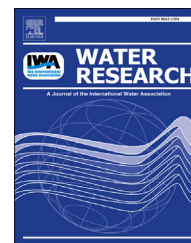


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A generalised chemical precipitation modelling approach in wastewater treatment applied to calcite



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ABSTRACT

Process simulation models used across the wastewater industry have inherent limitations due to over-simplistic descriptions of important physico–chemical reactions, especially for mineral solids precipitation. As part of the efforts towards a larger Generalized Physico-chemical Modelling Framework, the present study aims to identify a broadly applicable precipitation modelling approach. The study uses two experimental platforms applied to calcite precipitating from synthetic aqueous solutions to identify and validate the model approach. Firstly, dynamic pH titration tests are performed to define the baseline model approach. Constant Composition Method (CCM) experiments are then used to examine influence of environmental factors on the baseline approach. Results show that the baseline model should include precipitation kinetics (not be quasi-equilibrium), should include a 1st order effect of the mineral particulate state (X_{cryst}) and, for calcite, have a 2nd order dependency (exponent $n = 2.05 \pm 0.29$) on thermodynamic supersaturation (σ). Parameter analysis indicated that the model was more tolerant to a fast kinetic coefficient (k_{cryst}) and so, in general, it is recommended that a large k_{cryst} value be nominally selected where insufficient process data is available. Zero seed (self nucleating) conditions were effectively represented by including arbitrarily small amounts of mineral phase in the initial conditions. Both of these aspects are important for wastewater modelling, where knowledge of kinetic coefficients is usually not available, and it is typically uncertain which precipitates are actually present. The CCM experiments confirmed the baseline model, particularly the dependency on supersaturation. Temperature was also identified as an influential factor that should be corrected for via an Arrhenius-style correction of k_{cryst} . The influence of magnesium (a common and representative added impurity) on k_{cryst} was found to be significant but was considered an optional correction because of a lesser influence as compared to that of temperature. Other variables such as ionic strength and pH were adequately captured by the quasi-equilibrium description of the aqueous-phase and no further kinetic corrections were required. The baseline model is readily expandable to include other precipitation reactions. For simple representations, large values for k_{cryst}

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with $n = 2$ (or $n = 2$ or 3 for other minerals, as appropriate) should be selected without corrections to k_{cryst} . Where accuracy is required (e.g., in mechanistic studies), machine estimation of k_{cryst} should be performed with robust process data and k_{cryst} should at least be corrected for temperature.

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1. Introduction

In recent years, mathematical process modelling of wastewater processes has become an increasingly active field, with models being successfully used for research, process design, training, control and optimization of physical, chemical and biological processes. However, to date the focus of model development has largely been on the biological reactions that occur during wastewater treatment (Henze et al., 2000; Batstone et al., 2002). Much less attention has been given to the many non-biological chemical reactions that occur in wastewater treatment, even though such reactions are essential to achieve effective treatment (Batstone et al., 2012). Process simulation models used across the industry currently have inherent limitations due to simplistic and situation-specific representations of important physico-chemical reactions (Batstone, 2009). A key neglected area is liquid–solid chemical precipitation modelling, due to its widespread occurrence in wastewater treatment processes (Doyle and Parsons, 2002; Chen et al., 2008; Batstone and Keller, 2003; van Langerak et al., 2000) and a general under-representation in existing standardised models (Batstone et al., 2012). Chemical precipitation is also particularly significant from a modelling perspective, because of strong interactions with other physico-chemical reactions in wastewater such as the weak acid–base system and ion complexation. A model containing chemical precipitation therefore automatically requires representation of other physico-chemical reactions, which is a key limitation of (for example) the ASM2d (Henze et al., 2000) which models precipitation without considering pH.

Several studies have used mathematical modelling to improve the understanding of chemical precipitation mechanisms in wastewater treatment (Barat et al., 2009; Maurer et al., 1999; Musvoto et al., 2000; Smith et al., 2008; Szabó et al., 2008; Tait et al., 2009; van Rensburg et al., 2003). Typically, unique modelling approaches have been applied to specific experimental datasets. Key differences between the various modelling approaches have included:

- (a) an assumption that precipitation reactions are occurring at sufficiently rapid rates to be effectively at equilibrium (Smith et al., 2008; Hanhoun et al., 2011; Loewenthal et al., 1995; Ohlinger et al., 1998; Scott et al., 1991; Wrigley et al., 1992) or instead treating them as kinetic reactions in the dynamic state equation set (Maurer et al., 1999; Musvoto et al., 2000; van Rensburg et al., 2003);

- (b) accounting for the effect of the available mineral surface area on the overall rate of precipitation (Smith et al., 2008; Tait et al., 2009) or not (Musvoto et al., 2000); and
- (c) assuming competitive or synergistic interactions are occurring between multiple chemical precipitation reactions occurring in parallel (Barat et al., 2011) or not (Musvoto et al., 2000).

In particular, more complex models that include multi-step precipitation with a broad range of controlling mechanisms tend to focus on specific applications, with generalised approaches being simplified to equilibrium and simple kinetics. To date, there has not been substantial experimental-based work focussed on systematically developing a general precipitation modelling approach. With increasing interest in correctly predicting precipitation such as struvite for phosphorus resource recovery (Rahaman et al., 2014; Galbraith et al., 2014), and with the rise in plant-wide model descriptions (Germaey et al., 2011) to develop new control strategies that consider nutrient recovery, a generally applicable and robust model approach is required for both detailed mechanistic descriptions and broader engineering analysis.

In this paper, a baseline precipitation model approach is developed in the context of calcite precipitation and further analysis then focuses on clarifying key environmental factors that influence precipitation modelling. The model approach is intended to form part of a larger Generalized Physicochemical Modelling Framework (Batstone et al., 2012) but is also intended for use across a wider range of wastewater applications. The paper is structured to first present the baseline precipitation model validated via dynamic pH titration tests, after which Constant Composition Method (CCM) experiments and robust statistics are used to examine the influence of environmental factors.

2. Materials and methods

Experiments investigated the precipitation of calcite (a crystalline form of calcium carbonate) from synthetic aqueous solutions. Two experimental platforms were used, namely, dynamic pH titration tests with precipitation, and the Constant Composition Method (CCM). Titration was used to identify the baseline model approach across a range of pH values and CCM tests investigated the influence of environmental factors on the baseline model approach. In continuous pH titration, the aqueous solution is titrated from a low pH to a

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