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Full Length Article

Flotation separation of lithium–ion battery electrodes predicted by a long short-term memory network using data from physicochemical kinetic simulations and experiments

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ABSTRACT

Anode and cathode active materials from spent lithium–ion batteries may be recovered and potentially used in new batteries to promote recycling and resource circulation. Froth flotation was applied to pristine active materials and the black mass obtained from pretreated spent batteries. Flotation kinetics was simulated with the use of computational fluid dynamics and surface chemistry. Bubble surface coverage and entrainment in the flotation kinetics model were selected and optimized by systematic fitting to experimental data. Entrainment influences the recovery and grade of the active materials. The optimized flotation kinetics model was used for generating additional data that, along with the fitted data, were used to train a deep learning neural network. The trained network was validated using anode–cathode and black mass flotation experiments, and its predictions showed a maximum residual error of 0.18 ± 0.11 recovery. The simulation framework was developed into a desktop application that predicts the flotation behavior of active materials. It provides information for estimating results following operational and physicochemical changes and for optimizing flotation processes. Finally, recovered anode active materials from black mass were selected for coin cell tests. The coulombic efficiency of these coin cells was initially lower (86.8 %) than that of cells made with pristine graphite particles (98.4 %).

1. Introduction

Battery technologies include Li–ion, lead acid, solid–state, nickel–cadmium, and nickel–metal hydride batteries [1,2]. Li–ion batteries (LIBs) are a popular choice for electric cars, mobile phones, and laptops owing to their advantages over other battery types, such as energy per weight ratio, despite their high cost and temperature sensitivity [3]. Li iron phosphate, Li manganese oxide, Li nickel manganese cobalt oxide (NMC), Li cobalt oxide (LCO), and Li nickel cobalt aluminum oxide (NCA) are cathode active materials that are used in various types of LIBs [2,3]. An LIB consists of an anode active material (graphite), a cathode active material, binder (carboxymethyl cellulose or polyvinylidene fluoride), electrolyte ($LiPF_6$ or $LiBF_4$), separator (polyethylene or polypropylene), current collectors (copper foil for anode and aluminum foil for cathode), and various additives [4–6]. However, as the popularity and use of LIBs increase, so does their disposal. Therefore, the recycling of spent LIB batteries, including the recovery of anode and cathode active materials, is crucial for the environment and the recirculation of mineral resources as ores become depleted.

Pyrometallurgy (e.g., pyrolysis, incineration, calcination, roasting, and microwave reduction) and hydrometallurgy (acid leaching, precipitation, and solvent extraction) are used to recycle spent LIBs [5,6]. Pyrometallurgy is simple but involves high energy consumption, while hydrometallurgy yields high metal recovery but also requires high acid consumption [7,8]. Moreover, they produce physical and chemical

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Highlights

- Entrainment recovery was empirically included in an advanced flotation model.
- Experiment and simulation data were used to train a deep long short-term memory neural network.
- Software package integrating the neural network was developed to predict flotation hydrodynamics and probabilities, as well as pulp and entrainment recoveries.

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