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Modeling of $LiCoO_2$ Leaching Reaction using COMSOL Multiphysics

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Lithium-ion batteries (LIBs) are increasingly being used as energy storage in portable electronic devices and electric vehicles. The growing demand of these batteries involves an increase of disposed LIBs waste, which contains hazardous metals and harmful organic electrolytes that are a threat to the environment. Furthermore, spent LIBs contain high value-metals such as Li, Co, Ni, Al and Cu. Some of these elements are included in the EU's list of Critical Raw Materials due to their high economic importance and high supply-risk. Hence, recycling spent LIBs is important not only to reduce the environmental impact, but also to preserve mineral resources.

Currently, the most popular LIBs recycling processes are either pyrometallurgical and hydrometallurgical. Although the former is the most used method on an industrial scale, hydrometallurgical has become a promising process due to its recovery rate, high purity of the metals and a lower energy consumption. The main step of the hydrometallurgical process is the leaching, where acid is used as an extracting agent to recover metal from the waste LIBs. Different factors influencing the leaching process are the extracting agent concentration, temperature, solid-liquid ratio, reaction time and reductant agent concentration. Determine the reaction rate and the rate controlling step is essential to optimize leaching parameters and improve the process efficiency.

In this work, a mathematical model is presented with the aim of determine the leaching reaction kinetic of LIBs components, namely, $LiCoO_2$ particles. The model is based on a solid-liquid reaction model, in particular on the shrinking core model, due to the formation of Co_3O_4 in the outer part of the $LiCoO_2$ particle when is used an inorganic acid as extracting agent in absence of an external reducing agent. In this model, the diffusion of the reactant through the product layer and the chemical reaction at the surface of the unreacted core are defined as the rate controlling step. A series of extraction analyses were carried out and their results were used to adjust the formulated model. In batch experiments, hydrochloric acid was used as the extracting agent and its concentration was modified from 0.1M to 2.5M while solid-liquid ratio (50 g/L), temperature (25 ºC) and reaction time (2 h) were fixed in all of them.

COMSOL Multiphysics 5.5 program was used to adjust the kinetic model with the experimental results, obtaining as result the value of the kinetics and diffusion constant. The implemented model for simulation of the lithium and cobalt leaching from $LiCoO_2$ reproduces the experimental results, predicting the non-equimolar proportion between Li^+ and Co^{2+} and verifying the hypothesis of the Co_3O_4 layer formation.

Keywords

Lithium-ion batteries, batteries recycling, acid leaching, kinetics, modelling, COMSOL Multiphysics.

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