Title: A model-based approach for estimating PAO activity in aerobic granular sludge

Author(s): Giacomo Rizzardi*[1], Arianna Catenacci[1], Roberto Canziani[1], Andrea Turolla[1]

[1] Department of Civil and Environmental Engineering (DICA), Politecnico di Milano, Piazza Leonardo Da Vinci 32, 20133 Milano, IT, Italy (giacomo.rizzardi@polimi.it; arianna.catenacci@polimi.it; roberto.canziani@polimi.it; andrea.turolla@polimi.it)

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Abstract

Enhanced biological phosphorus removal (EBPR) systems offer a technological solution for high phosphorus (P) recovery with reduced resource consumption. These systems promote the selection of polyphosphate accumulating organisms (PAOs) by recirculating sludge through sequential anaerobic and aerobic conditions and thus favouring those organisms capable of exploiting feast-famine phases. Among EBPRs, aerobic granular sludge (AGS) systems are currently spreading worldwide. However, the use of mathematical models to optimize and control process performances remains underdeveloped due to both the complexity of process modelling and the difficulty to easily and accurately identify the kinetic parameters featuring the different microbial groups involved. With a specific focus on P fate, this study is aimed at the development of a model-based methodology to properly select operating test conditions for lab-scale batch activity assays targeted at accurately estimating PAOs kinetic parameters.

Introduction

Historical data on phosphorus (P) production and consumption, along with future trends, highlight the need for enhanced P recovery systems to meet the growing agricultural demand. Technologies for P removal from wastewater, aimed at limiting environmental damages resulting from nutrient spread, offer interesting opportunities for P recovery and recycling [1]. Currently, a great number of wastewater treatment plants still apply chemical precipitation using alum or lime for P removal. However, enhanced biological P removal (EBPR) systems emerged as enabling technological solution to achieve high P recovery with reduced resource consumption [2].

EBPR processes involve sludge recirculation through anaerobic and aerobic conditions to select for polyphosphate-accumulating organisms (PAOs). These microorganisms are essential in aerobic granular sludge (AGS) systems, an innovative biological treatment that is quickly spreading worldwide, based on microbial aggregation into dense and spherical structured biofilm [3]. In non-continuous AGS systems, the formation of granular sludge is promoted by specific environmental conditions and operational parameters, including cyclic feast-famine phases coupled with alternate anaerobic/aerobic conditions, favoring the growth of PAOs within the biofilm [2].

However, despite AGS systems spreading, involved processes are still scarcely interpreted by available mathematical models, particularly regarding P removal. Indeed, the fate of P in AGS systems may be affected not only by biological but also by physico-chemical (ion pairing and solid precipitation) removal mechanisms [4]. In addition, due to the complex model structure, accurate parameters estimation with datasets available from full-scale facilities is significantly challenging without falling into the risk of

overfitting (i.e., a model with more parameters than can be estimated from datasets).
In this study, data collected from a field pilot-scale plant were compared with predictions from an AGS model, which includes a one-dimensional (1D) description of granules and uses default kinetic parameters from the literature. Despite achieving a satisfactory fit for soluble COD, ammonium ($N\text{-}NH_4^+$), and nitrate ($N\text{-}NO_3^-$) concentrations, significant deviations from the measured P concentrations were detected. To address the challenge of properly describing P concentration in AGS systems, the objective of this study is to improve the predictive ability of models through the development of batch activity assays for the accurate estimation of PAOs kinetic parameters that can serve as a support tool for the robust application of modelling tools. In detail, following the development of an AGS modelling framework, a methodology based on sensitivity analysis was defined for the detection of the best operating test conditions to be applied to maximize parameters identifiability. The obtained outcomes can be used to set up batch activity tests at the lab-scale, whose estimated parameters can be later applied to calibrate the AGS system model of a pilot-scale plant facility.

Materials and methods

Pilot-scale

A Nereda® field pilot-scale plant (1.45 m^3 volume) was used as reference case study, being operated for six months by a water utility in the north of Italy in collaboration with Royal HaskoningDHV. The volume exchange ratio was 0.69 and the cycle time 4 hours, consisting of a simultaneous anaerobic feeding and effluent withdrawal period (1 h), a reaction period (2 + 0.5 h, aerobic with about 2 mg DO/L + anoxic with less than 0.5 mg DO/L), and a settling/sludge withdrawal/idle period (0.5 h). The reactor was equipped with five sampling ports over its height, spaced 1-m apart and samples at the end of the aerobic phase and during the anaerobic feeding phase were collected at different heights and characterized for soluble components, among which phosphate ($P\text{-}PO_4^{3-}$).

Modelling framework

A 1D granule model was developed based on [5] and [6]. The granule model was then implemented in a Sequency Batch Reactor model for the comparison of data collected at the pilot-scale facility with model predictions. Such model was then applied to simulate batch activity tests at the lab-scale and then subjected to a sensitivity analysis (relative-relative sensitivity index, equation 1), which was carried out on different parameters at varying operating test conditions, in order to identify the most suitable settings capable of maximising the magnitude of $rrSI$ and minimizing the correlations of parameters sensitivities.

$$rrSI = \frac{\partial y_i}{\partial \theta_j} \cdot \frac{\theta_{j,0}}{y_{i,0}} \quad \text{eq. 1}$$

where y_i is the *i-th* state variable ($y_{i,0}$ its nominal value) and θ_j is the *j-th* analyzed parameter ($\theta_{j,0}$ its nominal value).

Batch activity tests

Based on [7], preliminary batch activity tests were carried out using approximately 2-3 g VSS collected from the pilot reactor, and pretreated to completely remove from PAOs or saturate them with $P\text{-}PO_4^{3-}$ for aerobic and anaerobic tests, respectively. To assess P release under anaerobic condition, dissolved O_2 was removed by sparging N_2 gas into the nutrient solution. Subsequently, the bottle was sealed, and a concentrated solution of sodium acetate was injected into the bottle to have an initial concentration of 400 mg sCOD/L. Conversely, to evaluate the aerobic P uptake, a dissolved oxygen concentration of 2.5 mg O_2/L was maintained with intermittent aeration. At the test onset, a concentrated solution of K_2HPO_4

and KH_2PO_4 was injected to achieve an initial concentration of 8 mg $P\text{-}PO_4^{3-}$/L. Both tests lasted 150 minutes and liquid samples were regularly collected every 30 minutes to measure the P and soluble COD concentrations. The results from the sensitivity analysis may prompt modifications to the test settings and procedures of future experiments, with the aim of enhancing the identifiability of kinetic parameters.

Results and discussion

The distribution of microbial groups within the granules was determined by fitting model predictions at steady state with the measured effluent concentrations outlined in Table 1. Predicted microbial group distributions and concentrations of soluble components are shown in Figure 1, where S_{PO4} is predicted with concentrations of about 70 mg $P\text{-}PO_4^{3-}$/L at the external layer in contact with the bulk volume.

Table 1. Influent and effluent concentrations provided as average values with, in brackets, the standard deviation.

Parameter	Unit	Case study B
TSS concentration in the reactor	g TSS·L^{-1}	7.0 (±0.7) (81% VSS/TSS)
Influent / Effluent bCOD	mg COD·L^{-1}	300 (± 28) / 26 (± 2.9)
Influent / Effluent $P\text{-}PO_4^{3-}$	mg P·L^{-1}	2.3 (± 0.75) / 0.84 (± 2.7)
Influent / Effluent $N\text{-}NH_4^+$	mg N·L^{-1}	31 (± 11) / 0.68 (± 0.47)
Influent / Effluent $N\text{-}NO_3^-$	mg N·L^{-1}	0.32 (± 0.03) / 2.66 (± 2.5)

The concentrations of soluble compounds at the end of simulated aerobic phase are comparable those measured at the pilot-scale plant. In contrast, the concentrations measured at all heights at the end of the feeding phase (Fig. 2c) were poorly predicted by the model, which failed to accurately reproduce P release and COD uptake.

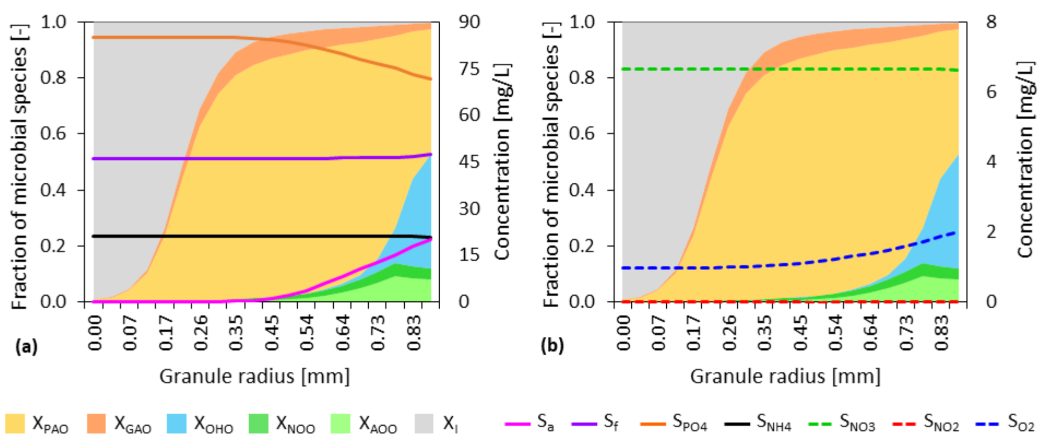

Figure 1. Relative distribution of active microbial groups at steady state as a function of distance from the granule centre. Overlaid lines represent concentrations of soluble components, predicted at the end of the anaerobic (a), and aerobic (b) phases.

In view of this, the AGS model requires further calibration and refinements specific to P dynamics. This could involve adjusting kinetic parameters related to phosphorus or incorporating additional processes or mechanisms that influence phosphorus behaviour in the system. To address the first aspect, highly informative batch activity tests can be carried out by selecting proper substrates and biomass concentrations. Regarding the second, the deviations in P concentrations might suggest that certain biological or chemical processes affecting phosphorus were not fully captured in the model [4].

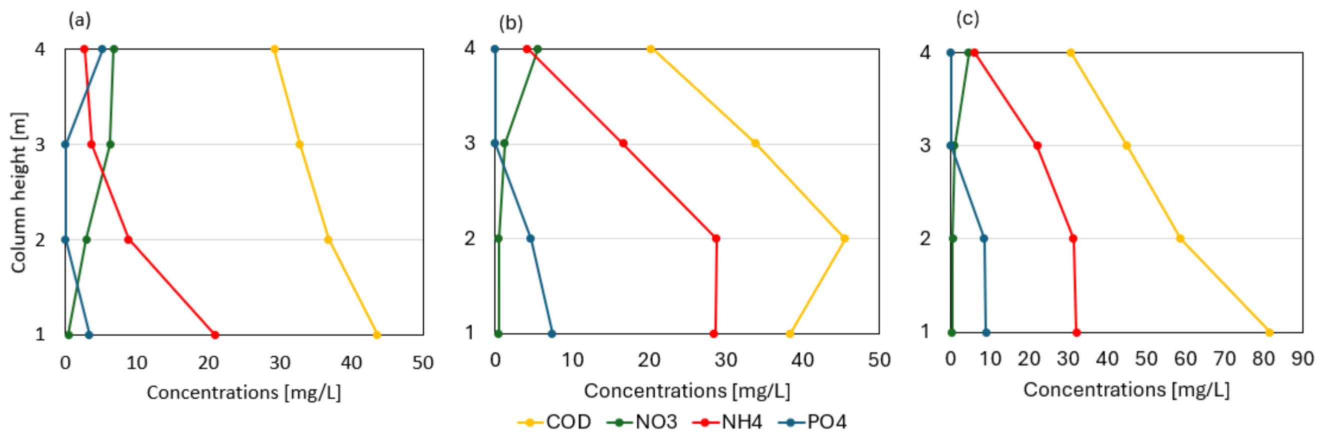

Figure 2. Concentration gradients of CODs, N-NO_3^-, N-NH_4^+ and P-PO_4^- along the column's height during the feed phase after (a) 20 minutes, (b) 40 minutes, and (c) 60 minutes.

To improve the robustness and predictive ability of the AGS model regarding phosphorus fate, thereby offering a reliable tool for understanding phosphorus removal in AGS systems and optimizing the process, this work will proceed with the following actions:

- integrating the 1D granule model with a batch reactor model to simulate batch activity tests;
- providing guidance on setting up batch activity tests to estimate PAO kinetic parameters through modelling and sensitivity analysis of batch lab-scale tests.

If the model cannot fully describe the treatment process and phosphorus mass balances, the objective will be to integrate additional processes and conditions, including:

- incorporating vertical concentration gradients during the anaerobic phase (plug flow reactor);
- distinguishing between floc and granule biomass aggregates;
- accounting for precipitation and ion pairing phenomena, following the approach outlined by Batstone and Flores-Alsina [8].

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