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Simultaneous determination of nucleation and crystal growth kinetics of struvite using a thermodynamic modeling approach

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HIGHLIGHTS

- ▶ This work concerns the controlled struvite formation by precipitation.
- ▶ We model nucleation and growth kinetics.
- ▶ A thermodynamic model is coupled with a population balance.
- ▶ The model predicts particle size distribution vs. experimental time.
- ▶ It allows the identification of nucleation and particle growth kinetics parameters.

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ABSTRACT

This work concerns the controlled struvite formation ($MgNH_4PO_4{\cdot}6H_2O$) by precipitation as an alternative removal of phosphorus and, consequently, of ammonium from wastewater discharges. A new method, based on an integrated methodology, is proposed here for predicting and controlling struvite nucleation and growth rate. Experiments were conducted in an isothermal stirred batch reactor at a temperature of 25 °C from a synthetic aqueous solution at different pH levels (8.5–9.6). The initial concentrations of Mg, PO_4 and NH_4 are fixed at 3 mmol/L, then at 4 mmol/L, with a molar ratio of $Mg/NH_4/PO_4$ equal to 1. Crystal size is determined by laser granulometry and morphometry. A population balance-based model coupled with a thermodynamic model predicts particle size distribution vs. experimental time using a reconstruction model. This approach is particularly numerically stable for the identification of nucleation and particle growth kinetics parameters that are used to predict crystal size distribution. The methodology is based on a thermodynamic model previously developed for which pH control and supersaturation constitute key parameters. The obtained results are of major importance for the design of struvite precipitation reactor, and for the development of crystal growth control methodology.

1. Introduction

The cost of environmental protection and pollution prevention is increasing above all because of stringent effluent quality standards. In this context, phosphate impact on water pollution plays a major role since it promotes eutrophication. One proposed solution to this problem is the recovery of phosphate using crystallization. This work addresses the problem of phosphorus recovery from synthetic wastewater by precipitation of struvite. The general objective is to develop a methodology for optimal design of an automated pilot reactor for wastewater treatment.

Two major crystallization processes have been developed for phosphorus recovery from wastewater, respectively the so-called calcium phosphate (CP) precipitation process and the magnesium ammonium phosphate (MAP) or struvite precipitation which is a crystalline substance consisting of magnesium, ammonium and phosphorus in equal molar concentrations ($MgNH_4PO_4{\cdot}6H_2O$). Struvite forms according to the following reaction [1]:

$$Mg^{2+} + NH_4^+ + PO_4^{3-} + 6H_2O \rightarrow MgNH_4PO_4 \cdot 6H_2O \quad (1)$$

It is important to understand and optimize the precipitation process in order to improve product quality, thus minimizing the associated production costs. A previous study [2–5] based on a thermodynamic model was developed to predict the quantity of

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