AN EXPERIMENTALLY VALIDATED CFD MODELLING APPROACH FOR THE SIMULATION OF ALUMINA PRECIPITATION TANK REACTORS

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ABSTRACT

The aluminothermic reduction of ores and residues is a process that has gained a lot of interest over the past years. During this process, a metal phase and a calcium aluminate slag are formed. The latter can be leached with Na_2CO_3 for the recovery of aluminum. The produced sodium aluminate solutions differ from the ones produced through the Bayer process and thus they can't be efficiently used for the traditional seeding precipitation. Instead, carbonation precipitation is applied to obtain aluminum, where CO_2 gas is inserted, lowering the pH and resulting in alumina trihydrate precipitation. Such a process involves gas, liquid and solid-phase interactions, increasing the degree of complexity. For better understanding the phenomena occurring, a three-dimensional CFD model is developed for the precipitation tank and the impeller, considering the main physicochemical mechanisms of the process and the dynamics of the liquid solution during the precipitation process are simulated. A two-phase dispersed flow approach is employed for the simulation of the CO_2 gas flow within the tank, in the form of gas bubbles. The CO_2 mass transfer between the two phases, as well as the CO_2 dissolution reactions, are also taken into account by the CFD model. The computational approach is validated by comparing theoretical predictions for the CO_2 outflow and solution pH with experimental measurements. The model is capable of reproducing the experimental results, illustrating the process dynamics for the CO_2 bubble flow and dissolution. More importantly, the good agreement between predictions and experimental measurements provides a solid basis for the development of an integrated model, which will take into account the simulation of the whole chain of chemical reactions, yielding the targeted alumina hydrate precipitate. The integrated model will provide an insight into the effect of the interplay between the different mechanisms occurring within the precipitation tank, such as the impeller rotation, the CO_2 bubble flow, the mass transfer between phases and the dissolution reactions. This, in turn, will enable the efficient optimization of the whole process regarding reactor design and process conditions.

KEYWORDS: CFD, precipitation process, two-phase flow, rotating domain, aluminothermic reduction

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