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Estimation of kinetic parameters of an anaerobic digestion model using particle swarm optimization

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ABSTRACT

Calibrating parameters of an anaerobic digestion model is often difficult and time consuming. In order to reduce the complexity of tuning a complex anaerobic digestion model, a particle swarm optimization-based smart algorithm was developed to estimate all parameters of an anaerobic digestion model. A glucose anaerobic digestion model was refined and applied to test the feasibility of the smart algorithm. A reactor was continuously fed with glucose until a steady state was achieved. The steady state and a transient state of the reactor were simultaneously included in the smart algorithm. Results shows that the algorithm acceptably estimated activated sludge concentrations and 14 sensitive parameters, though the glucose anaerobic digestion model was complex. The values of most estimated parameters were close to those reported data, while the values of four sensitive parameters deviated a little from reported data. By applying the estimated parameters, the glucose anaerobic digestion mode matched experimental data well. This verifies the applicability of the algorithm as well as the validity of the model structure.

1. Introduction

Activated sludge models ASMs have been widely applied in biological wastewater treatment, but the model parameters need calibration. Model calibration is necessary because the characteristics of influent and other factors such as temperature affect the model parameters [1–3]. In addition, since a parameter value covers a wide range, choosing different values for a parameter may result in significantly different predictions [4]. Moreover, calibration has become necessary because the complexity of the models has increased considerably with the discovery of new processes [5–7].

A number of protocols and guidelines have been established for calibrating ASMs [8–10]. These protocols and guidelines require data collection, manual parameter estimation, and model validation [4]. Nevertheless, manual parameter calibration is laborious, may result in erroneous estimations, and may not even be possible for poorly identifiable parameters [1].

Alternatively, mathematical approaches have been applied to estimate the values of ASMs [4,11–13]. Among these mathematical approaches, the genetic algorithm, as a kind of smart algorithm, could efficiently estimate the model parameters [1,14–16].

Compared to the genetic algorithm, the particle swarm optimizer (PSO) is a different smart algorithm that resembles a school of flying particles, and could be applied to estimate ASMs. In a PSO, each particle consists of parameters that need to be estimated. Parameter values determine the particle's position that evolves by cooperation and competition among the particles through generations, according to its own flying experience and its companions' flying experience [17]. A range of values could be selected for each parameter in an anaerobic digestion model [18], but it is difficult to determine a value for each parameter without performing necessary experiments. Furthermore, since default values for most parameters in aerobic sludge models can be applied directly [2,19], calibrating an anaerobic model is more challenging. A PSO has been applied to estimate a few anaerobic hydrolysis processes [20]. Nevertheless, apart from hydrolysis processes, an anaerobic sludge digestion model consists of many other different bioprocesses such as acidogenesis and methanogen processes.

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To the best of our knowledge, estimation of the kinetic parameters of a full anaerobic sludge model by PSO has not yet been reported.

An anaerobic digestion model usually includes a few sensitive parameters and some of them correlate with each other, which makes manual and experiment-based model calibration difficult and time consuming. In order to reduce the complexity of tuning a complex anaerobic digestion model, a particle swarm optimization-based smart algorithm was developed to efficiently estimate all parameters of an anaerobic digestion model. If successful, the smart algorithm could be applied to estimate parameters of other activated sludge models.

2. Methods and materials

2.1. Experiments

A glucose solution was pumped into a complete stirred continuous reactor that was operated under a steady state condition (refer to CSTR experiment). The concentration of the glucose solution was 10 g/L. When the steady state was achieved, additional glucose was once pulse added into the reactor so that the effluent glucose concentration immediately increased to 4 g/L (refer to PULSE experiment). The reactor was then allowed to return to its previous steady state. In the two experiments, the glucose solution (10 g/L) was always supplied. Aquino and Stuckey [22] conducted experiments and developed a model to simulate the response of the reactor in the PULSE experiment (refer to original model). The experimental data were adopted from Aquino and Stuckey [22] work.

2.2. Refined glucose digestion model

A few lumped parameters are applied in the original model, which reduced the complexity of the model but increased the difficulty in the model calibration. For instance, the decay coefficients of acidogenic bacteria and methanogenic archaea, which are different, were the same in the model. In this study, the lumped parameters were refined, which resulted in a refined model that is shown in Fig. 1. Comparing with the original model, other improvements were made in the refined model and are summarized below.

a) In the original model, active biomass and bound extracellular polymeric substances (bEPS) were modelled separately. Nevertheless, in the refined model, nominal bacteria and archaea (X_a, X_m), which consisted of active biomass (M1, M2) and bEPS, were modelled.
b) In the refined model, nominal bacteria and archaea rather than active biomass produced bacterial associated products and bEPS. Furthermore, bEPS were converted to BAP. Because nominal bacterial and archaea consisted of active biomass and bEPS, transferring materials from active biomass to bEPS, which produced bEPS, did not have an impact on the concentrations of nominal bacterial and archaea.

Table 1 summarizes bioprocesses shown in Fig. 1. Corresponding differential equations can be found in supplementary material. Table 2 summarizes the parameters applied in the original model and the refined model. Table 3 compares the lumped parameters in the original model and the corresponding refined parameters in the refined model.

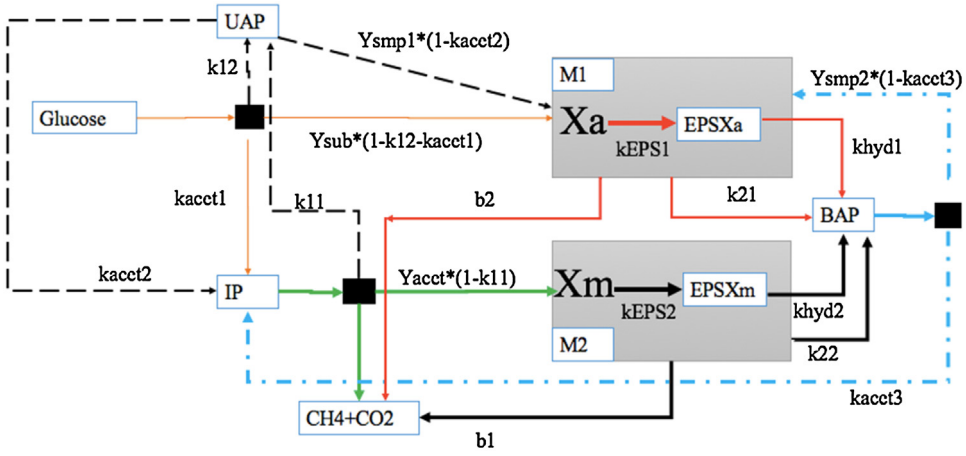

Fig. 1. Structure of the refined model. Adopted from [21] and parameters were refined. M_1: active hydrolysis bacteria; M_2: active methanogenic archaea; X_a: nominal hydrolysis bacteria; X_m: nominal methanogenic archaea; UAP: utilization associated products; BAP: bacterial associated products; IP: intermediates products; EPSXa: bound extracellular products on Xa; $EPSX_m$: bound extracellular products on X_m; r_{utuap}: utilization rate of UAP; r_{utsub}: utilization rate of glucose; r_{utacet}: utilization rate of acetate; $r_{utbap:}$ utilization rate of BAP.

Table 1
Bioprocesses in anaerobic glucose degradation.

Process	S	IP	UAP	BAP	X_a	X_m	$EPSX_a$	$EPSX_m$	rate
Glucose degradation	-1	k_{acet1}	k_{12}		$Y_{sub}(1-k_{12}-k_{acet1})$				X_a qs S/(K_s + S)
IP degradation		-1	k_{11}			$Y_{acet}(1-k_{11})$			X_m q_{IP} IP/(K_{IP} + IP)
UAP degradation		k_{acet2}	-1		$Y_{smp1}(1-k_{acet2})$				X_a q_{uap}UAP/(K_{uap} + UAP)
BAP degradation		k_{acet3}		-1	$Y_{smp2}(1-k_{acet3})$				X_a q_{bap} BAP/(K_{bap} + BAP)
BAP formation				$k_{21}X_a + k_{hyd1}X_a + k_{22}X_m + k_{hyd2}X_m$	$-k_{21}X_a - k_{hyd1}X_a$	$-k_{22}X_m - k_{hyd2}X_m$	$-k_{hyd1}X_a$	$-k_{hyd2}X_m$	1
X_m decay						$-b_1X_m$			1
X_a decay					$-b_2X_a$				1
$EPSX_a$ formation							$k_{EPS1}X_a$		1
$EPSX_m$ formation								$k_{EPS2}X_m$	1