

Application Strategy of the Genetic Algorithm to Parameter Estimation in Biofiltration

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(Received April 14, 2021; Revised May 18, 2021; Accepted May 18, 2021)

ABSTRACT

The mathematical modeling of a biofilter for effective biological gas removal has been problematic because of uncertain parameters incorporated into complicated equations. These parameters represent the critical factors in biofilter design and operation, such as mass transfer, biodegradation, and subsequent biofilm growth. Such parameters, which are highly site specific, should be estimated in biofilter operation. To resolve this issue, the application of the original Genetic Algorithm (GA) and its modified technique, an improved differential evolution method, was investigated as a global optimization technique, for optimal estimation of the parameters. Previous studies on the application of GA to biofiltration modeling were reviewed. Based on the review, a proper GA application strategy was developed by integrating GA with other conventional optimization and scientific/engineering-based models for enhanced computational efficiency. Thereby, the optimality of the strategy for parameter estimation was confirmed.

Key words : Biofiltration, Genetic Algorithm (GA), Improved Differential Evolution (IDE), Parameter Estimation, Optimization

1. Introduction

While real biofiltration performances of gas removals have often been tested with experiments, modeling has been applied to predict the performances. The modeling is normally implemented with assessing treated contaminant gas concentrations as response variables depending on the behaviors of the parameters and given inlet data. The parameters influencing the biofiltration performances are regarded as the critical factors on mass transfer and biodegradation of contaminant gases or their relevant compounds. Various types of the models have been developed such as the primitive model with zero-order growth along biodegradation in fixed film biofilters [1,2]. Some models focused on biofiltration of insoluble

gases (alkane compounds) at the steady state condition [3-5]. In contrast, dynamic and pseudo-steady state models to simulate transient biofilter operations were proposed by Deshusses et al. [6,7] and Alonso et al. [8,9], respectively.

The developed models are helpful to understand biofiltration mechanisms and performance predictions, but there are several challenges in model implementation. One of the most critical challenge is necessity of the unknown or site-specific parameter estimation. The optimal parameter estimation should be complicated primarily because of the parameter uncertainty in the model [10]. The parameter estimation was addressed using a conventional gradient-based optimization method, which is often not desirable for the parameters in complicated models [9,11]. Batch experimental or literature data other than biofiltration can be regarded for direct extraction of some key parameters such as biodegradation kinetics but the microbial structure and thereby degradation behaviors are highly site-specific so the batch experimental results may

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not correspond to those of biofiltration [10-12]. To resolve those issues, non-gradient based optimization methods, especially AI (Artificial Intelligence)-based models, have been useful to find global optimization from any kinds of equations [13,14]. A popular AI method is GA (Genetic Algorithm) to solve the global optimization problems with non-gradient basis [14-16]. Unfortunately, there are some previous GA applications of the inverse model approach for parameter estimation in conventional bioprocesses as fermentation [17-19], but, based on our best knowledge, only two studies addressed the original and the modified GA application for biofiltration modeling; one is Lee et al.'s and the other is Bhata et al.'s studies, respectively [10,11]. This study would review the two studies and propose a proper GA application strategy to biofiltration modeling.

2. Conceptual Description of Biofiltration

Prior to the review on AI (Artificial Intelligence) application, a brief explanation on the basics on biofiltration and the potential contribution AI to biofiltration performance would be introduced. In biofiltration, contaminated gas in the reactor normally moves via convection transport along a reactor bed. The contaminant in the gas phase with the gaseous concentration C_A is transferred into biofilm phase with the concentration C_S . The biodegradable contaminants in the biofilm phase are eliminated by microbial degradation. The concentration gradients of gas contaminants exist through the two (gas and biofilm) or three phases (gas, liquid, and biofilm) of a biofilter. The gradient of the concentrations of contaminants in the biofilm phase depends on mass transfer, diffusion, and microbial uptake. Among those, the gas solubility to biofilm (normally hydrophilic) is considered to be a critical factor. Hydrophilic contaminants can easily be transferred through the liquid phase surrounding the microbial biofilm phase. In contrast, a strongly hydrophobic compound is hardly transferred to biofilm phases, because of mass transfer resistance under the presence of thick liquid film around biofilm. Intriguingly, dried biofilm produces EPS (Extracellular Polymeric Substances) which often contain hydrophobic compounds to absorb nearby hydrophobic gases [20].

The dynamic mass transfer of the gas contaminant through filter media can be described as follows:

$$\frac{\partial C_A}{\partial t} = -v_z \frac{\partial C_A}{\partial z} - P_{1(i)} \frac{\partial C_S}{\partial x} \Big|_{x=L} \quad (1)$$

where the variable C_A represents the concentrations of the gas contaminant at a filter depth z and time t . The variable C_S means the contaminant concentration in the biofilm phase. When the contaminant is strongly insoluble to water (hydrophobic), the contaminant molecules in the liquid phase is assumed not to exist. The unknown parameter $P_{1(i)}$ is a characteristic parameter related to the contaminant mass transfer (flux along x-direction) through the active surface area of the biofilm-covered media and should be estimated using GA and the experimentally measured data. The variable L represents biofilm thickness along x-direction.

Both the diffusion and the microbial degradation of the contaminant in the biofilm phase (C_S) can be presented as follows:

$$\frac{\partial C_S}{\partial t} = D \frac{\partial^2 C_S}{\partial x^2} - V_B \frac{C_S}{K + C_S} \approx D \frac{\partial^2 C_S}{\partial x^2} - P_{2(i)} C_S \quad (2)$$

where the coefficient D is the diffusivity of the contaminant in the biofilm phase. The contaminant diffusivity in the water (or biofilm) phase could be easily found literature [8,9,11]. K is the half saturation coefficient of the contaminant in the biofilm phase. The parameter V_B contains the specific microbial degradation rate, the microbial cell density, and the yield coefficient. The boundary conditions for Eq (1) include the inlet contaminant concentration ($C_{A,in}$) entering the media in the biofilter reactor, the outlet contaminant concentration ($C_{A,out}$) as a primary indicator for the estimation. The optimal estimation is often defined as the removal efficiency ($= 1 - C_{A,out}/C_{A,in}$) obtained by modeling to be approximated to the corresponding measured one ($= 1 - C_{m,out}/C_{m,in}$) as much as possible. Another boundary condition should be relevant to the phase transfer between the gas and the biofilm phases. For this, the coefficient K_{AO} (Air-octanol partition), which is the contaminant partition between air and octanol, can be used [11]. Fig. 1 illustrates a schematic description of the contaminant distributions at the air and the biofilm phases in a hypothetical biofilter.

The dynamic change of the biofilm thickness in the hypothetical biofilter, which is proposed by Alonso et al. and Lee et al. [8,9,11,20], can be described as follows:

$$\frac{\partial L}{\partial t} = P_{3(i)} \frac{\partial C_S}{\partial x} \Big|_{x=L} - P_{4(i)} L \quad (3)$$

The unknown parameters $P_{3(i)}$ and $P_{4(i)}$ represent the diffusional flux and biofilm decay constants [8,9,11,20]. As noticed, the mathematical modeling for biofiltration incorporates complicated equations to express biodegradation and mass transfer.

For example, the Monod equation which is a typical form of microbial biodegradation presents the biokinetic and biofilm growth behaviors as a function of substrate (contaminant) concentrations. Furthermore, the mass transfer of the contaminant should include the differential equations to describe convention-diffusion-reaction mechanisms.

In addition to the complexity of the equations, a critical issue is the uncertainty of the key parameters included in the equations. The various parameters on biodegradation, biofilm growth, and mass transfer to solve the equations are mostly empirical and site-specific, and sometimes show random behaviors. Those characteristics with high degrees of variety and uncertainty result in requirement of considering various scenarios or modes in biofiltration design and operation. Therefore, biofiltration modeling should consider this point and utilize a proper parameter estimation technique before solving the model equations, in order to predict the biofiltration performances.

3. Application of GA for Estimation of Biofilter Parameters

GA explores an optimal solution through imitating the principles of genetics and evolution on natural selection. The biological genetic evolution in life science includes chromosomes, each of which consists of genes. A set of multiple chromosomes is contained in a population for a generation. Each chromosome undergoes evolution processes such as survival, extinction, mutation, or mating with others throughout generations. Based on certain criteria, some chromosomes with higher fitness to meet specified requirements are selected to survive as the generation elapsed, while others with lower fitness should be discarded in the process of natural selection [14]. GA includes mathematical formation of individual parameters, parameter sets, a group of parameter sets and an iteration stage mimic the biological genes, chromosome, a population, and a generation, respectively. Each parameter set undergoes the computational evolution processes, such as survival, extinction, mutation, or mating with other parameter sets throughout iteration stages (or generations). Based on certain criteria, some parameter sets with higher fitness range are chosen to survive in the generation but others become extinct, in the process of GA [11]. A criterion for the fitness can be generated by specifying an indicating value (i.e. biofiltration removal efficiency). If a modeling results with a given parameter set predicts a low indicating

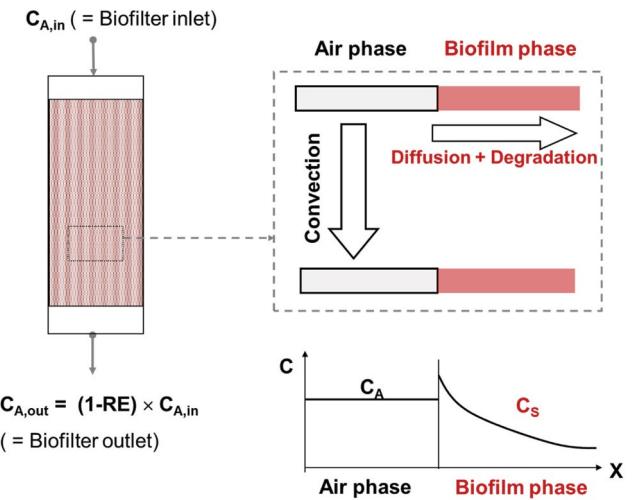


Fig. 1. A schematic illustration of the contaminant distributions at the air and the biofilm phases in a typical biofilter: inlet/outlet contaminant concentrations (Left), mass transfer directions (Top-right), and the contaminant concentration gradients (Bottom-right).

value, implying poor removal performances of biofiltration, the parameter set should be discarded from the current iteration stage. In contrast, the parameter sets with high fitness values (good biofiltration removal efficiencies) can be retained in the stage and advantageous in selection for mating and survival. Fig. 2 exhibits a typical conceptual description of GA, which was proposed for the parameter estimation in biofiltration by Lee et al. [11]. They created a random initial population which consisted of 400 parameter sets and set the maximum iteration number as 500. The initial values for the parameters were randomly specified between the maximal and the minimal values, which was given prior to initiation of GA. For certain, other constraints can be specified in regrading a high flexibility of modifying the algorithm. The unknown parameters to be estimated in GA were relevant to initial biofilm thickness, media specific surface area, contaminant mass transfer and biodegradation kinetics. The fitness of the parameter sets was decided by how the predicted model results were approximated to their corresponding measured ones. Specifically, the mean squared errors between the model and the experimentally measured data were regarded as cost values and the fitness should be high with low cost values. The biofiltration experiment to obtain the measured data incorporated the highly transient biofiltration operation as well as the normal steady operations.

Next, the individual parameter sets from the current population with high fitness or low cost values were selected to go to the subsequent iteration stage. In this stage, a parameter sets

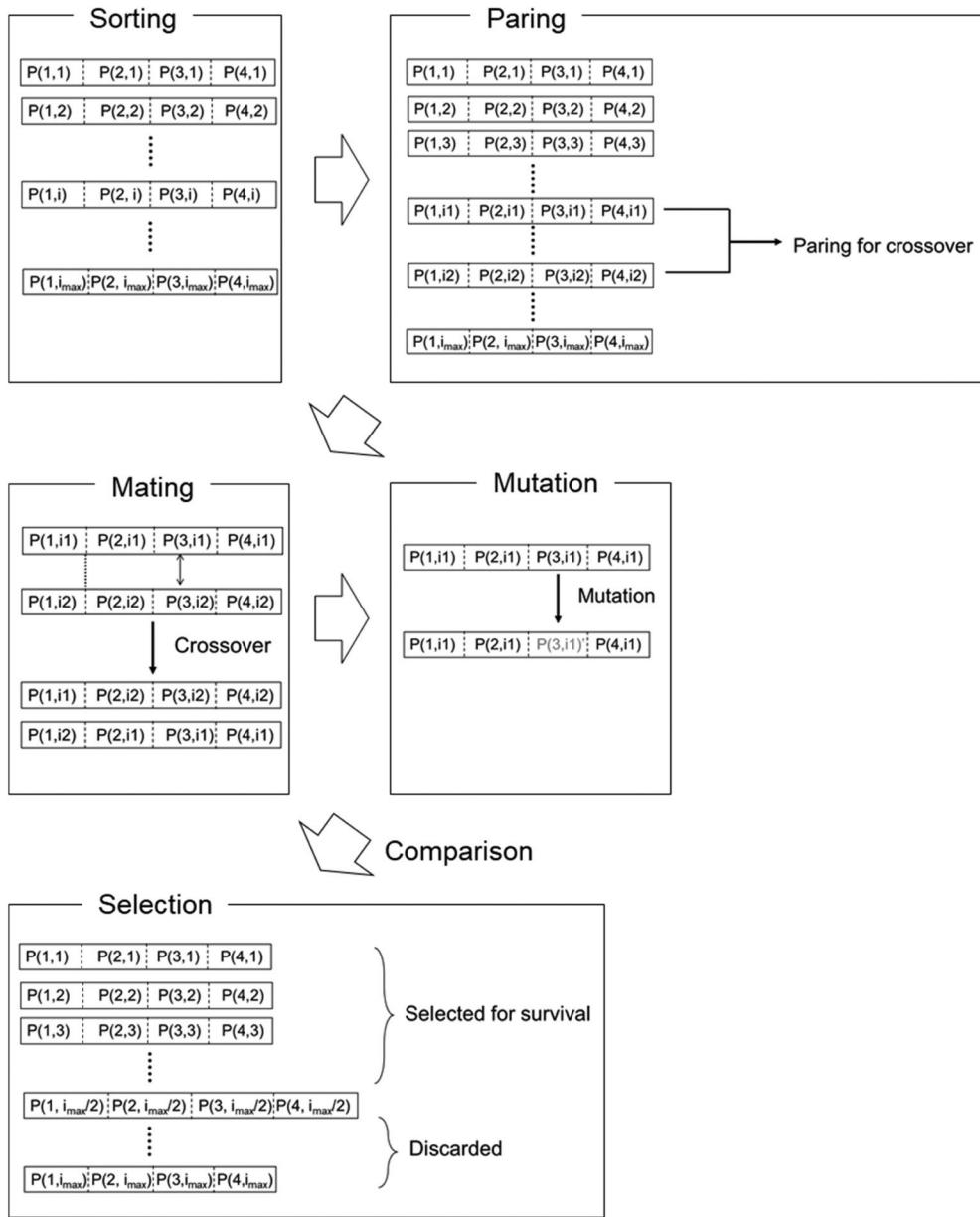


Fig. 2. A conceptual description of the genetic algorithm process for the parameter estimation on biofiltration model.

in survival has an opportunity to have one or more offspring parameter sets by copying their own parameter values. In Lee et al. study, half of the total parameter sets with low cost values and high fitness in a generation were chosen and considered for mating in the next generation [11]. The mating (or pairing) in GA means creation of a new parameter set (chromosome) through random selection of the values in the two parameter sets for mating. Another genetic processing, the mutation, was implemented simply by changing the value of one parameter with a low probability of occurrence as 0.1.

As a result of implementation of the algorithm, among the total 500 generation of the iteration stage, the values of the parameter sets in survival were approximated to those of the optimal parameter sets at the 200~400 generation numbers. The cost values for the first generation were 0.042~0.14 but those decreased to 0.06~0.020 and around 0.007 by the 10th and the 200th generations. To enhance the computation efficiencies, they could reduce, in a stepwise, the minimum and the maximum range for each parameter in the computation, as the generations elapsed. At the final stage, the 20 parameter

sets with the highest fitness (or the lowest cost values) were selected. Thereafter, further optimization processing with the gradient-based optimization was conducted with the 20 sets as the initial guess values [8,9].

Bhat et al. conducted another similar study for biofiltration with IDE (Improved Differential Evolution) method, which is slightly different to the original GA [10]. Prior to the optimization with the algorithm, they constructed a steady-state one dimensional mathematical model on transfer, dissolution and biodegradation on phenol biofiltration. Then, the target parameters were selected to represent biofilm thickness, biodegradation kinetics and air/biofilm partition coefficient for phenol and its relevant compounds in the biofilters. The improved differential evolution method was applied to optimally estimating the critical parameters. The optimization was confirmed by comparing the fitness similar to Lee et al.'s study [11]. Also, the effective biofilm thickness in prediction was proposed according to the phenol inlet loading and the gas flow rates. Bhat et al.'s study also noticed the major drawback of the original differential evolution algorithm of the convergence slow-down near the global optima [10]. Thus, they added another conventional optimization program of the Simplex method after the solutions of the differential evolution method approached to the global optimization with the slow convergence. When computation for the optimal solution searching progress is slow down, GA can be switched to the Simplex method to quickly reach the global optimum in a shorter computation time. The Simplex method obtained the optimal solution of the parameter set by sorting the parameter sets and calculating new ones by a sliding window approach [10]. The new method combining GA and the Simplex methods showed the computation speed twice as fast as the identical GA without the Simplex method.

4. Future Directions

The two case studies on the application of GA to biofiltration parameter estimation appear to be successful but require further research progresses as follows:

(1) The major disadvantage of GA is the slow computation speed near the convergence points near optimal solutions. Thus, the two case studies implemented the gradient-based optimization and the Simplex methods to enhance the computation efficiency. Such efforts should be continued to explore the model integration with GA and other traditional optimization or artificial intelligence (i.e. neural network or fuzzy) techniques.

(2) As proposed in the case studies for the review, the contribution of GA is expected to be desirable with the biofiltration models with the process engineering basis rather than for the other empirical ones as the black-box model [11,21,22]. For example, typical convection-diffusion-reaction models are straightforward to be understood in the relevant phenomena, and the model parameters contain their own scientific validity. This may facilitate validation of the model parameters and the GA algorithm performances, because a modeler may address the dual-confirmation of the optimality of the estimated parameters through scientific or engineering interpretations as well as the mathematical processing. In contrast, even if other types as the statistical models with purely empirical parameters or the black-box models may also apply GA or other optimization techniques for parameter estimation or performance prediction, the optimality or the reasonability of the parameters, with respect to the scientific or the engineering aspects, cannot be guaranteed for those models. Therefore, it is recommendable that the future research on GA application to biofiltration should be integrated with other typical optimization and science/engineering models. This strategy is suitable for the computational efficiency and the confirmation of optimality through GA.

5. Conclusion

An application strategy of an original GA and an improved differential evolution method to biofiltration modeling was proposed in this study. To prepare an effective strategy, the previous relevant studies were searched and intensively reviewed. As a result of the review, all of the two previous biofiltration modeling studies integrated GA with the subsequent typical optimization techniques of the gradient based or the Simplex methods mainly for enhancing computation efficiency. The specific objectives of GA application were the optimal estimation of the parameters on contaminant mass transfer, biodegradation and biofilm growth occurring in biofilters for both of the studies. In this context, a desirable strategy of GA to biofiltration modeling is (1) the integration of GA with other optimization techniques to enhance computational efficiency and (2) GA application to optimal estimation of the scientific or the engineering parameters for dual confirmation of the optimality based on reasonableness of not only mathematical but also scientific and engineering aspects.

Acknowledgements

Funding from Daegu Green Environment Center under (DARPA) under Grant No. B20160140-20200149 is acknowledged.

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