



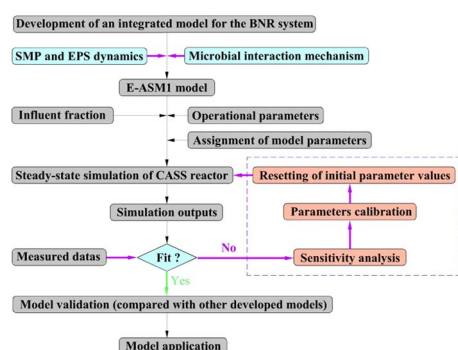
Modeling and simulation of a biological process for treating different COD:N ratio wastewater using an extended ASM1 model



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GRAPHICAL ABSTRACT



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ABSTRACT

The aim of this study was to establish a mathematical model for simulating a biological nutrient removal (BNR) process for treating wastewater with different COD:N ratios. Through phylogenetic analysis, the microbial communities in a cyclic activated sludge system (CASS) reactor under different COD:N ratios were quantitatively characterised, while the necessity of incorporating the microbial interaction mechanism in the extended ASM1 (E-ASM1) was validated. Since the newly introduced parameters affected the original kinetics in the activated sludge model No. 1 (ASM1), the poorly defined parameters were altered based on the batch experimental data taken from a lab-scale CASS and the results of a root-mean-square sensitivity analysis. The simulation results indicated that effluent COD and biopolymer concentrations decreased with an increase in influent COD:N ratio, while the trend was opposite for nitrification. Compared to the ASM1-SMP-EPS model, the extended ASM1 (E-ASM1) proved to be a preferable reference for the simulations of the CASS performance in substrate degradation and biopolymers formation mechanism, strongly suggesting that the interactive relationship among different bacteria and the biopolymer dynamics should be simultaneously included in this model.

1. Introduction

Owing to the increasing focus on environmental issues, as well as more stringent regulations governing the discharge of organic matter and nitrogen in contaminated wastewater, the utilisation of biological

nutrient removal (BNR) process for wastewater treatment is becoming more widespread. However, the major issues with biological technology are low operational efficiency and high consumption of time and energy, which hinder its further application in wastewater treatment plants (WWTPs). A deeper understanding of the BNR process can

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enhance the treatability, while reducing the operational cost. Model simulation is an ideal method to achieve this objective, having gained significant popularity in the past decades [1]. Activated sludge models No. 1–3 (ASMs), which were established by the International Water Association Task Group and can account for the nutrient metabolism mechanism in the BNR process, were proven to be valuable tools for process engineers to optimise WWTP operation while reducing the expenditure incurred [2]. Among the ASM-family models, the ASM1 model is the primary created model [3], and has been widely applied in scientific activities for predicting municipal WWTP behaviour [4]. This model assumes that the biodegradable substrate is initially hydrolysed by biomass with extracellular enzymes before being assimilated for growth. In particular, due to the introduction of the death-regeneration concept, the ASM1 model can analyse the nutrient removal mechanism quantitatively, often being adapted as a fundamental model for further development, aimed at describing the new experimental phenomena more reasonably.

One weakness of the ASM1 model is that it assumes that the inert soluble substance (S_I) is a key component of the effluent, and that its concentration does not depend on the influent chemical oxygen demand (COD), leading to poor predictions of effluent COD concentrations at low influent COD/N ratios [5]. In recent years, many researchers have recognized the crucial importance of biopolymers including soluble microbial products (SMP) and extracellular polymeric substances (EPS) in the BNR system because of the following three reasons: firstly, the biopolymers are characterised by a complex organic compound, while being considered to be a major component of effluent COD [6]. Secondly, there is a strong relationship between the biopolymers and microbial activities, i.e., SMP originates from substrate utilisation and biomass decay, while the term EPS refers to extracellular stored polymer, which is closely associated with the flocs in activated sludge. Thirdly, the presence of biopolymers not only sets the lower limit for effluent quality [7], but also accelerates membrane fouling, influencing some properties of sludge, including dewaterability, settleability, and compressibility [8]. Therefore, it is of considerable interest to develop kinetic models that are essentially a coupling of the ASM1 and the biopolymer formation process in order to advance its predictability of the BNR behaviour and the description of the influence of the biopolymers on this system. To date, several attempts have been made to establish a series of ASM-based models capable of modelling the biopolymer formation mechanism. These are briefly described below.

Lu et al. built an SMP model that was based on the ASM1 model and was used to simulate a membrane bioreactor (MBR) at high sludge concentrations [9]. This model assumed that the biomass-associated SMP production in the MBR system were generated only from cell lysis. In fact, both the biomass growth and EPS hydrolysis processes contributed to the SMP production. Lee et al. developed a modified model for a submerged membrane bioreactor (SMBR) by combining ASM1 with four process equations related to SMP degradation and production [10]. Results demonstrated that both the F/M ratio and SRT had a significant effect on the fate of SMP in the reactor. Nevertheless, the prediction accuracy of this model's state variables was reduced because its parameter values were directly derived from other literature, suffering from the absence of an appropriate calibration procedure. Ahn et al. integrated the SMP and EPS concepts with the ASM1 model, which was applied to describe the dynamic variation of the two biopolymers under three sludge retention times (SRT) [11]. However, their model was focussed on interpreting biopolymer dynamics, while neglecting the description of some relevant biological processes, such as carbon oxidation and nitrification. To account for the accumulation of SMP during the transient condition, which was not based on any ASM model, Aquino et al. further developed an anaerobic chemostats model based on the SMP kinetic model of Barker and Stuckey [8], that incorporated the unified theory of production and degradation of EPS as described by Laspidou and Rittmann [12], whereas their model was not

established based on any ASMs model [13]. Di Bella et al. created a modified ASM1 which considered the influence of SMP in a submerged MBR, further linking them with membrane fouling equations [14]. Their model suffered from an overestimation of the effluent nitrate (NO_3) concentration by ignoring the presence of the anoxic zone. The above-mentioned short review indicates that several researchers have attempted to obtain a better understanding of the BNR system, as well as the biopolymer concentrations, with several meaningful achievements in the process. However, upon studying their work closely, some flaws have been found in the published ASM-based models. For instance, (i) a lack of the relationship between substrate metabolism and biopolymer formation processes; (ii) a lack of interaction mechanisms among aerobic heterotrophs and autotrophs; and (iii) the absence of appropriate parameter calibration.

In another way, increasingly more scientists have found that influent COD to nitrogen (COD:N) ratio is a crucial factor affecting the biological process, resulting in one kind of functional bacteria obtaining a competitive advantage and dominating the living environment, while the activity of another functional bacteria was inhibited [15–17]. As is well-known, two major groups of bacteria (i.e. heterotrophs and autotrophs) exist in the activated sludge system under aerobic conditions, with different proliferation rates and metabolic functions. Moreover, due to the higher oxygen affinity, the heterotrophs obtain oxygen more easily than the autotrophs under the conditions of high COD and limited DO. As a result, the former bacteria, which possess a high growth rate, cell yield, and oxygen affinity, have a competitive advantage over the latter, as illustrated in Table 1 [17], and cause a higher rate of carbon metabolism than nitrogen metabolism. Most of the previous revised ASM1 models assumed that the carbon oxidation process, associated with heterotrophic activity, was unrelated to the nitrification induced by autotrophs, thus failing to appropriately predict the effluent quality. Therefore, there is an urgent need for a complete ASM1 model, advanced by considering the interaction mechanism among the two bacterial groups for a better description of the BNR performance. In addition, although there is an abundance of previously reported works [9,10,18,19] involving SMP and/or EPS concepts in the ASM matrix that focus on influential factors like DO, SRT, HRT, and temperature, information on microbial communities in BNR systems at different influent COD:N ratios is limited. Moreover, the effects of different COD:N ratios on both nutrient utilisation and biopolymer dynamics have not yet been discussed, as they continue to be absent from the ASM1-based models. It is therefore of considerable interest to improve the ASM1 model by coupling it with the biopolymer kinetics in order to obtain a comprehensive understanding of the influence of different influent COD:N ratios in a BNR system.

The objective of this study was to obtain a deeper understanding of the BNR system at different influent COD:N ratios with a mechanistic model, namely Extended Activated Sludge Model No. 1 (E-ASM1), which was improved by taking the bio-polymers (i.e. SMP and EPS) kinetic modelling into account in the ASM1 model, and including the interactive relationship between heterotrophic and autotrophic biomass. A 16S rRNA gene sequencing analysis was subsequently conducted to investigate the variation in the microbial community of the BNR system at different influent COD:N ratios. For model evaluation, this model was employed to predict the effluent and biopolymer concentrations in a lab-scale CASS reactor under different influent COD:N

Table 1
The comparison of the proliferation rate between heterotroph and autotroph [17].

Bacteria	Maximum growth rate (h^{-1})	Cell yield	Generation time (h)
Aerobic heterotroph	0.3–0.5	0.5–0.7	2.31–8.69
Nitrosomonas	0.04–0.08	0.02–0.06	8–36
Nitrobacteria	0.04–0.13	0.02–0.07	12–15

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