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A New Approach of Solving the Nonlinear Equations in Biofiltration of Methane in a Closed Biofilter

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Abstract

In this paper, a new mathematical steady state model which describes the methane biofiltration process is discussed. The model involves the impact of various parameters, such as the inlet methane concentration, the gas superficial velocity and the packing bed average temperature, on the methane biofilter efficiency. Simple and an approximate expression of concentrations and elimination capacity are derived for general non-linear Monod kinetics models. The analytical results are compared with the numerical results and are found to be in good agreement. This analytical result helps as to estimate the overall biofilter efficiency in terms of the conversion, elimination capacity and carbon dioxide production.

Keywords: New homotopy perturbation method; Mathematical modeling; Nonlinear equations; Biofiltration; Methane; Carbon dioxide

Nomenclature: *A*: Specific surface of the packing material (m^2/m^3); C_P: Concentration of *P* within the gas phase (g/m^3); *D*: Biofilter inlet diameter (m); D_P: Diffusion coefficient of *P* in the biofilm (m^2/s); *EC*: Elimination Capacity ($g/m^3/h$); *H*: Height of the packing material within the biofilter (m); H_P: Henry coefficient of *P* (dimensionless); S_{CH_4}: Concentration of methane in the biofilm phase; S_{CO_2}: Concentration of carbon dioxide in the biofilm phase; C_{CH_4}: Concentration of methane in the gas phase; C_{CO_2}: Concentration of carbon dioxide in the gas phase; D_{CH_4}: Diffusion coefficient of methane in the biofilm; D_{CO_2}: Diffusion coefficient of carbon dioxide in the biofilm; *IL*: Inlet Load ($g/m^3/h$) in inlet flow; *k*(*T*): Maximum substrate utilisation rate at a *T* Temperature (1/s); K_m: Monod Constant (g/m^3) out outlet flow; *P*: CH_4 or CO_2; P_{endo}: Endogenous Production of CO_2 ($g/m^3/h$); P_{CO2}: CO_2 Production ($g/m^3/h$); *Q*: Gas Flow Rate (m^3/h); *r*: CH_4 Consumption rate (g/m^3 (filter bed)/s); S_P: Concentration of *P* within the Biofilm (g/m^3); *T*: Time (s); *T*: Temperature (°C); u_g: Gas Superficial velocity within the Biofilter ($m^3/m^2/s$); *V*: Biofilter Bed Volume (m^3); *x*: Depth coordinate in the Biofilm (m); X_b: Density of Biomass in the Biofilm (g/m^3); *X*: Conversion (%); *Y*: Biomass Yield Coefficient (g biomass/gCH_4); *z*: Biofilter Height Coordinate (m).

Greek symbols

α_{CO_2/CH_4}: Yield of CO_2 (g gaseous CO_2 produced/gCH_4 consumed); δ: Biofilm thickness (m); ε: Filter bed porosity (dimensionless); *μ*: Specific growth rate of the microorganisms within the biofilm (1/s); μ_m: Maximum specific growth rate of microorganisms within the biofilm (1/s); σ: CH_4 Consumption rate (g/m^3 (filter bed)/s); *θ*: Temperature Coefficient (dimensionless).

Introduction

A methane is assimilated by the methanotrophs: these bacteria use the methane as their sole and unique carbon source to satisfy their metabolic needs. In addition to the methanotrophic population, the availability of nutrients (mainly as nitrogen and phosphorus elements) and supportive operating conditions, such as the moisture of the packing material, the gas superficial velocity and the inlet CH_4 concentration, are all to be accounted for among the factors needing to be closely controlled for operating a successful bioprocess. During the past 3 decades, several mathematical models dealing with the biofiltration of pollutants, such as volatile organic or inorganic compounds, have been developed in order to predict the efficiency of the bioprocess and the behaviour of the pollutants, and products. In general, models take into account physical, chemical and biological phenomena occurring in biofilteration such as diffusion, mass transfer of the pollutants and biodegradation kinetics, which have been described in detail in the review conducted by Devinny and Ramesh [1].

Mohseni and Allen [2] have reported that the constituents of the biofilm have a significant impact on the solubility of the hydrophobic substrates in the biofilm. In their view, air/biofilm distribution coefficient, which accounts for the lipophilic characteristics of the biofilm, should be used, instead of the usual air/water distribution coefficient, for modeling the biofiltration of hydrophobic VOCs. Important parameters, mathematical modeling of biofilters looks quite challenging. Kiranmai et al. [3] have applied the differential evolution method for determining the biokinetics in their fixed-film reactor modeling problem.

Among these researches, the direct route that converts methane into high hydrocarbons in one step by the oxidative coupling reactions is more economically attractive and consequentially has been thoroughly studied [4,5]. The mathematical modeling of catalyst pellet in OCM process which is considered the heart of catalytic fixed bed reactor is the most important model used in describing the behavior of fixed bed reactor [6-17].

Many important physical phenomena on the engineering and science fields are frequently modeled by nonlinear differential equations.

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Such equations are often difficult or impossible to solve analytically. Nevertheless, analytical approximate methods to obtain approximate solutions have gained importance in recent years [18]. There are several methods employed to find approximate solutions to nonlinear problems like homotopy perturbation method (HPM) [19,20], homotopy analysis method (HAM) [21,22], Adomian decomposition method (ADM) [23,24] and Picard's iterative method [25,26] etc. Recently, Rajendran et al. solved the nonlinear differential equations in biosensor and biofuel cells using various analytical method [27-33].

However, to the best of our knowledge, till date there was no rigorous analytical expression of the concentrations for methane and carbon dioxide in a closed biofilter for all possible values of reaction-diffusion parameters have been reported [17]. The purpose of this communication is to derive approximate analytical expressions for the concentrations methane and carbon dioxide for all possible values of parameters using new approach of homotopy perturbation method.

Mathematical Formulation of the Boundary Value Problem

The general assumption of the mathematical models for methane bioelimination involving the closed biofilter is described [17]. Figure 1 denotes the phenomena occurring within the biofilter and considered in the present model. It contains the two components CH_4 and CO_2 through the gas phase and biofilm phase. During steady state operations, there is no accumulation of the pollutant, of the by-products or of the products within the biofilter. The general mass balances within the gas phase involve essentially three terms: an accumulation term, a convection term, and a mass exchange term through the interface of the gas phase with the biofilm. Within the biofilm phase, CH_4 becomes biodegraded, forming CO_2 among others. The mass balances equation of CH_4 and CO_2 gives as follows [17]:

$$D_{CH_4}\frac{d^2S_{CH_4}}{dx^2}-\sigma\left(S_{CH_4},T\right)=0, \tag{1}$$

$$D_{co2}\frac{d^2S_{co_2}}{dx^2}-\sigma\left(S_{CH_4},T\right)=0, \tag{2}$$

The boundary conditions are:

$$S_{CH_4}(0,z)=\frac{C_{CH_4}(z)}{H_{CH_4}(T)},\ \frac{dS_{CH_4}(\delta,z)}{dx}=0 \text{ for } 0<x<\delta, 0<z\le H \tag{3}$$

$$S_{co_2}(0,z)=\frac{C_{co_2}(z)}{H_{co_2}(T)},\ \frac{dS_{co_2}(\delta,z)}{dx}=0 \text{ for } 0<x<\delta, 0<z\le H \tag{4}$$

Where,

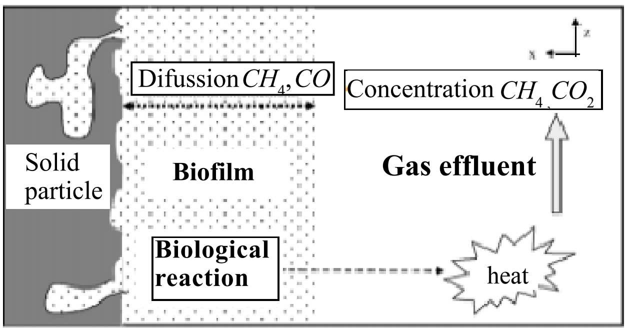

Figure 1: Schematic diagram for biofilter.

$$\sigma\left(S_{CH_4},T\right)=\frac{X_b\,k(T)S_{CH_4}}{K_m+S_{CH_4}};H_{CH_4}(T)=\left[4.559(T+273.15)\times10^{(675.74/(T+273.15)-6.880)}\right]^{-1}$$

$$H_{CO_2}(T)=\left[4.559(T+273.15)\times10^{(1012.40/(T+273.15)-6.606)}\right]^{-1};K(T)=1.464\times10^{-5}\times1.104^{T-20} \tag{5}$$

where S_{CH4} and S_{CO2} represents the concentration of methane and carbon dioxide in the biofilm phase. X_b and K_m represents density of biomass in the biofilm and Monod constant. *H(T)* depends on the temperature *T* in °C, *K(T)* is the temperature dependent maximum substrate utilization rate and σ is the consumption rate of CH_4. The concentrations CH_4 and CO_2 within the gas phase described by the following equation:

$$-u_g\frac{dC_{CH_4}}{dz}+D_{CH_4}\,A\left(\frac{dS_{CH_4}}{dx}\right)_{x=0}=0,\quad 0<z\le H \tag{6}$$

$$-u_g\frac{dC_{CO_2}}{dz}+D_{CO_2}\,A\left(\frac{dS_{CO_2}}{dx}\right)_{x=0}=0,\quad 0<z\le H, \tag{7}$$

The initial conditions for the Eqn. (6) and (7) are:

$$C_{CH_4}(z=0)=C_{CH_4,in} \tag{8}$$

$$C_{CO_2}(z=0)=C_{CO_2,in} \tag{9}$$

where C_{CH_4} and C_{CO_2} represents the concentration of methane and carbon dioxide in the gas phase. D_{CH_4} and D_{CO_2} represents the diffusion coefficient of methane and carbon dioxide in the biofilm respectively. u_g and *A* represents the gas superficial velocity within the biofilter and specific surface of the packing material. The elimination capacity (EC) is:

$$EC=IL\,\frac{X}{100} \tag{10}$$

Where,

$$IL=\frac{Q}{V}C_{CH_{4,in}}\ \text{ and }\ X=\frac{C_{(CH_4),in}-C_{(CH_4),out}}{C_{(CH_4),in}}\times100 \tag{11}$$

Analytical Expression of the Concentration of *CH_4* and CO_2 in the Biofilm and Gas Phase Using New Homotopy Perturbation Approach

In recent days, new homotopy perturbation approach is often employed to solve several nonlinear problems in physics, chemistry and biochemical engineering. Furthermore, new homotopy perturbation approach is a simple, accurate and efficient method. The analytical solution of nonlinear equation is of great importance due to its wide application in scientific research. The new homotopy perturbation approach [34,35] is used to obtain the approximate analytical solution of non-linear reaction/diffusion Eqns. (1-2). Using the new homotopy perturbation approach (Appendix A), we can obtain the of the concentrations for methane and carbon dioxide in a closed biofilter as follows:

$$S_{CH_4}(z,x)=\frac{\dfrac{C_{CH_4}(z)}{H_{CH_4}(T)}\cosh\sqrt{\dfrac{X_bk(T)}{K_m+\dfrac{C_{CH_4}(z)}{H_{CH_4}(T)}}}(x-\delta)}{\cosh\sqrt{\dfrac{X_bk(T)}{K_m+\dfrac{C_{CH_4}(z)}{H_{CH_4}(T)}}}\,\delta} \tag{12}$$

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$$S_{CO_2}(z,x) = -B(z)x^2 + 2\delta B(z)x + \frac{C_{CO_2}(z)}{H_{CO_2}(T)} \quad (13)$$

where
$$B(z) = \frac{-\alpha_{CO_2/CH_4} X_b k(T) \frac{C_{CH_4}(z)}{H_{CH_4}(T)}}{D_{CO_2}\left(K_m + \frac{C_{CH_4}(z)}{H_{CH_4}(T)}\right)} \quad (14)$$

Also solving Eqns. (6-7) and (8-9) using the analytical method, we can obtain the concentration of CH_4 and CO_2 in the gas phase are as follows:

$$C_{CH_4}(z) = C_{CH_{4,in}} - \exp\left(\frac{-A\sqrt{D_{CH_4}}\, P \tanh P\delta}{u_g\; H(T)} z\right) \quad (15)$$

$$C_{CO_2}(z) = C_{CO_2,in} + \frac{2\, D_{CO_2}\, A\, \delta}{u_g} \frac{\alpha_{CO_2/CH_4} X_b k(T) \frac{C_{CH_4}(z)}{H_{CH_4}(T)}}{D_{CO_2}\left(K_m + \frac{C_{CH_4}(z)}{H_{CH_4}(T)}\right)} z \quad (16)$$

where
$$P = \sqrt{\frac{X_b k(T)}{K_m + \frac{C_{CH_4,in}}{H_{CH_4}(T)}}} \quad (17)$$

Using the Eqns. (10), (11), and (16) we can also obtain the elimination capacity.

Discussion

Equations (12) and (13) are the new and simple approximate analytical expressions of the concentrations of the methane and carbon dioxide in biofilm base calculated using homotopy perturbation method. The concentration profiles of methane versus height coordinate are expressed in Figures 2a-2c. From these Figures, it is inferred that the value of the concentration decreases when A and δ increase. The concentration of methane is increases when Monod constant K_m is increases. The concentration profiles of carbon dioxide versus height coordinate are expressed in Figures 3a-3c. From these figures, it is observed that the value of the concentration of carbon dioxide decreases when K_m increase. The concentration of carbon dioxide is increases when A and δ is increases (Table 1).

Equations (15) and (16) are represent the new and simple approximate analytical expressions of the concentrations of the methane and carbon dioxide in gas base. The concentration profiles of methane versus height coordinate are expressed in Figures 4a-4c. From these Figures, it is inferred that the value of the concentration of methane decreases when A and δ increase or Monod constant K_m is decreases. Also, the concentrations of the methane in gas phase decreases slowly from its initial value for all values of parameters due to biodegradation of methane in gas phase.

The concentration profiles of carbon dioxide versus height coordinate is represented in Figures 5a-5c. From these figures, it is observed that the value of the concentration of carbon dioxide increases

Parameters	Values
A	2750 m²/m³
D	0.015 m
D_{CH4}	1.49 × 10⁻⁹ m²/s
D_{CO2}	1.96 × 10⁻⁹ m²/s
K_m	5.37 g/m³
Pendo	7 g/m³/h
V	0.0177 m³
X_b	100,000 g/m³
Y	0.34 g biomass/g CH_4
H	1 m
CO_2/CH_4	2.01 g CO_2/g CH_4
ε	0.40
δ	85 × 10⁻⁶ m
μ_m	4.98 × 10⁻⁶ S⁻¹
θ	1.104

Table 1: Numerical value of parameters used in this work.

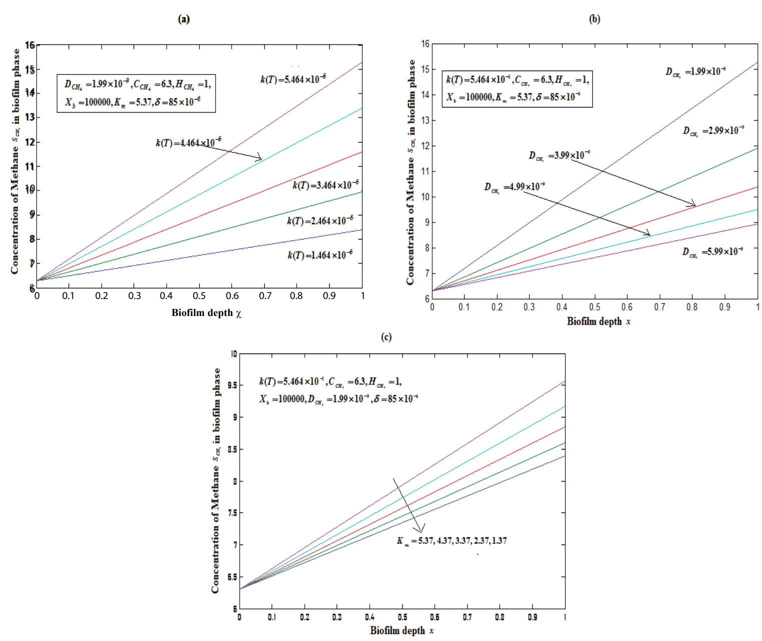

Figure 2: a-c. Concentrations of methane in biofilm phase versus coordinate of biofilm depth for different values of the parameters using Eqn.(12).

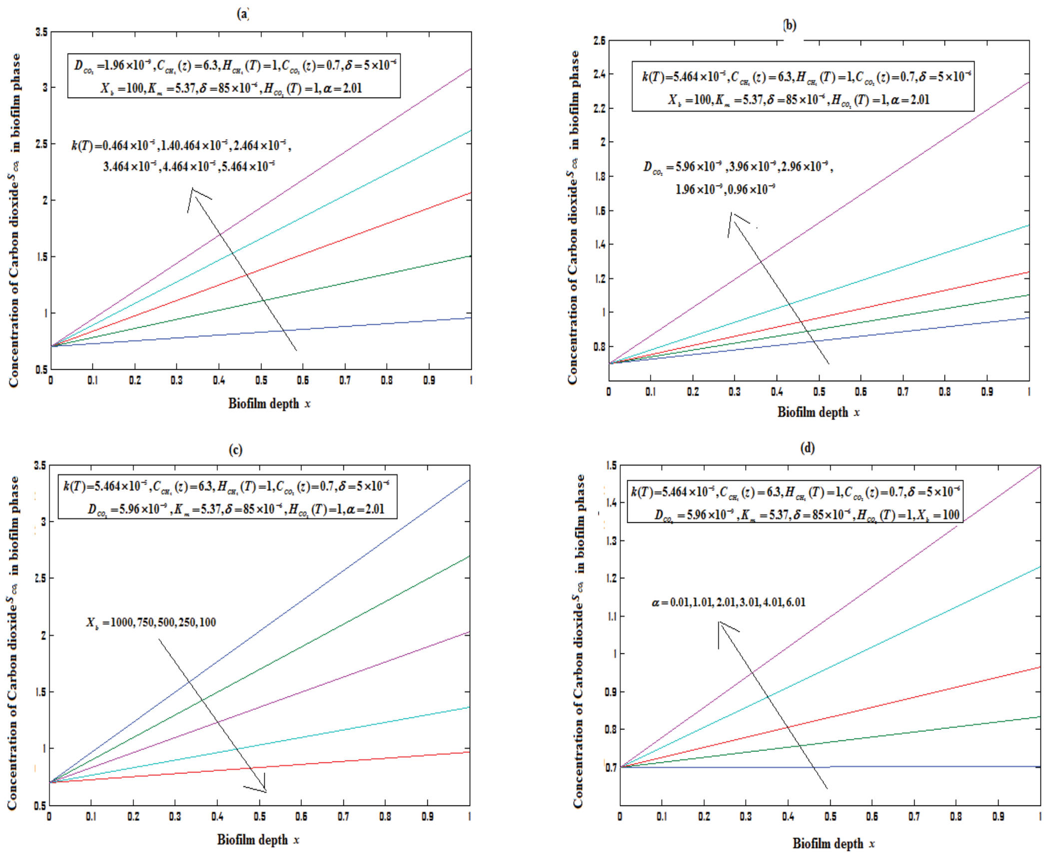

Figure 3: a-d. Concentrations of the Carbon dioxide in biofilm phase versus coordinate of biofilm depth for different values of the parameters using Eqn.(13).

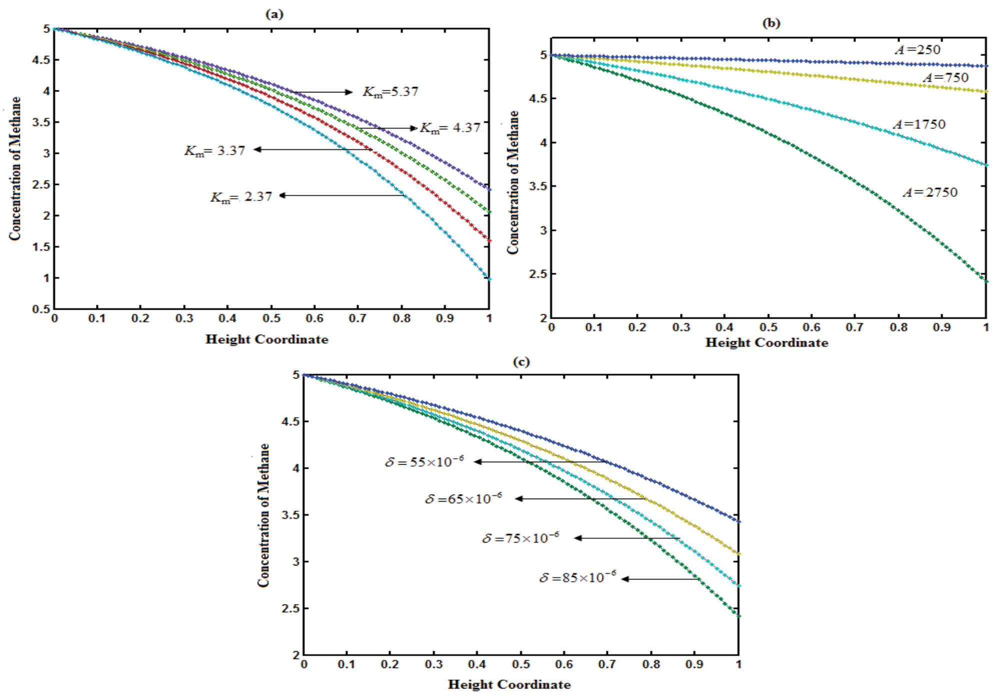

Figure 4: a-c. Concentrations of the Methane in gas phase methane versus coordinate of height for different values of the parameters using Eqn. (15).

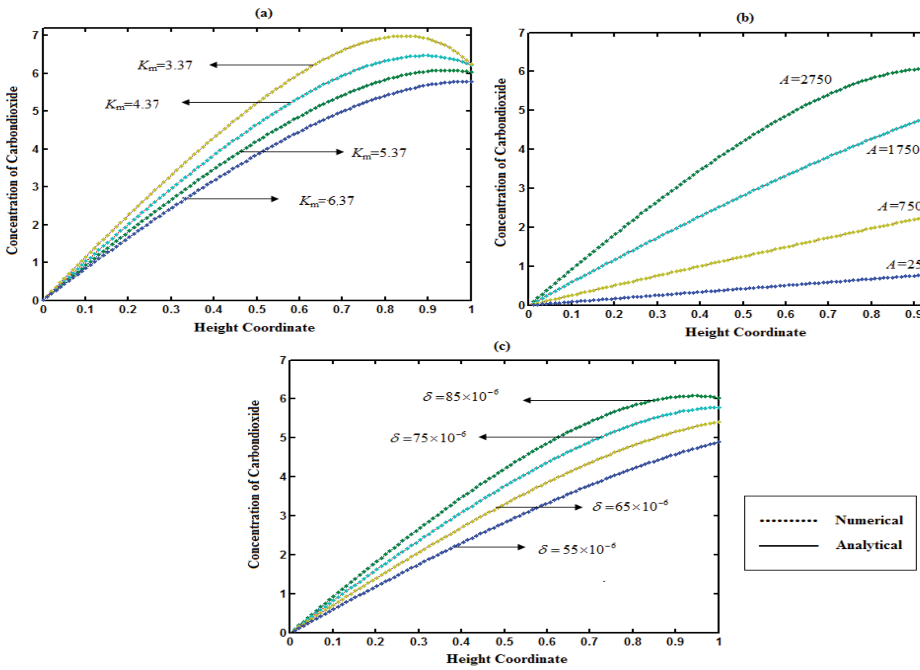

Figure 5: a-c. Concentrations of the Carbon dioxide versus coordinate of height for different values of the parameters using Eqn. (16).

when *A* and δ is increases or *K* decreases. The concentration of carbon dioxide is always increases due to production of carbon dioxide in gas phase. Our analytical results for the concentration of methane and carbon dioxide in gas phase is compared with simulation results (Matlab). Satisfactory agreement is noted.

Conclusions

In this paper, steady-state of solutions of a nonlinear reaction equations arising in elimination of methane has been studied. The theoretical model of biofilms Monod-type inhibition kinetics for the steady state condition is discussed. The nonlinear differential equation for methane and carbon dioxide has been solved analytically using the new homotopy perturbation method. The obtained results have a good agreement with those obtained using numerical methods. Theoretical results obtained in this paper can also be used to predict the response of biofilms.

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