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# Dynamic Modelling and Identification of Precipitation Reactions in Full-Scale WWTP

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## Abstract

Current process models used across the wastewater industry have inherent limitations due to limited description of physicochemical processes such as precipitation. As part of the overall effort towards more general and robust physicochemical models applicable to the broad range of problems, this paper evaluates plant-wide modelling of precipitation reactions using a generic approach integrated within activated sludge and anaerobic models. Preliminary results of anaerobic digester sludge in batch system suggest that the model is able to simulate the dynamics of precipitation reactions. Kinetic rate coefficients, identified by mathematical optimization, were  $4.65(\pm 0.74)$  hrs<sup>-1</sup> and  $2.98(\pm 0.48)$  hrs<sup>-1</sup> for struvite and amorphous calcium phosphate (ACP), respectively. The joint parameter confidence regions found were highly nonlinear and asymmetric, indicating that the model was more tolerant to a fast kinetic coefficient. Nonlinearity of the confidence regions also indicates that nonlinear and iterative techniques for parameter identification are required in estimating real parameter uncertainty. Additional experimental results and model analysis in full-scale WWTP will be presented in the full paper.

## Keywords

Physico-chemical modelling, Precipitation kinetics, Parameter estimation

## 1. INTRODUCTION

There is a need to improve the standardized models of wastewater treatment processes (Henze et al. 2000, Batstone et al. 2002) and plant-wide simulation platforms such as Benchmark Simulation Model (BSM2) (Gernaey et al., 2014) with improved precipitation descriptions relevant to activate sludge and anaerobic digestion processes. The modelling of precipitation processes in plant-wide context presents the opportunity to model the physico-chemistry of major chemical compounds as they go through the different part of the wastewater treatment plant (Ge et al. 2013). The application of the physico-chemical model with standard biological models will result in an extended model able to predict with high accuracy the pH, the precipitation reactions and biological processes. An important first step has been the implementation of the physical chemical model without precipitation reactions within the ADM1 model (Solon et al. 2015). This study has demonstrated that the application of an improved physicochemical model and the use of proper corrections have paramount important when evaluating control / operational strategies at plant-wide level. To this end the modelling approach, systematically analysed and tested in a simple system (Kazadi Mbamba et al. 2015a) and validated in a multicomponent system (Kazadi Mbamba et al. 2015b), is applied at plant-wide through coupling the physical and chemical model framework (in particular precipitation) to ASM2d and ADM1, creating a model extension able to represent jointly the physical, chemical and biological processes at plant scale. A companion paper

(Flores-Alsina et al. 2015) introduces and describes in details the rational of plan-wide model integration with upgraded ADM1 and new interface between the models.

## 2. MATERIALS AND METHODS

### *Full scale system*

The full scale WWTP, located in South East Queensland, was designed for removal of organic matter (COD), nitrogen (N) and phosphorus (P) from domestic wastewater serving approximately 750000 EP. The plant consist of inlet work, 6 primary settling tanks, 6 parallel bioreactors (5-stage Barden-pho), 12 final settling tanks, 2 rotary sludge thickener, 4 dissolved Air floatation units, 6 primary digesters and 2 storage digester, 2 co-generation units, 3 dewatering units. The ASM2d standard was used for influent characterization (Henze et al. 2000).

### *Batch precipitation system*

In order to assess the potential for mineral precipitation of the full-scale facility, batch precipitation was carried out on the primary anaerobic digester sludge (ADS). The ADS was aerated to strip carbon dioxide (CO<sub>2</sub>) to raise the pH and induce precipitation.

### *Plant-wide model structure and parameter estimation*

The new plant-wide Benchmark Simulation Model with a bio-P process (BSM2-P), described in the companion paper (Flores-Alsina et al. 2015), was used after minor modification to fit the layout of the full scale system under study. Briefly the new model structure integrates a precipitation model (Kazadi Mbamba et al. 2015a), a modified version of ASM2d (Henze et al. 2000), an upgraded ADM1 and a new ASM2d/ADM1 interface (Nopens et al. 2009).

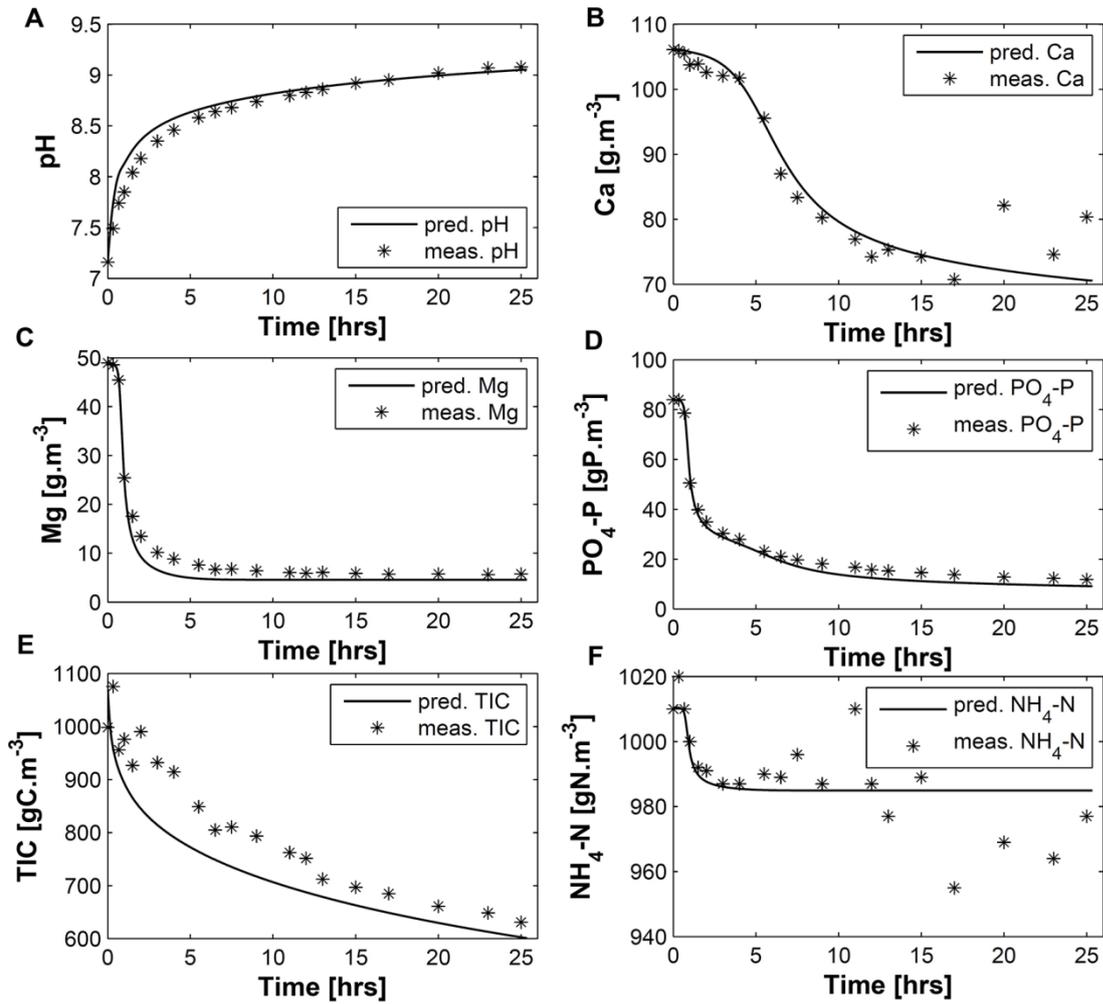
The parameter estimation evaluation with a 95 % confidence level applied used a non-linear local optimization, while the joint confidence region was determined using an iterative surface searching to the residual sum of squares (RSS), selected as the base objective function (Lobry et al. 1991).

## 3. RESULTS AND DISCUSSION

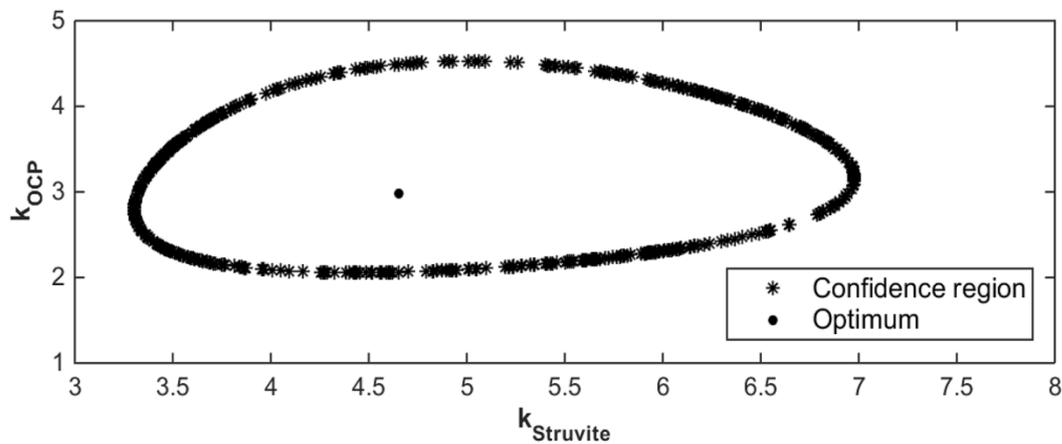
Fig. 1 presents simulation results together with the experimental data of the aeration experiment in ADS. In this experiment, as the pH increases due CO<sub>2</sub> stripping as a result of aeration, calcium, magnesium, phosphate and ammonia concentration decreased as a function of time. This could indicate that the ADS became supersaturated with respect to minerals such as struvite and ACP which might have precipitated from the anaerobic digester supernatant (ADS). An optimization analysis to determine the kinetic parameters and uncertainty was applied by simultaneously fitting the model to the experimental. The optimum estimated parameter values including CO<sub>2</sub> gas stripping rate at 95% confidence level describing struvite and ACP precipitation were 4.65(±0.74) hrs<sup>-1</sup> and 2.98(± 0.48) hrs<sup>-1</sup>, respectively All uncertainties in the linear uncorrelated confidence intervals for the parameters were estimated without initially considering any non-linearity of the objective functions.

Fig. 2 presents a summary of parameter confidence region. In general the structure of confidence regions in Fig. 4 shows strong asymmetry which suggests that the model is more tolerant to high values of kinetic coefficients as opposed to low values. To have the model reflect the fast process dynamics observed in the different experiment a quasi-equilibrium approach with high value of kinetic coefficient may be required. This is in close agreement

with other studies (Musvoto et al. 2000, van Rensburg et al. 2003, Ekama et al. 2006) that reported on dominance and fast process dynamics of mineral precipitation in a wastewater.



**Fig. 1 – Representative experimental and modelling data for aeration tests on wastewater AD sludge (ADS) with struvite and calcium carbonate (monohydrate). The dotted and solid lines represent the experimental and simulation results of the batch precipitation experiment.**



**Fig. 2 – Confidence region at the 95% confidence limit for kinetic parameters determined from model fits of data from Aeration of ADS.**

Although it is known that a great deal of minerals that can potentially precipitate in typical wastewater treatment (Batstone et al. 2012), preliminary study has shown that not all of these precipitating reactions take place at all wastewater conditions. The minerals to include in a model are not universal; they are site-specific and depend on the composition of the wastewater. Therefore, a wastewater treatment model needs to be selective in terms of minerals to include. A priori knowledge, mineral saturation, parameter estimation and confidence region of the parameters may play a key role in terms of selecting the relevant mineral in full scale WWTP. Furthermore, the formation of multiple minerals at full-scale can be modelled via a parallel competitive precipitation approach rather than a sequential approach, for reduced model complexity without loss in model performance. In full scale facility, continuous recycle of minerals will create an auto-nucleating environment, which means that the dependence of precipitation on existing seed material will become more important. It is expected that the implementation of the precipitation model at plant-wide will allow the identification of various minerals of interest in wastewater treatment works, will improve the plant-wide balance of phosphorus and will also foster the understanding of the influence of major ions and mineral precipitates on the biological systems. Such a work will be a first step in dynamic controls of precipitation reactions and optimization of nutrients recovery in wastewater treatment.

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