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Modelling green microalgal growth, nutrient uptake and storage in the ASM framework

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Summary of key findings

Recent research focuses on the development of cost-effective ways to recover nutrients, energy and fresh water from wastewater. Microalgal photobioreactors (PBRs) coupled with wastewater treatment processes offer an opportunity for efficient resource recovery. Several models with different complexities have been developed to simulate microalgal growth. However, none of these models can effectively describe all the relevant processes when microalgal growth is coupled to nutrient removal and recovery from wastewaters. We present a novel consensus model (ASM-A) developed in the activated sludge modelling (ASM) framework to predict photoautotrophic growth, nutrient uptake and storage, as well as heterotrophic microalgal growth, and decay of mixed green microalgae. A two-step model evaluation was carried out using independent data obtained in a 24-L sequenced batch PBR. Three hypothesis were answered comprising (I) Does culture history or substrate availability influence parameter values estimated to a significant extent?; (II) What are the practical consequences for model calibration, i.e., Can we use a mean parameter set?; (III) Can we explain discrepancy as a result of parameter variability?

Background and relevance

Due to an increasing global population, climate change and industrialization, we will be facing new global challenges, such as severe water scarcity, or the depletion of phosphorus rock, in the near future (4). While conventional wastewater treatment processes solely focus on the elimination of contaminants and nutrients, such as nitrogen and phosphorous, the cultivation of microalgae on wastewater resources offers a potential to recover nutrients present in wastewater (2). Recent research proposes systems to integrate microalgal cultivation as part of the wastewater treatment process. Design, operation and control of systems combining bacteria-based wastewater treatment processes with microalgal cultivation require mathematically consistent and reliable process models. The main objectives of this work are (i) to identify suitable biokinetic model for photoautotrophic and heterotrophic microalgal growth in the activated sludge modelling framework (ASM-A); (ii) to assess microalgal uptake and storage of nutrients; (iii) to assess kinetic parameter variability and sources of uncertainty.

The PBR was modelled using the consensus model for algal growth on wastewater ASM-A ((5), Table 1) and implemented in Matlab-Simulink (The MathWorks, Natick, MA). The units are expressed in chemical oxygen demand (COD), g-N and g-P. To make the integration of the algal model into the existing model structures straightforward, the activated sludge modelling (ASM, (1)) nomenclature was followed.

Sequential batch experiments were set up in 24-L airlift PBRs. In the first four cycles (descending cycles), the initial ammonia and nitrate concentration decreased in sequential cycles from 10 to 5 to 2.5 to 0.5 mg-N/L. In the following four cycles (ascending cycles), the initial ammonia and nitrate concentration increased from 0.5 to 2.5 to 5 to 10 mg-N/L. The experimental design used with different initial substrate to biomass ratio in each cycle allows decoupling the culture history from the substrate availability impact. Through the two-step model evaluation, in the first evaluation step, parameter sets obtained through each descending cycle were confronted with data obtained in the

corresponding (same initial substrate concentrations) ascending cycle. To evaluate the model accuracy, we used the Janus coefficient. In the second evaluation step, Monte Carlo simulations (3) were performed to infer confidence interval of model predictions using probability ranges assessed based on the descending cycles.

Results

ASM-A considers the microalgal uptake and storage of both ammonia (R1) and nitrate (R2) nitrogen (Table 1). The uptake and storage of nitrogen is dependent on the availability of external nitrogen (S_{NH4} or S_{NO}), as well as the internal cell quota of nitrogen ($X_{Alg,N}$). Typically, ammonia is preferred over nitrate for most algal species; hence an inhibition term for nitrate uptake is included when ammonia is available (R2, Table 1). The uptake and storage of phosphorus (R3, Table 1) is dependent on the availability of external soluble orto-phosphate in wastewater (S_{PO4}), and on the internal cell quota of phosphorus ($X_{Alg,PP}$). Nutrient limitations are described by the Droop model with growth dependent on the internal cell quota of the nitrogen and phosphorus. The consumption of inorganic carbon (S_{Alk}) is modelled using Monod kinetics. We assume that the microalgae are exposed to a constant average light intensity and the light dependence is modelled using the Steele equation (R4). Heterotrophic microalgal growth is modelled with the Monod kinetics (R5). Oxygen serves as a terminal electron acceptor for heterotrophic growth (S_{O2}), and its effect follows the Monod kinetics. Inhibition of the heterotrophic growth by light is modelled using the competitive inhibition term. The algal decay process includes all sources of biomass loss that will reduce the amount of active biomass in the culture (R6).

The first evaluation step indicates that, for those parameters influencing algal biomass, ammonia and phosphate concentrations as well as the phosphorus storage, the source of parameter variability is related to substrate availability and not to culture history (data shown in Wágner et al., (5)). In the second evaluation step, results obtained show that most of experimental values are in the proximity of the simulation results obtained using the mean values of parameters estimated using data from the first four cycles (descending). Therefore, practitioners can calibrate ASM-A using the mean parameter set as default to simulate mixed cultures with Chlorella and Scenedesmus as dominating species. The discrepancy between measured and simulated data can be explained by parameter variability (i.e. data falls within the confidence interval, Fig. 1 a, b, d, f).

Table 1. Process rate equations of the ASM-A microalgal model.

Process rates	
R1 [g N m^{-3} d^{-1}]	$k_{NH4} \cdot \frac{S_{NH4}}{S_{NH4} + K_{NH4,Alg}} \cdot \frac{X_{Alg,Nmax} \cdot X_{Alg} - X_{Alg,N}}{X_{Alg,Nmax} \cdot X_{Alg}} \cdot X_{Alg}$
R2 [g N m^{-3} d^{-1}]	$k_{NO} \cdot \frac{S_{NO}}{S_{NO} + K_{NO,Alg}} \cdot \frac{K_{NH4,Alg}}{K_{NH4,Alg} + S_{NH4}} \cdot \frac{X_{Alg,Nmax} X_{Alg} - X_{Alg,N}}{X_{Alg,Nmax} X_{Alg}} \cdot X_{Alg}$
R3 [g P m^{-3} d^{-1}]	$k_{PO4} \cdot \frac{S_{PO4}}{S_{PO4} + K_{PO4,Alg}} \cdot \frac{X_{Alg,PPmax} \cdot X_{Alg} - X_{Alg,PP}}{X_{Alg,PPmax} \cdot X_{Alg}} \cdot X_{Alg}$
R4 [g COD m^{-3} d^{-1}]	$\mu_{A,max} \cdot (1 - \frac{X_{Alg,Nmin} X_{Alg}}{X_{Alg,N}}) \cdot (1 - \frac{X_{Alg,PPmin} X_{Alg}}{X_{Alg,PP}}) \cdot \frac{S_{Alk}}{S_{Alk} + K_{Alk}} \cdot \frac{I_{Av}}{I_S} \cdot e^{1 - \frac{I_{Av}}{I_S}} \cdot X_{Alg}$
R5 [g COD m^{-3} d^{-1}]	$\mu_{H,max} \cdot (1 - \frac{X_{Alg,Nmin} X_{Alg}}{X_{Alg,N}}) \cdot (1 - \frac{X_{Alg,PPmin} X_{Alg}}{X_{Alg,PP}}) \cdot \frac{S_A}{S_A + K_A} \cdot \frac{S_{O2}}{S_{O2} + K_{O2}} \cdot \frac{K_I}{K_I + I_{Av}} \cdot X_{Alg}$
R6 [g COD m^{-3} d^{-1}]	$b_{Xalg} \cdot X_{Alg}$

This is not the case for predicting the internal nitrogen storage, i.e. data falls outside the confidence interval (Fig. 1e), and substrate availability is found to have an effect on parameter estimates. Hence, nitrogen storage measured through the ascending cycles can only be predicted by using parameter values estimated in the corresponding descending cycles (data shown in Wágner et al., (5)). The discrepancy between predicted and measured bulk nitrate concentration cannot be explained through parameter variability (i.e. most data falls outside the predictive confidence interval, Fig. 1c). Moreover, the bulk nitrate concentration prediction fails the first evaluation step (Janus >>1), suggesting that values of the parameters affecting this model output depend on the history of the culture.

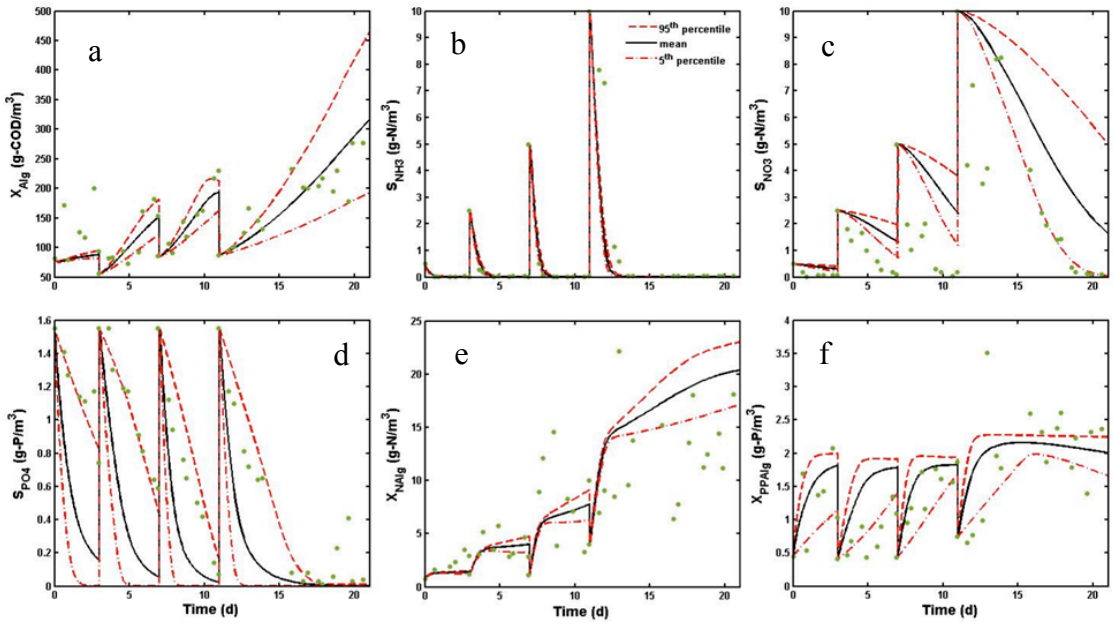

Figure 1 Evaluation of the ASM-A model identified in this study using a mean parameter set derived from experimental data and literature. Predictions for algal biomass growth (a), internal nitrogen (e) and phosphorus (f) quota and effluent ammonia (b), nitrate (c) and phosphate (d) concentration is shown.

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