al. [3] was rewritten for the case of ion exchange (NICA-IX). The two fitted model parameters for each species i are the affinity constant K_i and the non-ideality constant h_i . When setting h_i equal to 1, the NICA-IX model reduces to the competitive Langmuir isotherm model. Neither MAL, competitive Langmuir, nor NICA-IX models could explain the effect of the proton concentration with a fixed set of model parameters when the acid concentration changes 10 or 100 times, *i.e.* 1-2 steps on the pH scale. However, the experimental equilibrium data for an individual metal at a given pH was well correlated using the NICA-IX model.

The results help to understand ion exchange in concentrated battery metal solutions and provide a useful tool to estimate the equilibria of multi component solutions with chelating resin Lewatit TP260. The model also helps to reduce elaborate experimental work during process design and development of a continuous ion exchange process for battery metals purification.

References:

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