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Comparison of Regression Model and Modified Monod Kinetic Model to Predict the Removal of Ethanol in Trickling Biofilter

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Abstract

Ethanol is a toxic compound and a member of volatile organic compounds (VOCs). Ethanol is emitted to the atmosphere by several industries worldwide. Biotrickling filter technology is a well-known technology for removal of VOCs from air. The aim of this study is to compare two regression and modified monod models to predict the removal of ethanol using a biotrickling filter reactor (BTFR). The data of the previous study on ethanol vapor removal by bio-trickling filter were used for determination of r_{max} and K_m. Also by these data, a simple regression model was developed. Eventually, ethanol removal efficiency was predicted by both regression and kinetic models. All results were compared with actual data. Our results show that regression model could only predict the average of ethanol removal efficiency. However, kinetic model could additionally predict all changes in ethanol removal efficiency: it has had some good alignment with actual data.

Keyword: Ethanol, Kinetic coefficient, Modeling, Biotrickling filter, Biodegradation

1 Introduction

The rapid evolution of industries during the last few centuries has left a significant impact on the environment (1-3). The momentous scale of today's environmental challenges has urged countless number of researchers continuously working in order to provide the best solution for various types of man-made harms dealt to the environment (4-7). Among these is the issue of air pollution caused by the exhaust gasses including ethanol emitted from various industries such as petrochemical and alcoholic drinks manufacturers, often beyond the acceptable capacities (8-10). Ethanol is one of such pollutants and it is categorized into the volatile organic compounds (VOCs), posing threats to the environment (11). Ethanol is widely used in the production of petrochemical compounds. Thus it is only natural to address this issue by considering the threats of this pollutant and its wide-scale usage and generation. In order to achieve reductions in air pollution to attain air quality standards, a set of specific techniques and measures should be identified and implemented. In this particular case, various systems of physical, chemical and biochemical nature have already been utilized so as to treat this pollutant (12-16). However, some of procedures including the physical methods applied by utilizing various adsorbents (17) and the chemical methods (18) applied by utilizing chemical scrubbers, are often expensive–these possess even less efficiency in ethanol reduction (19). In contrast, biochemical methods, despite their complications, could prove to be highly appropriate substitutes for the physical and chemical methods (20). The biological methods mostly involve bio-filters. It is to be noted that amongst all these, the trickling biofilters are deemed the most optimum for the elimination of ethanol. The models proposed by researchers to determine the best conditions of applying trickling biofilters, are actually divided into two groups of Micro kinetic and Macro kinetic (21, 22). In Micro kinetic models, it is attempted to take into consideration all parameters involved (23). These may well include the specific surface of the substrate, the thinness of the applied biofilm, the dispersion coefficient of input polluted air into the biofilter, and the constant coefficient of Henry in Mass Transference. These models are usually very complex; they require a vast array of parameters and coefficients which are normally unavailable to the engineers (24). Ottengraf and Van den Over offered one of the most referred-to microkinetic models. The macrokinetic models often avoid defining or investigating partial parameters and would only focus on the most prominent parameters including the concentration of the pollutant, input pollutant debit, and the degree of moisture and temperature. Studying the effects of these parameters on the system efficiency and providing the mathematical relations in the form of macro kinetic models require laboratory experiments; thence they are referred to as the "Experimental models". Generally, in macro kinetic

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models having lower concentration of the input pollutant, the shifts in the fixation rate of the input pollutant within the system is linear. However, by increasing the concentration of the input pollutant, the fixation rate of the pollutant within the system shifts towards zero so that it can no longer remain linear. Strauss et al in 2000 provided the Eq. 1 for the determination of the biofilter's efficiency in eliminating VOCs, where a and b are the constant coefficients, t is the retention time within the biofilter, and ultimately u is the overall efficiency of the system. The constant coefficients in this equation are determined by calculating the log form from both sides of the equation and eventually by fitting the data based on the results obtained in the experiments within the various retention intervals.

$\mu = a\,(1\text{-}e^{-bt})$

Similar studies have also been conducted by Duplacis et al in 2003, leading to the successful modulation of an experimental model based on the completion of the previous equations. In all macro kinetic models, the efficiency of the biofilter depends on the concentration of input pollutant which is also, in its own turn, dependent on the input contamination rate into the system. It is worth mentioning that the rate of the input pollutant entering the biofilter is associated with the debit of the input contaminated air that gets into the totality of the system.

The main purpose of this study is investigating into the kinetic parameters of a biotrickling filter and also providing a simple regression model. Furthermore, a comparison between the obtained anticipatory results of the biokinetic equations and the regression model is provided. In the first step, piloting the biotrickling filter was kept under examination for 61 days after which the biosynthetic parameters were calculated by the resulting data. The re-examined monod equation and the regression model are propounded, too. In the end, the resolution of these models in anticipating the efficiency of the system within various conditions has come to the fore.

2 Materials and Methods

We began with designing a pilot for the biofilter, based on the descriptions provided by Goli et al. This was examined in 3 debits of input air into the ethanol vapor in 90, 291 and 1512 liters per hour. Previous studies have shown that the efficiency of the biofilter is highly associated with the hydraulic retention time and the pH of the environment. Therefore, based on the resulting conclusions, within 61 days the biofilter was subjected to 3 different uploads. Since the previous studies by Goli et al established the optimum pH for the highest efficiency at 7, the pH of system in this study is constantly maintained on 7 in all uploads. The uploads were maintained until the system came to be stabilized. The stable conditions for this study are defined in terms of stable or insignificant changes in system efficiency for at least 6 days. In each upload, the parameters of retention time, the input pollutant and the output pollutant were investigated. A simple model based on the linear regression and the reexamined monod equation was also studied based on the obtained data.

2.1 The calculation of the regression model

In order to provide a simple model based on the regression method, the daily efficiency of the system was obtained. After each cycle, the average efficiency within the upload was calculated. Therefore, in the end, 3 different efficiency rates for every 3 upload were arrived at. By applying the linear regression amongst these data, a simple model is achieved. In order to practicalize this simple model in the design of the biofilter, or even for purposes of anticipating various states of the biofilters, it is combined with another model.

2.2 The calculation of the kinetic parameters

In the first step of analyzing the resulting data from the experiments, the development of a suitable model is necessary. The development of such a model is conducted in the following steps:

The removal capacity (r) of the biofilter is determined by the following equation.

$r = ((Cin\text{-}Cout)Q)/V$

Where Q is the debit of the input flow into the biofilter in m^3h^{-1}, the concentration is in gm^{-3}, and the volume of the reactor is in cubic meter. Furthermore, based on the monod equation, the removal capacity could also be expressed by the following equation:

$r = (rmax \times Cg)/(Km+Cg)$

where C_g is the average concentration of the pollutant in gm^{-3}, r_{max} is the maximum reaction speed of the bio-decomposition associated with the bed volume in $gm^{-3}h^{-1}$ and K_m is the saturation constant in the gas phase in gm^{-3}. By combining the equation 1 and 2, and equalizing both, Eq.3 is attained for the calculation of the kinetic parameters.

$$\frac{(C_{in} - C_{out})Q}{V} = \frac{r_{max} \times C_g}{K_m + C_g} \quad (3)$$

By simplifying the Eq.3, Eq.4 is achieved:

$$\frac{V}{(C_{in} - C_{out})Q} = \frac{K_m}{r_{max}} \times \frac{1}{C_g} + \frac{1}{r_{max}} \quad (4)$$

where C_g is the average logarithmic concentration in the biofilter. The following equation could be applied in order to obtain the average logarithmic concentration. In the first step, Eq.1 is solved, which would then lead to Eq.5:

$$V = \frac{(C_{in} - C_{out})Q}{r} \quad (5)$$

The researchers also show that both r and the volume of the reactor could be expressed through the equations 6 and 7.

$$r = \frac{K_1 \times C_g}{1 + K_2 \times 豹_g} \quad (6)$$

$$V = \frac{ln\left(\frac{C_{in}}{C_{out}}\right) + K_2(C_{in} - C_{out})Q}{K_1} \quad (7)$$

By equalizing the two equations, Eq.8 is obtained:

$$\frac{(C_{in}-C_{out})Q}{r}=\frac{ln\left(\frac{C_{in}}{C_{out}}\right)+K_2(C_{in}-C_{out})Q}{K_1} \quad (8)$$

By replacing the Eq.6 with the r factor in Eq.8, Eq.9 is arrived at:

$$\frac{(C_{in}-C_{out})Q}{\frac{K_1\times \text{[illegible]}_g}{1+K_2\times C_g}}=\frac{ln\left(\frac{C_{in}}{C_{out}}\right)+K_2(C_{in}-C_{out})Q}{K_1} \quad (9)$$

The expansion of the Eq.9, simplifying it and ultimately solving it for C_g leads to the identification of the following equation as the average logarithmic concentration in bioreactor which is expressed as Eq.10:

$$C_g=\frac{C_{in}-C_{out}}{ln\left(\frac{C_{in}}{C_{out}}\right)} \quad (10)$$

By applying Eq.10 we can attempt to calculate the average logarithmic concentration, and by replacing it in Eq.4 we can obtain the synthetic parameters. In order to determine the kinetic coefficients in this study, the parameters of $V/[(C_{in}-C_{out})Q]$ is plotted against $1/C_g$ in Eq.4 which leads to r_{max} and K_m.

2.3 Experimental methods

In this study, an ethanol measurement device was utilized (Inters can company, model: 4160) which provided fast and direct examination of the ethanol present in the air.

3 Results and Discussions

3.1 Regression model

The previous studies by Goli et al suggested that the efficiency of the biological filter studied here is statistically associated with retention time and the pH of the environment. Since the optimum pH for the studied biofilter was established at 7, it is only natural that any future navigation is also the most efficient in neutral pH; therefore, the calculation of Eq.11 by the regression method is conducted based on this pH. It is noticeable that Eq.11 is achieved by considering the average efficiency of the system in each upload obtained during the 61 experiments conducted on each upload on a daily basis. The results of this regression are shown in Fig.1. As demonstrated there, the correlation coefficient in this equation is equal to 0.909.

$$y = 0.052x + 94 \quad 11$$

In this study, Eq.12 is applied in order to obtain the efficiency of the system. Where C_{out} is the output ethanol from the system in mg/l and C_{in} is the concentration of the input ethanol into the system in mg/l. Moreover, the retention time is obtained by Eq.13 in which V is the volume of the filter in l, Q is the debit of the input polluted air into the filter in l/h, and t is the hydraulic retention time in seconds. By replacing Eq.12 with F factor and by replacing Eq.13 with t factor in Eq.11 and the simplifying thereof, we can achieve Eq.14. Eq.14 allows us to determine the volume of the filter in industrial scale by providing it with the input and output concentration of ethanol and the debit of the input polluted air by ethanol.

Enough attention has to be paid to the fact that this equation will only be applicable if the utilized bed is identical to the bed used in this study. This is because different beds are characterized by different porosity rates and especial surfaces. As a result, the cultured biomass on these beds could be different. The input air into the system only contains ethanol. The bio-decomposition rate of the biofilter is of course different in the presence of other compounds. Finally, the concentration of ethanol must be within the scope of this study. In order to prove the interpolation capacity of this model and also the extrapolation resolution, further experiments are required.

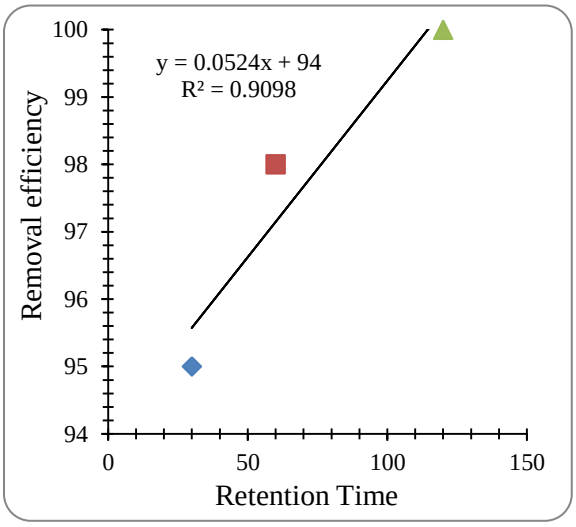

Fig.1: The dependence of filter efficiency on retention time

$$F=\frac{C_{in}-C_{out}}{C_{in}} \quad (12)$$

$$t=\frac{V}{Q} \quad (13)$$

$$V=\frac{Q[100\times(C_{in}-C_{out})-96.2]}{0.065C_{in}} \quad (14)$$

3.2 Calculation of the kinetic parameters

In this study, Eq.4 was used in order to determine the kinetic parameters. In Eq.4 the rates of r_{max} and K_m is obtained by plotting the $V/[(C_{in}-C_{out})Q]$ against $1/C_g$.

Table1: The calculation results of kinetic parameters

Volume	Debit of the input flow	Inlet Ethanol concentration	Outlet Ethanol concentration	Average logarithmic concentration (Cg)	$(V/Q)/(C_{in}-C_{out})$	1/Cg
0.00319	0.09	485	53.26	195.449	$8.209*10^{-5}$	$5.116*10^{-3}$
0.00319	0.291	485	18.32	142.447	$2.348*10^{-5}$	$7.020*10^{-3}$
0.00319	1.512	485	26.54	157.790	$4.601*10^{-6}$	$6.337*10^{-3}$

The above values are then applied in order to provide the linear regression between the $V/[(C_{in}-C_{out})Q]$ and $1/C_g$ columns and calculating the associated equation. Equation 15 is the result of the respective regression model in which the intercept was $1/r_{max}$, and the constant coefficient of X was K_m/r_{max} (thus allowing easy calculation of the kinetic parameters needed).

$$y = 24.58x - 0.011 \quad (15)$$

The results of this table illustrate that the biofilter r_{max} is equal to - 0.011 $gm^{-3}h^{-1}$ and K_m is equal to 24.58 gm^{-3}. The r_{max} is less than zero because of the relative increase of the efficiency against the increase of the formaldehyde concentration.

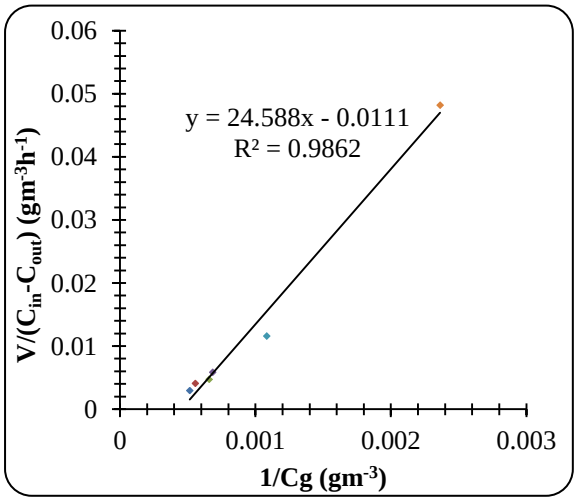

Fig.2: The results of the linear regression in 3 different loadings.

3.2 Comparing the results of the regression model and the kinetic model in anticipating the biofilter's efficiency

At this stage, equation 4 (the kinetic model) and 14 (the regression model) were solved in order to determine the efficiency of the biofilter. These equations were then applied in the forms of Eq.16 and Eq.17.

$$C_{out} = \frac{V}{Q\left(\frac{K_m}{r_{max}}\frac{1}{C_g} + \frac{1}{r_{max}}\right)} + C_{in} \quad (16)$$

$$C_{out} = \frac{C_{in}(-145.8t + 99.98) + 100 \times C_{in}}{100} \quad (17)$$

The data retrieved from various experiments were then inserted into these equations and the results were then compared with the real experimental results. It is worth mentioning that these data were applied to the system in three different loadings. The load shift was applied by changing the hydraulic retention time by increasing the debit. The range of retention time changes includes: 90, 291 and 1512 lit/h. The results of these experiments are presented in Fig.3. As it is illustrated in this figure, the real percentage of formaldehyde elimination by the biofilter shows severe shifts. On the other hand, the regression model has only determined the average of the formaldehyde removal without the capacity to anticipate the possible shifts. However, the accuracy of these models is still remarkable. Based on Fig.3, the provided results by Eq.4 are about 10% lower than the real experimental results; nonetheless, they were successful in anticipating the various shifts that occurred within the biofilter. This is considered as a big advantage in applying this equation.

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Competing interests

The authors declare that there is no conflict of interest that would prejudice the impartiality of this scientific work.

Author's contributions

It is certified that all of the authors have made the same contribution in the experiments and manuscript writing.

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Ethical considerations

Authors are aware of, and have complied with, best practices in ethics, specifically with regard to authorship (avoidance of guest authorship), dual submission, manipulation of figures, competing interests and compliance with policies on research ethics. Authors adhere to publication requirements that the submitted work is original and has not been published elsewhere in any language.

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