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RESEARCH ARTICLE

REMOVAL OF DIMETHYLSULPHIDE IN A BENCH-SCALE BIOFILTER: SOME ANALYTICAL SOLUTIONS

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ABSTRACT

A mathematical model describing the biofiltration of dimethyle sulphide (DMS) in a bench-scale biofilter is discussed. This model contains the diffusion of the compounds through the biofilm and degradation of the compound along the biofilter column. The model proposed here is based on the mass transfer in gas-biofilm interface and chemical oxidation in the gas phase. Analytical expressions pertaining to the dimethyl sulphide concentration in the gas phase and bio-film phase have been derived using the new homotopy perturbation method (NHPM) for all possible values of parameters. Furthermore, in this work the numerical simulation of the problem is also reported using the Matlab program to investigate the dynamics of the system. Our analytical result are compared with numerical result. Satisfactory agreement is noted.

INTRODUCTION

The biofiltration has been widely and efficiently applied during the recent period for the treatment of air streams contaminated by volatile organic compounds at low concentrations. Also it has been applied widely and efficiently in the removal of styrene from waste gas streams. (Bina *et al*., 2010). It work through absorbing noxious gases into a biofilm where microorganisms break down the gases into carbondioxide, water and salts and use the energy and nutrients to grow and reproduce. Biofiltration is an efficient biotechnological process used for waste gas abatement in various industrial processes. The odorous pollutants by this process was also investigated at a municipal wastewater treatment plant (Omri *et al*., 2013). Wood chips and bark mulch are commonly used biofilter media because they are generally available and inexpensive. These organic materials degrade and they require replacement every 2–5 years (Akdeniz *et al*., 2011). A bench scale biofilter packed with compost and wood chips on with potential DMS degrading culture (Bacillus sphaericus) which could efficiently remove DMS from ambient air. Further, the same biofilter operated for the treatment of vent gas generated from a P&P industry indicated DMS removal (Giri and Pandey, 2013). Dimethyl sulfide conversion depended both on gas residence time and inlet Concentration (Giri and Pandey, 2013). Biofilters are applied for odor reduction, but their operational control was limited. Dimethyl sulfide elimination depends up on the DMS inlet concentration, gas residence time, and membrane polymer (DeBo *et al*., 2003). This bioreactor performed well in terms of DMS gas removal, based on an evaluation of the apparent kinetics and maximal removal capacity of the system. Under different conditions the bioreactor inoculated with enhanced removal of high concentrations of DMS (Shu and Chen, 2009). The atmospheric oxidation of dimethyl-sulphide (DMS) derived from marine phytoplankton is a significant source of marine sulphate aerosol. DMS has been proposed to regulate climate by changes in cloud properties, also global cloud condensation nuclei (CCN) concentrations have only a weak dependence on the total emission flux of DMS (Woodhouse *et al*., 2013). Rahman *et al*. (Rahman *et al*., 2009) developed a one-dimensional biofilm model based on the basic principle of conservation of mass. Miller *et al*. (Stine *et al*., 2013) presents a mathematical model describing the growth of a biofilm and predicts the response of a biofilm to several basic treatment strategies. Laspidou *et al*. (Laspidou *et al*., 2014) discussed the mathematical modeling of biofilm mechanical properties.

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Alma Masic *et al*. (Masic *et al*., 2010) developed a mathematical modeling of the oxygen profile in a nitrifying moving bed biofilm reactor. Recentely Giri *et al*. (Giri and Pandey, 2013) developed the mathematical model for the removal of DMS from waste gas. The non-linear differential equation representing the degration of DMS along the thickness of the biofilm under steady state condition is solved by numerical method. However the best of our knowledge, analytical expression of concentration of dimethylesulphide in the gas phase and in the biofilm phase have been reported. The purpose of this comnication is to drive the approximate analytical expression for the dimethylsulphide concentration in both the phase using the New Homotopy perturbation method.

Mathematical modelling

The mathematical model describes the biofiltration of DMS based on the degradation of the compound with the biofilter column and diffusion of the compounds through the biofilm. There are no radial concentration gradients across the biofilter and the flow of air through the bed is viewed as plug flow. The biofilm grows on the outside surface of the packing material only. It uniformly covers the packing media, especially the compost and woodchip mixture over which the biofilm is formed and when compared to the size of the partical its thickness is very; hence, rectangular geometry might make utilized. DMS is the only substrate (carbon source) affecting the biodegradation rate. Oxygen is not a restricting substrate within the range of concentrations. There is no gas-phase boundary layer at the air/biofilm interface and henceforth, the gas-phase mass exchange can be ignored. Using air/biofilm partition coefficient DMS concentrations in the gas phase are related to their concentrations in the biofilm. The overall biofilm density, determined as kg of dried biomass per m^3 of biofilm, is constant for any period of experimental run on account of the biomass accumulation in the column is slow and additionally because under steady-state conditions the decay rate can be assumed to be equivalent to the growth rate. The schematic diagram of air-phase biofilter for treatment of waste gas containing DMS is represented in Fig.1. Let us consider the nonlinear differential equation for the removal of DMS from waste gas in the biofilm under steady-state conditions (Duan and Rach, 2011) as follows:

$$\frac{\partial S_{DMS}(x,t)}{\partial t} = D_e \frac{\partial^2 S_{DMS}(x,t)}{\partial x^2} - \frac{\mu_{\max} X\, S_{DMS}(x,t)}{Y_{x/s}(k_s + S_{DMS}(x,t))} \tag{1}$$

where S_{DMS} represents the liquid phase concentration of DMS in biofilm, X is the dry cell density in the biofilm which represents the overall population of micro- organisms that includes specific DMS degrading microorganisms , $\mu_{\max}$ is the maximum specific growth rate, K_s is the half saturation constant, $Y_{x/s}$ is the biomass yield coefficient, D_e is the effective diffusion coefficient of the DMS in the biofilm, and x is the position in the biofilm. Initial and boundary conditions for above equation can be represented as:

$$S_{DMS}(t=0) = 0 \tag{2}$$

$$S_{DMS}(x=0) = \frac{C_{DMS}(h)}{m_{DMS}} \tag{3}$$

$$\frac{dS_{DMS}(x=\delta)}{dx} = 0 \tag{4}$$

where C_{DMS} is DMS concentration in gas phase and m_{DMS} is the air/biofilm partition coefficient. The gas phase DMS concentrations , along the biofilter column, can be described by:

$$\frac{\partial C_{DMS}(h,t)}{\partial t} = U_g \frac{\partial C_{DMS}(h,t)}{\partial h} - A_s D_e \left[\frac{\partial S_{DMS}(x,t)}{\partial x}\right]_{x=0} \tag{5}$$

where U_g is superficial gas velocity, A_s is the biofilm surface area and h is position along the biofilter. The initial conditions is:

$$C_{DMS}(t=0) = 0 \tag{6}$$

$$C_{DMS}(h=0) = C_{DMSi} \tag{7}$$

where the subscript 'i' represents conditions at the inlet of the biofilter.

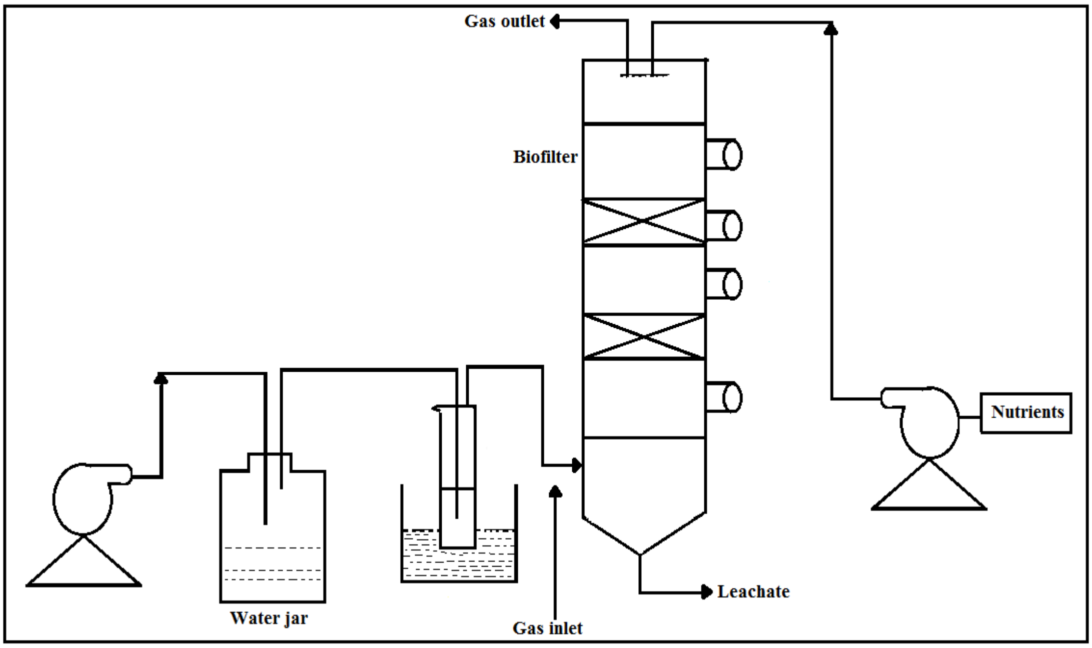

Fig. 1. Schematic diagram of air-phase biofilter for treatment of waste gas containing DMS (Giri *et al*., 2010)

Dimensionless form

Dimensionless form for the non-linear differential Eq (1) and Eq (5) is made by defining the following dimensionless parameters:

$$\overline{S}_{DMS}=\frac{S_{DMS}\,m_{DMS}}{C_{DMS}},\quad \overline{x}=\frac{x}{\delta},\ \alpha=\delta^{2}\,\frac{\mu_{\max}X}{Y\,D_e\,K_s},\ \beta=\frac{C_{DMS}}{K_s\,m_{DMS}},$$

$$\overline{C}_{DMS}=\frac{C_{DMS}}{C_{DMS_i}},\ \overline{h}=\frac{h}{\delta},\quad \gamma=\frac{A_s\,\delta}{m_{DMS}},\quad \tau=t\,\frac{D_e}{\delta^{2}},\ \eta=\frac{\delta U_g}{D_e}$$

Using the above dimensionless variables, Eq (1) and Eq (5) reduces to following dimensionless form:

$$\frac{\partial\overline{S}_{DMS}}{\partial\tau}=\frac{\partial^{2}\overline{S}_{DMS}}{\partial\overline{x}^{2}}-\frac{\alpha\,\overline{S}_{DMS}}{1+\beta\,\overline{S}_{DMS}}\tag{8}$$

$$\frac{\partial\overline{C}_{DMS}}{\partial\tau}=\eta\frac{\partial\overline{C}_{DMS}}{\partial\overline{h}}-\gamma\,\overline{C}_{DMS}\left[\frac{\partial\overline{S}_{DMS}}{\partial\overline{x}}\right]_{\overline{x}=0}\tag{9}$$

The corresponding dimensionless boundary conditions

$$\overline{S}_{DMS}(\overline{x}=0)=1\tag{10}$$

$$\frac{d\overline{S}_{DMS}(\overline{x}=1)}{dx}=0\tag{11}$$

$$\overline{C}_{DMS}(\overline{h}=0)=1\tag{12}$$

Approximate analytical solution to Eq. (8) and Eq. (9) using the New approach tohomotopy pertubrtion method

$$\overline{S}_{DMS}(\overline{x},\tau)=\frac{\cosh(\sqrt{A}(\overline{x}-1))}{\cosh(\sqrt{A})}-\sum_{n=0}^{\infty}\frac{(-1)^{n}(2n+1)e^{-f_n\tau}\cos(((2n+1)\pi(\overline{x}-1)/2))}{f_n}\tag{13}$$

$$\overline{C}_{DMS}\ (\overline{h},\tau) = \gamma\sqrt{A}\ \tanh\ \sqrt{A}\ \tau + \sum g_n \frac{(1-e^{-f_n\tau})}{f_n} \tag{14}$$

$$+\ \theta\,(\tau + \overline{h}/\eta)\{\,1-(\gamma\sqrt{A}\ \tanh\ \sqrt{A}\,(\tau-\overline{h}/\eta)) - \sum g_n \frac{(1-e^{-f_n(\tau-\overline{h}/\eta)})}{f_n}\}$$

$$A = \frac{\alpha}{1+\beta},\ f_n = \frac{\pi^2(2n+1)^2+4A}{4\pi},\ g_n = \left(\frac{(-1)^n(2n+1)^2\pi^2}{2f_n}\right) \tag{15}$$

Numerical simulation

In order to test the accuracy of the solution with a finite number of terms, the system of time dependent non-linear differential equations were solved numerically. To show the efficiency of the present method, our results are compared with numerical results in Table 1. The function pdepe (Finite element method) in Matlab software which is a function of solving the boundary value problems is used to solve the Eqs. (8) and (9). A comparitive study of the analytical solution of DMS concentrations in gas phase and biofilm phase and simulation results are shown in Figs. (1) and (2).

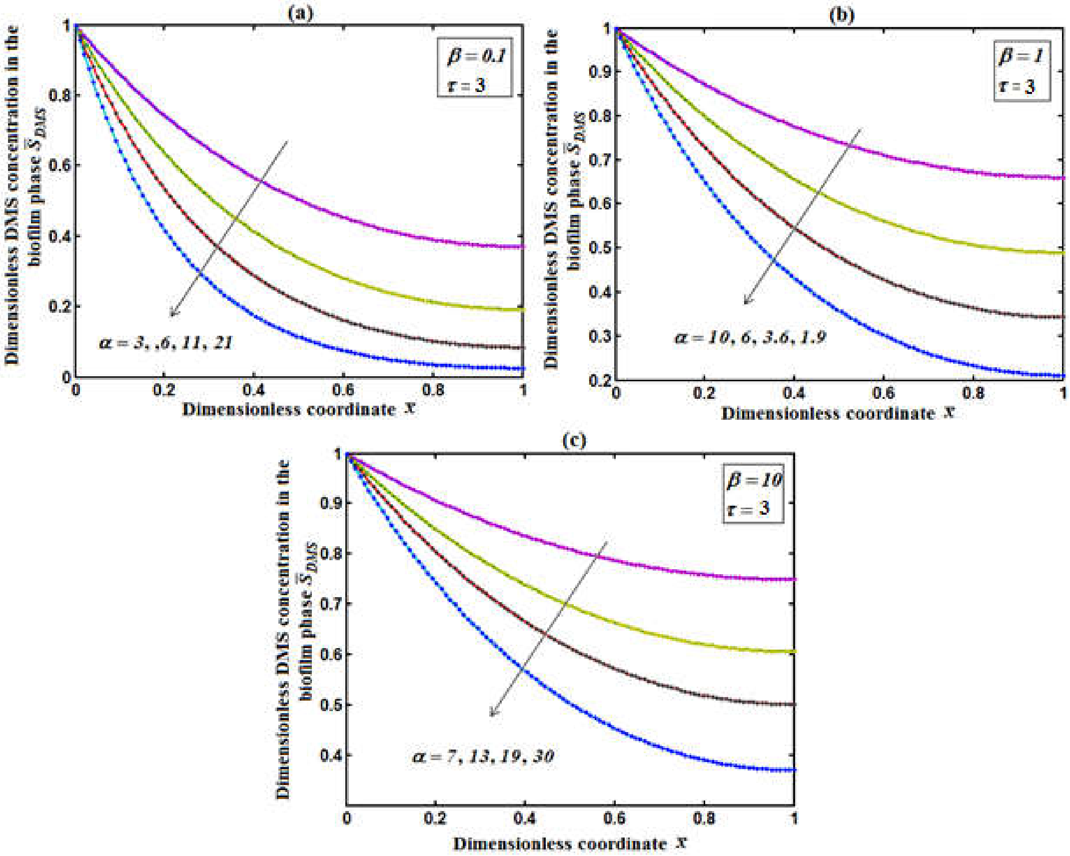

Fig. 2. Dimensionless DMS concentration in the biofilm phase $\overline{S}_{DMS}$ versus dimensionless coordinate $\overline{x}$ for various experimental values of α and for some fixed experimental values of the parameter β (Appendix B). The key to the graph, solid line represents the Eq.(13) and dotted line represents the numerical simulation

Table 1. Comparison of analytical result of dimensionless DMS concentration in the biofilm phase S_{DMS} $(g\ m^{-3})$with the numerical simulation for various experimental values of α and X using Eqn.(17)Eq.(13)when $\beta = 10,\ \tau = 3$

X	$\alpha=1$			$\alpha=5$			$\alpha=7$			$\alpha=0.4$		
	Analytical Eqn.(17)	Numerical	% of derivation	Analytical Eqn.(17)	Numerical	% of derivation	Analytical Eqn.(17)	Numerical	% of derivation	Analytical Eqn.(17)	Numerical	% of derivation
0	1	1	0	1	1	0	1	1	0	1	0	0
0.2	0.9836	0.9837	0.01	0.9194	0.9196	0.02	0.8878	0.8884	0.06	0.9935	0.9929	0.06
0.4	0.9710	0.9710	0.00	0.8568	0.8572	0.04	0.8009	0.8020	0.13	0.9883	0.9873	0.1
0.6	0.9619	0.9619	0.00	0.8122	0.8128	0.07	0.7389	0.7406	0.22	0.9847	0.9834	0.13
0.8	0.9565	0.9565	0.00	0.7855	0.7862	0.08	0.7018	0.7038	0.28	0.9826	0.981	0.16
1	0.9547	0.9547	0.00	0.7766	0.7773	0.09	0.6894	0.6915	0.30	0.9818	0.9802	0.16
	Average % of deviation		0.006	Average % of deviation		0.05	Average % of deviation		0.165	Average % of deviation		0.101

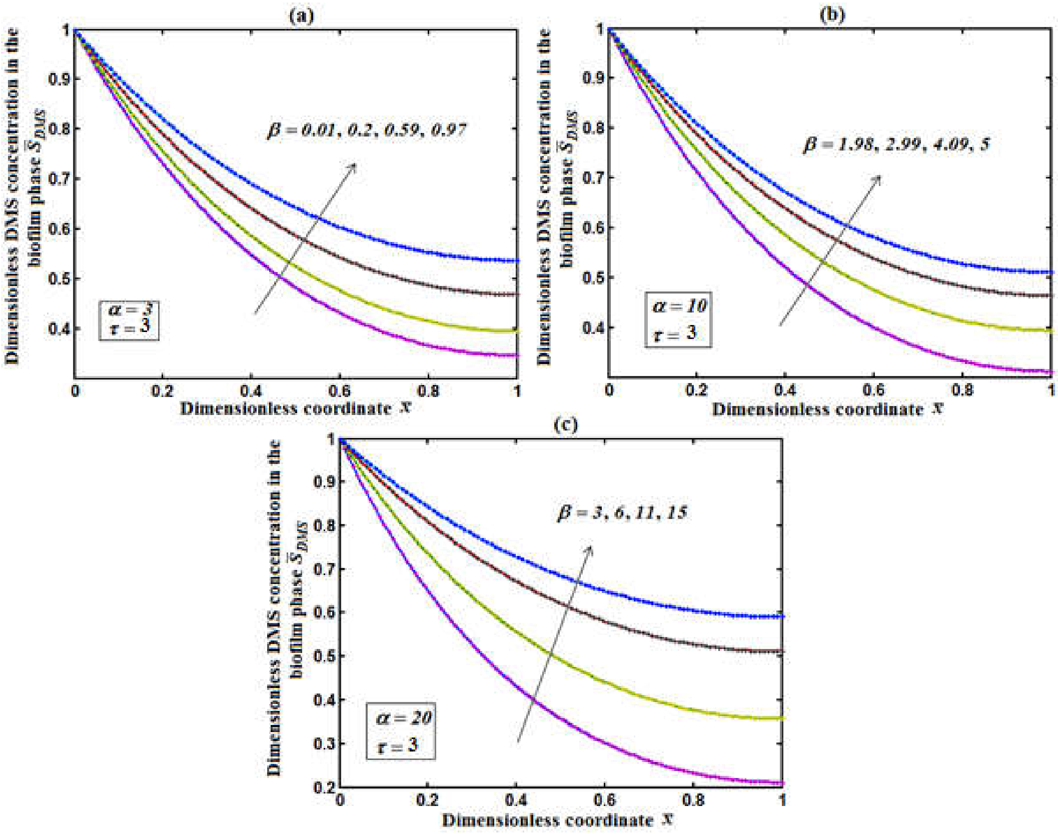

Fig. 3. Dimensionless DMS concentration in the biofilm phase ($\bar{S}_{DMS}$) versus dimensionless coordinate $\bar{x}$ for various experimental values of β and for some fixed experimental values of the parameter α (Appendix B). The key to the graph solid line represents the Eq. (13) and the dotted line represents the numerical simulation

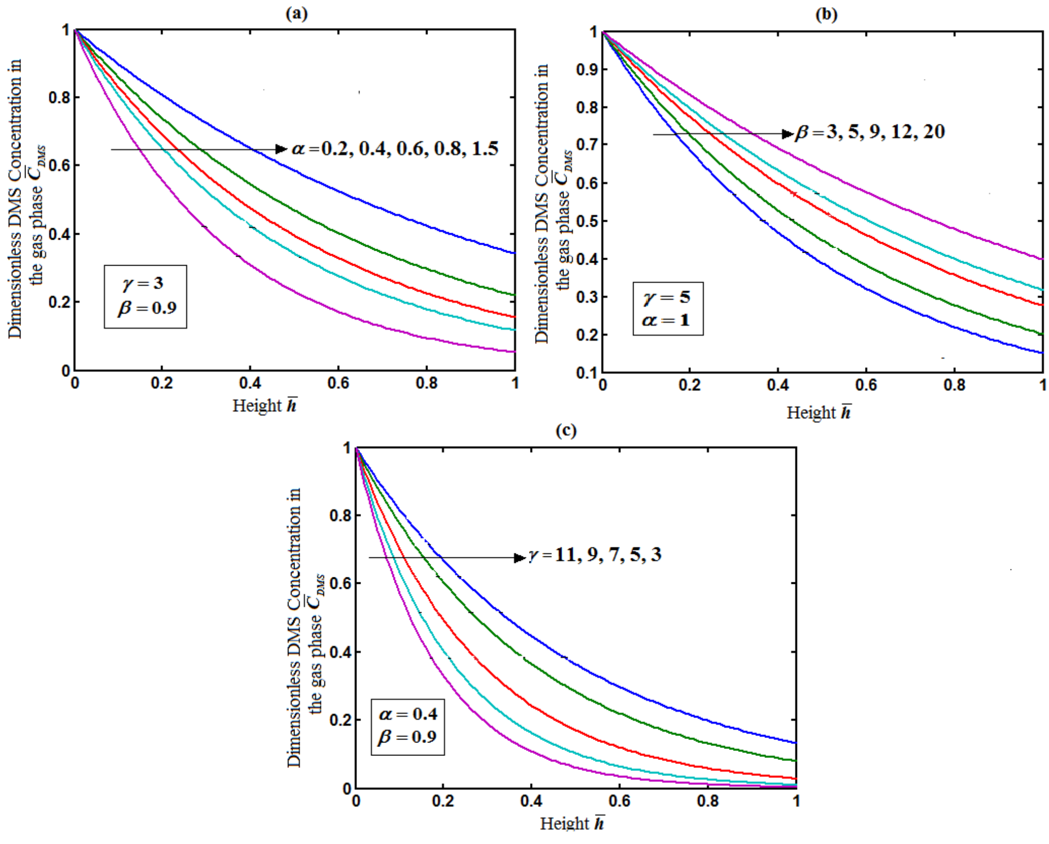

Fig. 4. Dimensionless DMS concentration in the gas phase $\bar{C}_{DMS}$ versus dimensionless height ($\bar{h}$) for various experimental values of $\alpha(a)$, $\beta(b)$, $\gamma(c)$ and for some fixed experimental values (Appendix B) of other parameters in Eq(14)

RESULTS AND DISCUSSION

Eqs. (13) and (14) represent the simple approximate analytical expressions of DMS concentration in the biofilm phase and the gas phase respectively. The concentration of dimethyl sulphide in the gas phase $\overline{C}_{DMS}$ depends up on the following three dimensionless parameters γ, α and β. The parameter γ depends up on specific surface area of the biofilm A_s, effective diffusion coefficient in the biofilm D_e, and superficial gas velocity U_g. The parameter α depends up on the biofilm thikness δ and β depends on inlet DMS concentration. The influence of the parameters α and β over DMS concentration in the biofilm phase $\overline{S}_{DMS}$ is shown in Fig. 2 and 3 respectively. In Fig. 2, the DMS concentration in the biofilm phase increases for various values of α and for some fixed values of β with time $\tau = 3$. In Fig. 3 it is inferred that the DMS concentration in biofilm phase increases when β decreases for some various values and for fixed value of α with time is fixed as 3. Fig. 4, shows the concentration of DMS in the gas phase $\overline{C}_{DMS}$ versus height $\overline{h}$ for various values of parameter γ, α and β is plotted. Here the value of $\overline{C}_{DMS}$ equal to 1 and the concentration of $\overline{C}_{DMS}$ increases with α. Also the $\overline{C}_{DMS}$ concentration is directly propotional to the parameter β whereas it is inversely propotionalto γ. Again the concentration of $\overline{C}_{DMS}$ increases with decrease in γ when α and β are small.

Conclusion

The system of time dependent nonlinear differential equations in bench-scale biofilter has been solved analytically in this paper. The model investigated the influence of parameters over the removal of DMS from the oxygen in the BTF reactor. Approximate analytical expressions pertaining to the concentration of DMS in the gas phase $\overline{C}_{DMS}$ and biofilm phase $\overline{S}_{DMS}$ for all values of the parameters α, β, γ, v are obtained using the new Homotopy Perturbation methods. The accurate expression of $\overline{C}_{DMS}$ also represented. This analytical result helps for the better understanding of the system. Our results are compared with the numerical simulations and it gives satisfactory agreement.

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Appendix A

Solution of equations (8) and (9) using complex inversion formula

In this appendix we indicate how equations (13) and (14) are derived. By solving a differential equation of second order with constant coefficients by using new Homotopy approach and also by applying Laplace transform in equations (8) and (9), and in conditions in equations (10 - 12) we obtained the solution of the equation (8) as

$$\bar{u} = \frac{\cosh\sqrt{s+A}(\bar{x}-1)}{s\cosh\sqrt{s+A}} \tag{A1}$$

In this appendix we indicate how equation (A1) may be inverted using the complex inversion formula. If $\bar{y}(s)$ represents the Laplace transform of a function $y(\tau)$, then according to the complex inversion formula we can state that

$$y(\tau) = \frac{1}{2\pi\int_{c-i\infty}^{c+i\infty}\exp[s\tau]\bar{y}(s)\,ds} = \frac{1}{2\pi i}\oint_c \exp[s\tau]\,\bar{y}(s)\,ds \tag{A2}$$

where the integration in equation (A2) is to be performed along a line $s = c$ in the complex plane where $s = x + iy$. The real number c is chosen such that $s = c$ lies to the right of all the singularities, but is otherwise assumed to be arbitrary. In practice, the integral is evaluated by considering the contour integral presented on the right-hand side of equation (A2), which is then evaluated using the so-called Bromwich contour. The contour integral is then evaluated using the residue theorem which states for any analytic function $F(z)$

$$\oint_c F(\bar{x})\,dz = 2\pi i\sum_n \operatorname{Re}s[F(\bar{x})]_{\bar{x}=\bar{x}0} \tag{A3}$$

where the residues are computed at the poles of the function $F(\bar{x})$. Hence from eq. (A3), we note that

$$y(\tau) = \sum_n \operatorname{Re}s[\exp[s\tau]\bar{y}(s)]_{s=s_0} \tag{A4}$$

From the theory of complex variables we can show that the residue of a function $F(\bar{x})$ at a simple pole at $\bar{x} = a$ is given by

$$\operatorname{Re}s[F(\bar{x})]_{\bar{x}=a} = \lim_{z\to a}\{(\bar{x}-a)F(\bar{x})\} \tag{A5}$$

Hence in order to invert equation (A1), we need to evaluate

$$\operatorname{Re}s\left[\frac{\cosh(\sqrt{s+A})(\bar{x}-1)}{s\cosh(\sqrt{s+A})}\right]$$

The poles are obtained from $s\cosh\sqrt{s+A}=0$. Hence there is a simple pole at $S=0$ and there are infinitely many poles given by the solution of the equation $\cosh\sqrt{s+A}=0$ and

So $s_n=\frac{-\pi^2(2n+1)^2-4A}{4}$ where n = 0,1,2,…….Hence we note that

$$u(X,\tau)=\operatorname{Re}s[s\cosh(\sqrt{s+A})]_{s=0}+\operatorname{Re}s[s\cosh(\sqrt{s+A})]_{s=s_n} \tag{A6}$$

The first residue in equation (A6) is given by

$$\operatorname{Re}s[s\cosh(\sqrt{s+A})]_{s=0}=\lim_{s\to 0}\left[\frac{\exp(s\tau)\cosh(\sqrt{s+A})(\bar{x}-1)}{s\cosh(\sqrt{s+A})}\right]=\frac{\cosh\sqrt{A}(\bar{x}-1)}{\cosh\sqrt{A}} \tag{A7}$$

The second residue in equation (A6) is given by

$$\operatorname{Re}s[s\cosh(\sqrt{s+A})]_{s=s_n}=\lim_{s\to s_n}\left[\frac{\exp(s\tau)\cosh(\sqrt{s+A})(\bar{x}-1)}{s\cosh(\sqrt{s+A})}\right]$$

$$=\lim_{s\to s_n}\left[\frac{\exp(s\tau)\cosh(\sqrt{s+A})(\bar{x}-1)}{s\frac{d}{ds}\cosh(\sqrt{s+A})}\right]$$

$$=-\sum_{n=0}^{\infty}\left[\frac{(-1)^n\pi(2n+1)e^{-f_n\tau}\cos\frac{(2n+1)\pi(\bar{x}-1)}{2}}{f_n}\right] \tag{A8}$$

Where f_n is defined in equation (14). Here we used $\cosh(i\theta)=\cos(\theta)$ and $\sinh(i\theta)=i\sin(\theta)$.From (A6), (A7) and (A8) we conclude that

$$u(\bar{x},\tau)=\frac{\cosh\sqrt{A}(\bar{x}-1)}{\cosh\sqrt{A}}-\sum_{n=0}^{\infty}\left[\frac{(-1)^n\pi(2n+1)e^{-f_n\tau}\cos\frac{(2n+1)\pi(\bar{x}-1)}{2}}{f_n}\right] \tag{A9}$$

Where f_n is defined as in equation (16). Similarly we can invert equation (9) by using complex inversion formula.

Appendix B. Numerical values of parameter used in this work and experimental (Giri *et al*., 2010)

Parameter	Description	Values
A_s	Surface area of biofilm (m^{-1})	526
D_e	Effective diffusion coefficient in the biofilm $(m^2\,h^{-1})$	1.74×10^{-6}
X	Over all population of microorganisms $(CFU\,g^{-1})$	83.515
K_s	Half saturation constant $(g\,m^{-3})$	0.0132
μ_{max}	Maximum specific growth rate of biomass (h^{-1})	0.012
H	Biofilter bed height (m)	0.55
δ	Biofilm thickness (m)	0.0001
m_{DMS}	Biofilm partition coefficient of DMS	0.84
U_g	Superficial gas velocity $(m\,h^{-1})$	0.018 - 0.791

Continue…..

Y	Yield coefficient of microorganisms (m^3)	1
h	Value of the Height which is calculated from the base of the packing materials (m)	-
x	Coordinate axis which is calculated from the surface of the biofilm (m)	-
S_{DMS}	DMS concentration in the biofilm phase $(g\,m^{-3})$	-
C_{DMS}	DMS concentration in the gas phase $(g\,m^{-3})$	-
α	Dimensionless parameter	0.4363
β	Dimensionless parameter	0.9090
γ	Dimensionless parameter	0.0018
$\bar{S}_{DMS}$	Dimensionless DMS concentration in the biofilm phase	0 to 1
$\bar{C}_{DMS}$	Dimensionless DMS concentration in the gas phase	0 to 1
$\bar{x}$	Dimensionless coordinate calculated from the surface of the biofilm	0 to 1
$\bar{h}$	Height calculated from the base of the packing material	0 to 1

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