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Comparison of optimization algorithms for modeling of Haldane-type growth kinetics during phenol and benzene degradation

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ABSTRACT

In this study, three optimization algorithms (discretized domain, Monte Carlo, steepest descent) were compared to determine the best algorithm for estimation of Haldane-type microbial growth kinetic parameters. Application of these algorithms to growth data measured during phenol and benzene degradation showed different results in the estimated parameters obtained under various boundary conditions and growth phases. Regardless of the specific algorithm used, the factor with the greatest influence on parameter estimation was the boundary condition for the half-saturation constant (K_S), although the parameters were also sensitive to the growth phase for phenol. Among the three algorithms, Monte Carlo was found to be the best and most consistent. The estimated parameters of phenol and benzene using an appropriate boundary value of K_S were comparable with the outputs reported in previous studies, but those derived with inappropriate boundary values were not consistent with previously reported data.

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1. Introduction

Phenol is one of the main toxic organic contaminants frequently detected in industrial effluents. When phenolic wastewater is discharged without treatment, the underground aquifer and ecosystem can be seriously damaged owing to the high solubility and toxicity of phenol. Therefore, numerous studies have been conducted to develop methods for the effective removal of phenol from wastewater, using the adsorption capacity of activated carbon [1], photo-catalysts such as TiO_2 and ZnO [2], and metabolism of phenol by microorganisms [3,4]. Recently, attention in this field has focused on biological treatments, which have advantages with respect to their cost-effectiveness and eco-friendly nature.

The relationship between microbial growth and phenol concentration has been considered to be a key factor in determining the efficiency of treating phenol existing at various concentrations in wastewater. In general, the specific growth rate of a microorganism, μ (1/h), shows a nonlinear relationship with substrate concentration, S (mg/L). Depending on the concentration range used, this nonlinear relationship can be estimated using either noninhibitory or inhibitory kinetic models. The Monod (1) and Haldane (2) models, which are well-known kinetics models used to express the noninhibitory and inhibitory behavior of microorganisms, respectively, can be defined as follows:

$$\mu = \mu_{\max} \frac{S}{K_s + S} \quad (1)$$

$$\mu = \mu_{\max} \frac{S}{K_S + S + S^2/K_I} \quad (2)$$

where $\mu_{\max}$ is the maximum growth rate (1/h), K_S is the half-saturation constant (mg/L), and K_I is the inhibitory constant (mg/L). When the Haldane model is used to estimate kinetic parameters, the change of any one parameter can lead to a simultaneous change of the other two parameters, implying that multiple sets that satisfy the optimization problem can exist for a given experimental dataset.

One way to resolve this dependency problem of estimated parameters would be to use a discretization method by which the parameter domain is discretized so that the effect of the boundary values and intervals on model outputs can be systematically

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Table 1
Boundary values and intervals of kinetic parameters used for algorithm optimization.

Constraints			Kinetic parameter					
			μ_{max} (1/h)		K_S (mg/L)		K_I (mg/L)	
Boundary[a]			$a_{1(min)}$	$b_{1(max)}$	$a_{2(min)}$	$b_{2(max)}$	$a_{3(min)}$	$b_{3(max)}$
	Type A	(Phenol)	0	1	0	800	0	800
		(Benzene)	0	1	0	400	0	400
	Type B	(Phenol)	0	1	0	50	0	800
		(Benzene)	0	1	0	15	0	400
Interval[b]	Type A		0.01		10		10	
	Type B		0.01		1		10	
Initial value[c]	(Given)	Optimized parameter set obtained from DD						
	(Random)	Randomly selected values from Eq. (8)						

[a] Boundary values used in DD, MC, SD.
[b] Intervals used in DD.
[c] Initial values used in SD.

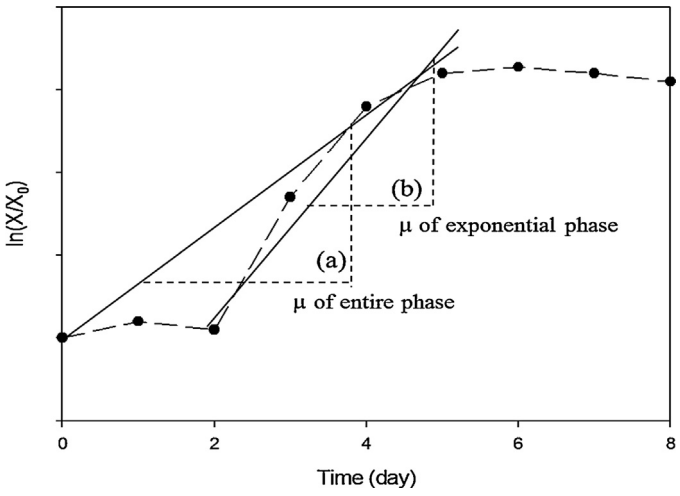

Fig. 1. Effect of growth phase on the determination of specific growth rate (μ).

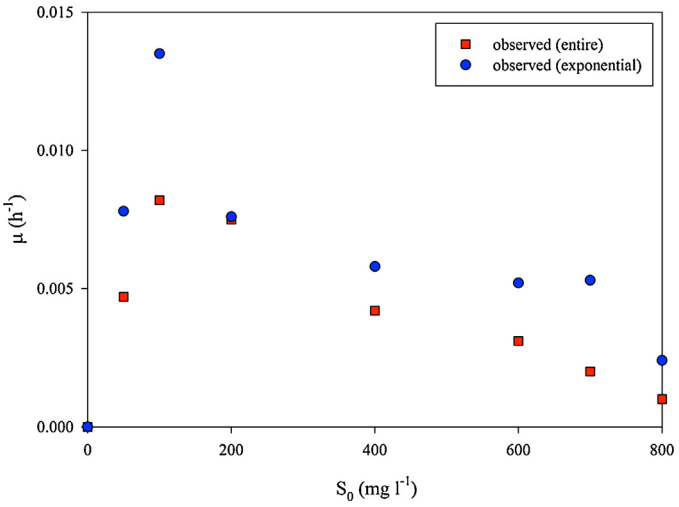

Fig. 2. Comparison of the observed growth rates determined from the entire and exponential growth phases.

explored. For example, the discretized domain (DD) technique was applied to a simulation of a variable and fluctuating traffic signal system [5]. This method was also applied to an unsaturated groundwater flow problem by discretization of variable vertical grid spacing [6]. These exemplary studies indicate that discretization is a useful technique for transferring a continuous parameter domain into discrete points to make it suitable for numerical evaluation. However, the discretization method becomes inefficient when the spacing of grid points is wide or if a solution point exists between grid points. To overcome this problem, the steepest descent (SD) method can be used. SD is a mathematical algorithm in which a sequence series is generated to push the gradient towards the direction that minimizes the value of the error function. Since the determination of the gradient is taken from the mathematical calculation of an earlier step, the entire problem domain has an equal possibility to be tested. The use of the SD technique was reported in a study of the cell growth kinetics during substrate interactions between phenol and *m*-cresol [7].

In addition to these two methods, the Monte Carlo (MC) algorithm is another alternative for simple optimization when a kinetic model is complex, nonlinear, or includes more than two parameters. This method evaluates the error function using a uniform distribution of probability for a given random number by simplifying the mathematical procedure. This simplicity of the MC method was demonstrated in a study of the geophysical inversion problem as a control-searching method to test the effectiveness of complicated algorithms [8].

To date, numerous studies on the estimation of Haldane-type growth kinetic parameters for phenol degradation have been conducted. However, with the exception of only two studies – Alexievaa et al. [17] and Kumar et al. [18] that defined the algorithms of Hooke and Jeeves, and Levenberg-Marquardt, respectively – none of the other studies [19–23] mentioned the specific algorithm used or the associated boundary values of the kinetic parameters. In addition, to our knowledge, no study has been conducted to evaluate the effect of specific optimization algorithms on the estimation of growth kinetic parameters showing a nonlinear inhibitory pattern. Therefore, the aim of this study was to estimate the growth kinetic parameters of two biodegradable organics (phenol and benzene) using three optimization algorithms (DD, SD, and MC) for various boundary values and growth phases.

2. Materials and methods

2.1. Microorganism and culture medium

The bacterial strain *Pseudomonas putida* F1 (Korea National Environmental Microorganisms Bank, Suwon, Korea) was pre-cultured in 2 L of Luria-Bertani medium (10 g/L tryptone, 5 g/L yeast extract, 5 g/L NaCl) at 30 °C in an incubator for 2 days. The bacterial cells in the late exponential growth phase were harvested by centrifugation at 10,000 rpm and 4 °C for 15 min, washed twice with mineral salt medium (MSM), and re-suspended in MSM. The composition of MSM was determined from a previous study [9] as follows (per liter): K_2HPO_4 0.095 g, KH_2PO_4 0.1055 g, $(NH_4)_2SO_4$ 0.488 g, $CaCl_2H_2O$ 3.676 g, $FeCl_36H_2O$ 0.10 g, NaCl 0.060 g, $MgSO_47H_2O$ 0.123 g. The re-suspended cells were adjusted to a final optical den-

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