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Transport and Kinetics in Biofiltration Membranes: New Analytical Expressions for Concentration Profiles of Hydrophilic and Hydrophobic VOCs Using Taylor's Series and Akbari- Ganji methods.

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The mathematical models of biofiltration of mixtures of hydrophilic (methanol) and hydrophobic ($\alpha -$ $\alpha -$pinene) volatile organic compounds (VOCs) are explored in this paper. This model is based on diffusion equations that contain a nonlinear term linked to the enzymatic reaction's Michaelis-Menten kinetics. An approximate analytical expression of methanol and $\alpha -$pinene concentration profiles in the air and biofilm phase were derived using Taylor's series and Akbari-Ganji's methods. In addition, the numerical simulation of the problem using the Matlab programme to investigate the system's dynamics is reported in this work. Graphic results are presented to illustrate the solution, and numerical data is analyzed. The analytical and numerical data are in good agreement.

Keywords: Methanol; Biofilters; VOC's; Mathematical modeling; Non-linear differential equations; Taylor's series method; Akbari Ganji's method

1. INTRODUCTION

Several technologies for cleaning gaseous effluent have been developed. Biological methods are increasingly being used to treat air pollution caused by various types of contaminants. Biofiltration is without a doubt the most widely used natural gas treatment technology. Microorganisms immobilised in biofilm over a porous substrate such as peat, soil, compost, synthetic substances, or a mixture are used in biofiltration. In terms of oxygen, temperature, moisture, nutrients, and pH, the medium provides a hospitable habitat for microorganisms. As the polluted airstream travels through the filter bed, pollutants are transported from the vapour phase to the biofilm that forms on the packing particles [1,2].

VOC emissions into the atmosphere have been discussed by Li et al. [3] and other research groups [4-10]. As a result, biological control processes are now a well-established technology for air pollution control. This method has many improvement over existing methods, including fewer operating costs and less secondary pollution, which is true in some cases for removing rapidly biodegradable VOCs at low concentrations. As a result, these systems have attracted significant research and are widely disseminated. Bioreactors for VOC removal are classified as biofilters, bioscrubbers, biotrickling filters, and rotating drum biofilters, with reactors were chosen based on various factors, including the properties of the target VOCs [11-4].

Biofilters are used instead of the chemical complex absorption technique to control the emission of volatile organic chemicals such as methanol and $\alpha-$ pinene from industries [15-20]. Although there are various efficient numerical techniques for solving nonlinear equations, the ultimate goal of analyzing the effect of various parameters on the governing system remains to get approximate analytical solutions. Furthermore, numerical solutions have a few significant limitations, such as achieving numerical stabilities and the difficulty of changing parameters to match the numerical data [21]. The homotopy perturbation method [22, 23], homotopy analysis method [24], variational iteration method [25], Akbari-method Ganji's [26], Green's function method [27], Adomian decomposition method [28], and Taylor series method [29] are among the most commonly used analytical methods.

Recent uses of the Taylor series method (TSM) and the Akbari-method Ganji's (AGM) for solving nonlinear models in multiple sciences and engineering domains have proven effective and accurate. They are generally available for study with a basic knowledge of mathematics. TSM has been used to solve the fractal Bratu equation [30], Lane–Emden equation [31], the nonlinear reaction-diffusion equation in the electroactive polymer film [32],porous catalysts particle of arbitrary shape [33], mass transfer processes [34], electroanalytical chemistry [35], electrostatic interaction [36], and Poisson–Boltzmann equation [36]. The Akbari-Ganji method (AGM) has also been used to derive semi-analytic solutions to nonlinear equations. Berkan [25], for example, investigated the steady three-dimensional problem of condensation film on an inclined rotating surface that used AGM. Nirmala et al. [35] estimated the steady-state substrate and product concentrations for non-Michaelis-Menten kinetics in an amperometric biosensor through using the hyperbolic function technique, a subset of the Akbari-Ganji method. AGM was applied by Manimegalai et al. [37] to generate approximate analytical solutions to nonlinear equations describing diffusion-limited reactions within the film. Dharmalingam et al. [38] used AGM to solve nonlinear reaction-diffusion equations governing substrate concentration in electroactive polymer films. More AGM method applications can be found in [39,40].

In this paper, we use both the Taylor series and the Akbari-Ganji methods to obtain of methanol and $\alpha-$ pinene concentration profiles in the air stream and bio-film phase. This paper presents a numerical simulation of the problem using the Matlab tool. To illustrate the method, graphical and quantitative data are provided. The analytical and numerical data are in good agreement for small Thiele modulus values and all values of other parameters.

2. MATHEMATICAL FORMULATION OF THE BOUNDARY VALUE PROBLEM

The biophysical model proposed by Madjid Mohseni et al., and Meena et al.[15-17] served as the foundation for the mathematical model about the biofiltration of hydrophilic and hydrophobic VOCs. It consists of two major diffusion processes of the compound's methanol and α – pinene via the biofilm, as well as their decay in the biofilm. Figure 1 shows a single particle in a biofilter covered in a homogeneous coating of biofilm. Methanol and α – pinene are both biodegrading at the same time.

The governing equations for removing mixed VOCs (methanol and α – pinene) in biofilters are based on the following assumptions: (i) There are no radial concentration gradients throughout the biofilter, and the airflow is modelled as a plug flow. (ii) Biofilm forms on the particle's outer surface. Biodegradation does not occur in the inner pores of the particles because microorganisms do not exist there. (iii) Because the biofilm evenly covers the packing media and has a minimal thickness compared to the particle size, a rectangular shape may be employed. (iv) The only substrates that impact the biodegradation rate are methanol and α – pinene.

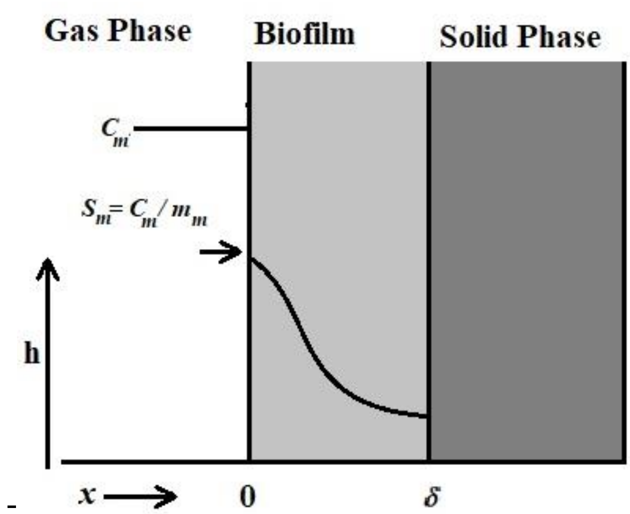

Figure 1. Biophysical model for the biofilm structure based on biofilter packing materials and concentration profiles across the biofilm [15-17].

2.1. Mass balance in the biofilm phase

The removal of methanol and α – pinene in the biofilm at steady-state is described by the following system of non-linear differential equations [15-17]:

$$D_{em}\frac{d^2S_m}{dx^2} = \frac{X}{Y_m}\frac{\mu_{\max(m)}\ S_m}{K_m+S_m} \quad (1)$$

$$D_{ep}\frac{d^2S_p}{dx^2} = \frac{X}{Y_p}\frac{\mu_{\max(p)}\ S_p}{K_p+S_p} \quad (2)$$

where S_m and S_p represent the concentration of methanol and α –pinene respectively. Here μ_{max}, K, Y, D and x are maximum specific growth rate, half saturation constant, yield coefficient, effective diffusion coefficient and the distance from one end of the gas phase respectively. Subscripts m and p represent methanol and $\alpha -$ pinene respectively. The dry cell density in the biofilm X represents the overall population of microorganisms that consist of methanol and $\alpha -$ pinene degraders. The boundary conditions are

$$S_m = \frac{C_m}{m_m} = S_{im} \text{ and } S_p = \frac{C_p}{m_p} = S_{ip} \text{ at } x = 0 \quad (3)$$

$$\frac{dS_m}{dx} = \frac{dS_p}{dx} = 0 \text{ at } x = \delta \quad (4)$$

The concentration of methanol and $\alpha -$pinene in the interphase of gas phase and biofilm phase are S_{im} and S_{ip}. The concentration gradient of methanol and $\alpha -$ pinene in biofilm and solid phase are zero which is represented by the boundary conditions Eq. (4). Here δ denotes the biofilm thickness.

2.2 Mass balance in gas phase

The concentrations of methanol and $\alpha -$ pinene in the air, along the biofilter column are described by

$$U_g \frac{dC_m}{dh} = A_s D_{em} \left[\frac{dS_m}{dx}\right]_{x=0} \quad (5)$$

$$U_g \frac{dC_p}{dh} = A_s D_{ep} \left[\frac{dS_p}{dx}\right]_{x=0} \quad (6)$$

where C_m and C_p represents the concentration of methanol and $\alpha -$pinene in the air phase. Here U_g, A_s, D_{em}, D_{ep} and h are the superficial gas velocity, biofilm surface area, effective diffusivity of methanol, effective diffusivity of $\alpha -$pinene and position along the height of the biofilters respectively. The corresponding initial conditions are

$$C_m = C_{im} \text{ and } C_p = C_{ip} \text{ at } h = 0 \quad (7)$$

where the subscript i represent the concentration of the VOCs at the biofilters inlet.

2.3 Dimensionless mass balance equation in the biofilm phase

The dimensionless mass balance equation in the biofilm phase with corresponding boundary conditions and dimensionless variables are given in the Table A.

Table A. Mass balance equation and corresponding boundary conditions with dimensionless variables in the biofilm phase

Mass balance equation	Boundary conditions	Dimensionless variables
$\frac{d^2u}{dy^2} = \varphi\left(\frac{u}{1+\beta u}\right)$ $\frac{d^2v}{dy^2} = \alpha\varphi_1\left(\frac{v}{1+\beta_1 v}\right)$	$u = 1, v = 1$ at $y = 0$ $\frac{du}{dy} = \frac{dv}{dy} = 0$ at $y = 1$	$\beta = \frac{S_{im}}{K_m}, \varphi = \frac{X\,\mu_{\max(m)}}{Y_m}\frac{\delta^2}{D_{em}K_m}, y = \frac{x}{\delta}, u = \frac{S_m}{S_{im}}$ $\beta_1 = \frac{S_{ip}}{K_p},$ $\varphi_1 = \frac{X\,\mu_{\max(p)}}{Y_p}\frac{\delta^2}{D_{ep}K_p}, v = \frac{S_p}{S_{ip}}$

2.4 Dimensionless mass balance equation in the gas phase

The dimensionless mass balance equation in the gas phase with corresponding boundary conditions and dimensionless variables are given in the Table-B.

Table B. Mass balance equation and corresponding boundary conditions with dimensionless variables in the gas phase.

Mass balance equation	Boundary conditions	Dimensionless variables
$\frac{da}{dz} = \gamma\left(\frac{du}{dy}\right)_{y=0}$ $\frac{db}{dz} = \alpha\gamma_1\left(\frac{dv}{dy}\right)_{y=0}$	$a = 1$ and $b = 1$ at $z = 0$	$\gamma = \frac{H\,A_s\,D_{em}\,S_{im}}{U_g\,\delta\,C_{im}}, \gamma_1 = \frac{H\,A_s\,D_{ep}\,S_{ip}}{U_g\,\delta\,C_{ip}},$ $z = \frac{h}{H}, a = \frac{C_m}{C_{im}}, b = \frac{C_p}{C_{ip}}$

3. ANALYTICAL EXPRESSION FOR THE CONCENTRATION OF METHANOL AND α −PINENE IN BIOFILM PHASE USING THE TAYLOR'S SERIES METHOD (TSM)

TSM is used in this part to solve the nonlinear boundary value problems (3) - (4). TSM [27-34] provides a semi-analytical solution in the form of a fast converging series that does not involve linearization. The analytical expression for the concentration of methanol and $\alpha -$ pinene using the TSM is obtained as follows (Appendix 1):

$$u(y) = \sum_{i=0}^{\infty} \frac{d^i u}{dy^i}\frac{(y-1)^i}{i!}\bigg|_{y=1} = u(1) + \frac{(y-1)}{1!}\frac{du}{dy}\bigg|_{y=1} + \frac{(y-1)^2}{2!}\frac{d^2u}{dy^2}\bigg|_{y=1} + \frac{(y-1)^3}{3!}\frac{d^3u}{dy^3}\bigg|_{y=1} \tag{8}$$

$$= u(1) + u_1(1)(y-1)^2 + u_2(1)(y-1)^3 + u_3(1)(y-1)^4$$

$$v(y) = \sum_{i=0}^{\infty} \frac{d^i v}{dy^i}\frac{(y-1)^i}{i!}\bigg|_{y=1} = \left(v(1) + \frac{(y-1)}{1!}\frac{dv}{dy}\bigg|_{y=1} + \frac{(y-1)^2}{2!}\frac{d^2v}{dy^2}\bigg|_{y=1} + \frac{(y-1)^3}{3!}\frac{d^3v}{dy^3}\bigg|_{y=1} + ..\right) \tag{9}$$

$$= \alpha(v(1) + v_1(1)(y-1)^2 + v_2(1)(y-1)^3 + v_3(1)(y-1)^4)$$

where

$$u_1(1) = \frac{\varphi\,u(1)}{(1+\beta\,u(1))}\frac{1}{2!},\; u_2(1) = \frac{\varphi^2\,u(1)}{(1+\beta\,u(1))^3}\frac{1}{4!},\; u_3(1) = \frac{\varphi^3\,u(1)\,(1+\beta\,u(1)-7\,u(1))}{(1+\beta\,u(1))^5}\frac{1}{6!} \tag{10}$$

$$v_1(1) = \frac{\alpha\varphi_1\,v(1)}{(1+\beta_1\,v(1))}\frac{1}{2!},\; v_2(1) = \frac{(\alpha\varphi_1)^2\,v(1)}{(1+\beta_1\,v(1))^3}\frac{1}{4!},\; v_3(1) = \frac{(\alpha\varphi_1)^3\,v(1)\,(1+\beta_1\,v(1)-7\,v(1))}{(1+\beta_1\,v(1))^5}\frac{1}{6!} \tag{11}$$

where $u(1)$ and $v(1)$ satisfies the following relation

$$1 = u(1) + u_1(1) - u_2(1) + u_3(1) \tag{12}$$

$$1 = \alpha(v(1) + v_1(1) - v_2(1) + v_3(1)\;) \tag{13}$$

The above equation can obtain using the boundary condition in Table A.

3.1. Analytical expression for the concentration of methanol and α −pinene in air phase using the Taylor's series method (TSM)

The mathematical expression for methanol and α -pinene concentrations using the TSM is as follows:

$$a(z) = \int_0^z \gamma\left(\frac{du}{dy}\right)_{y=0} dz = 1 + \gamma\left(\frac{\varphi\,u(1)}{(1+\beta\,u(1))} + \frac{\varphi^2\,u(1)}{(1+\beta\,u(1))^3}\frac{1}{6} + \frac{\varphi^3\,u(1)\,(1+\beta\,u(1)-7\,u(1))}{(1+\beta\,u(1))^5}\frac{1}{120}\right)z \tag{14}$$

$$b(z) = \int_0^z \alpha\gamma_1\left(\frac{dv}{dy}\right)_{y=0} dz = 1 + \alpha\gamma_1\left(\frac{\alpha\varphi_1\,v(1)}{(1+\beta_1\,v(1))} + \frac{(\alpha\varphi_1)^2\,v(1)}{(1+\beta_1\,v(1))^3}\frac{1}{6} + \frac{(\alpha\varphi_1)^3\,v(1)\,(1+\beta_1\,v(1)-7\,v(1))}{(1+\beta_1\,v(1))^5}\frac{1}{120}\right)z \tag{15}$$

4. ANALYTICAL EXPRESSION OF CONCENTRATIONS IN BIOFILM PHASE USING THE AKBARI-GANJI'S METHOD

As stated in the introduction, Akbari- Ganji's method [35-39] is a powerful algebraic approach that yields semi-analytic approximation solutions to nonlinear differential equations. The method does not require linearization and provides solutions in the form of convergent series. Therefore, a derived analytical expression of the concentration is given by

$$u(y) = \cosh(my) - \tanh m \sinh(m\, y). \tag{16}$$

$$v(y) = \alpha \cosh(ny) - \tanh n \sinh(n\, y). \tag{17}$$

$$\text{where} \quad m = \sqrt{\varphi\left(\frac{1}{(1+\beta)}\right)} \quad \text{and} \quad n = \sqrt{\alpha\varphi_1\left(\frac{1}{(1+\beta_1)}\right)} \tag{18}$$

4.1. Analytical expression of concentrations of mass balance in the gas phase using the Akbari-Ganji's method

The analytical expression for the concentration of methanol and $\alpha -$ pinene in gas phase using the eqns. (16) and (17) is obtained as follows:

$$\frac{da}{dz} = \gamma\left(\frac{du}{dy}\right)_{y=0} = \gamma(-m \sinh m\,) \tag{19}$$

$$a(z) = \int \gamma\left(\frac{du}{dy}\right)_{y=0} = 1 + \gamma(-m \sinh m\,)z \tag{20}$$

$$\frac{db}{dz} = \alpha\gamma_1\left(\frac{dv}{dy}\right)_{y=0} = \alpha\gamma_1(-n \sinh n\,) \tag{21}$$

$$b(z) = \int \alpha\gamma_1\left(\frac{dv}{dy}\right)_{y=0} = 1 + \alpha\gamma_1(-n \sinh n\,)z \tag{22}$$

5. RESULT AND DISCUSSION

The nonlinear Eqs. (1)- (7) are solved using two simple, efficient, and reliable analytical approaches: The Taylor series and the Akbari-Ganji methods. Semi-analytical approximate concentrations were obtained for all values of parameters.

5.1 Validation of analytical methods.

To assess the accuracy of the TSM and AGM solutions with a finite number of terms, the system of differential equations was numerically solved. Our analytical data are graphically compared with numerical results to demonstrate the efficacy of the present method. The analytical solution of the concentrations of methanol and α-pinene in air phase and biofilm phase are compared with simulation results in Figs. 3–4 and Tables 1 and 4. Figures 3 and 4 show that there is a strong agreement between the TSM and numerical results for small Thiele modulus values ($\varphi_1 \leq 1$ *and* $\varphi \leq 1$) and all values of other parameters.

5.2 *Previous result*

Recently Meena and Co-workers [15,17] obtain the analytical expression concentration of methanol and α- pinene in the biofilm phase using ADM as follows:

$$u(y) = 1 + \frac{\varphi}{(1+\beta)}\left(\frac{y^2}{2} - y\right) \tag{23}$$

$$v(y) = 1 + \frac{\alpha\varphi_1}{(1+\beta_1)}\left(\frac{y^2}{2} - y\right) \tag{24}$$

Similarly, Meena and colleagues used ADM to determine the concentrations of methanol and -pinene in the air phase [15, 17].

$$a(z) = 1 - \frac{A\ \varphi}{(1+\beta)} z \tag{25}$$

$$b(z) = 1 - \frac{\alpha A_1 \varphi_1}{(1+\beta_1)} z \tag{26}$$

The analytical expression of the concentrations of methanol and α-pinene in the biofilm phase are compared with simulation results and previously available ADM results in Tables 5 and 6. The average error percentage in TSM and AGM is significantly less than in the ADM method.

Compared to TSM and AGM methods, the series in the ADM method does not converge quickly for the significant value of parameters. The Taylor series method yields a rapidly convergent, easily computable, and readily verifiable sequence of analytic approximations convenient for parametric simulations. The process of solving nonlinear equation(s) using TSM and AGM will be straightforward and convenient compared to the other methods.

5.3 Effect the parameter on the concentrations

Eqs. (19–22) represent the simple and new analytical expression of the concentrations of methanol and α-pinene in biofilm phase and in the air phase respectively. The concentrations of methanol and α-pinene in the biofilm and air phases depend on the parameters φ and β.

Eqs. (19–22) give a simple and innovative analytical expression of methanol and α-pinene concentrations in the biofilm and air phases, respectively. Methanol and α-pinene concentrations in the biofilm and air phases are affected by the parameters φ and β. The Thiele modulus φ can be varied by altering the biofilm thickness or dry cell density. The parameter β is affected by the initial concentration as well as the half-saturation constant.

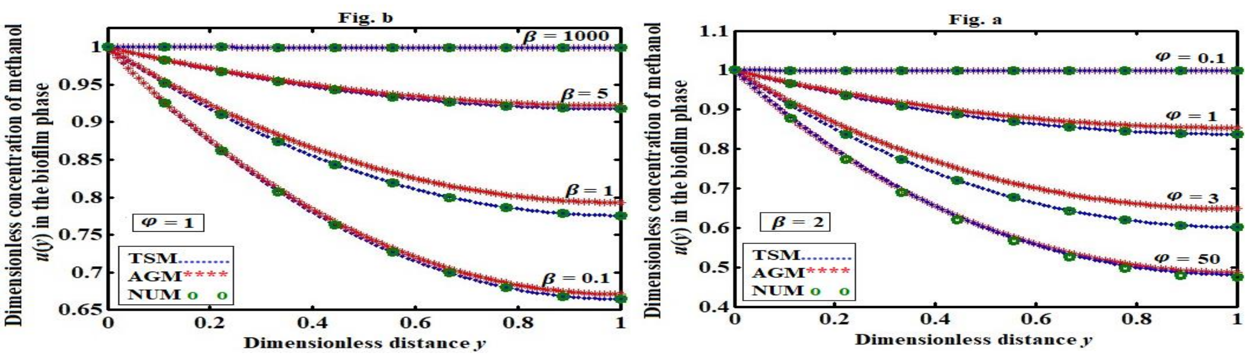

Figure 2. Dimensionless concentration of methanol $u(y)$in the biofilm phase versus, dimensionless distance y. (a) various values of φ. (b) various values for β.

Fig. 2 exhibits the concentration of methanol $u(y)$ in the biofilm phase versus dimensionless distance y for different values of φ and β. From Fig. 2a, b, it is inferred that the concentration of methane increases when the Thele modulus φ decreases or the saturation parameter β increases . For large value of β or very small values of φ the concentration of methane is uniform.

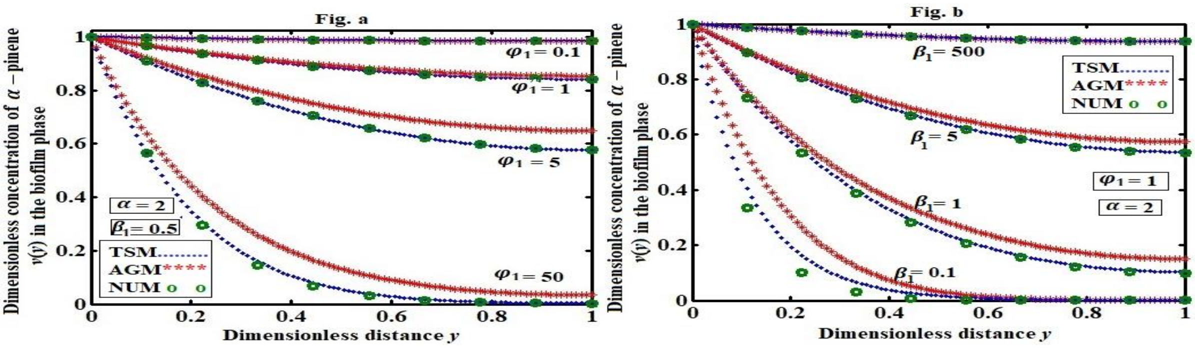

Figure 3. Dimensionless concentration of α-pinene v(y)in the biofilm phase versus, dimensionless distance y . (a) for fixed values of β and various values for φ. (b). for fixed values of φ and various values for β. The key to the graph: solid line represents analytical result and dotted line represent the numerical result.

In Fig. 3a, b, we show that the concentration of α-pinene in the biofilm phase for various values of Thiele modulus φ_1 and parameter β_1. From this figure, we conclude that the concentration of α-pinene increases when φ_1 decreases. The concentration of α-pinene is equal to one when $\varphi_1 \ll 0.1$ or $\beta_1 \gg 500$.

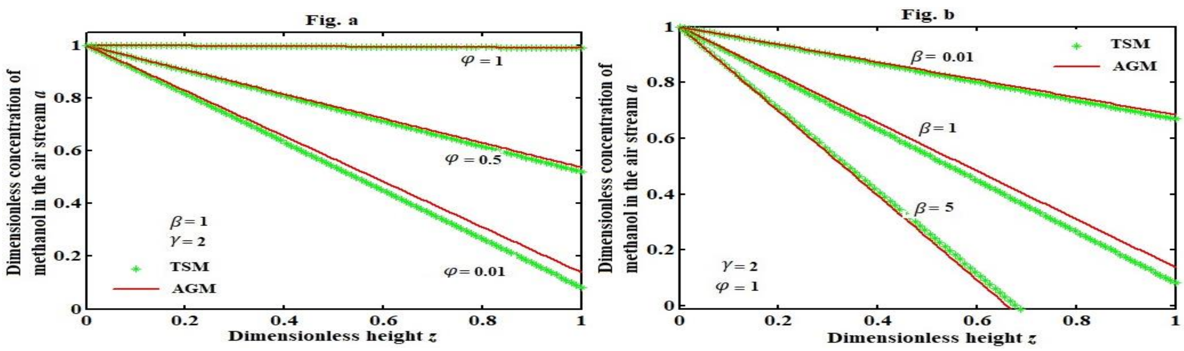

Figure 4. Dimensionless concentration of methanol in the air stream *a v*ersus dimensionless height *z* for some experimental values of the parameters. (a) for various values of the parameter φ . (b) for various values of the parameter β. The key to the graph: solid line represents Eq. (15) and (20) and dotted line represent the numerical result.

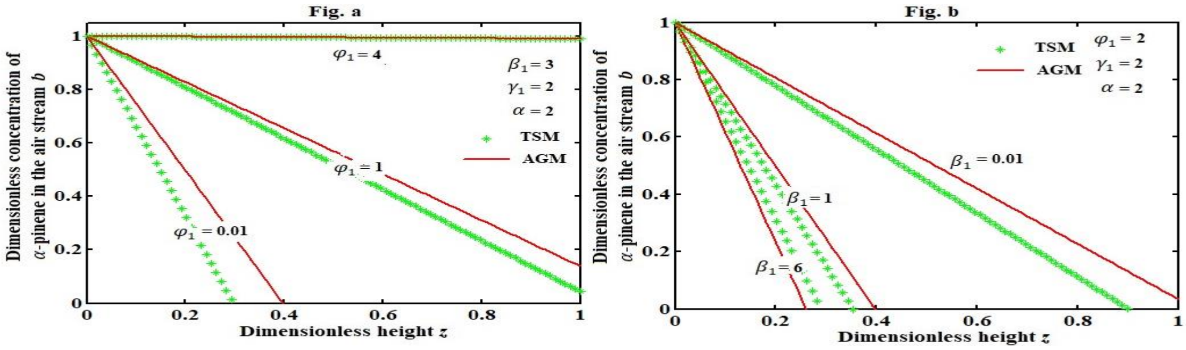

Figure 5. Dimensionless concentration of methanol in the air stream a versus dimensionless height z for some fixed experimental values of the parameters. (a) for various values of the parameter φ . (b) for various values of the parameter β. The key to the graph: solid line represents Eq. (17) and (22) and dotted line represent the numerical result.

Figures 5,6 illustrate the concentrations of methanol and α-pinene in the air phase as a function of height z for a given experimental parameter value. From these figures it is inferred that the concentration is linearly proportional to the height of the biofilter. And also the concentration of methanol and α-pinene decrease when the height of the biofilter increases.

Table 1. Comparison of numerical solution of dimensionless concentration of methanol $u(y)$ with the analytical solutions by TSM and AGM methods for different values of β when $\varphi = 2$.

	$\beta = 1$					$\beta = 10$					$\beta = 50$				
y	**NUM**	**TSM Eq.(8)**	**Err % of TSM**	**AGM Eq.(16)**	**Err % of AGM**	**NUM**	**TSM Eq.(8)**	**Err % of TSM**	**AGM Eq.(16)**	**Err % of AGM**	**NUM**	**TSM Eq.(8)**	**Err % of TSM**	**AGM Eq.(16)**	**Err % of AGM**
0.0	1.0000	1.0000	0.00	1.0000	0.00	1.0000	1.0000	0.00	1.0000	0.00	1.0000	1.0000	0.00	1.0000	0.00
0.2	0.8502	0.8516	0.16	0.8667	1.90	0.9964	0.9963	0.01	0.9965	0.01	0.9929	0.9929	0.00	0.993	0.01
0.4	0.7380	0.7399	0.26	0.7682	3.93	0.9936	0.9936	0.00	0.9937	0.01	0.9874	0.9875	0.01	0.9876	0.02
0.6	0.6604	0.6623	0.29	0.7006	5.74	0.9916	0.9916	0.00	0.9917	0.01	0.9834	0.9835	0.01	0.9838	0.04
0.8	0.6154	0.6167	0.21	0.6611	6.91	0.9904	0.9904	0.00	0.9906	0.02	0.9811	0.9812	0.01	0.9815	0.04
1.0	0.6016	0.6016	0.00	0.6481	7.17	0.9900	0.9900	0.00	0.9902	0.02	0.9804	0.9804	0.00	0.9807	0.03
Average			**0.15**		**4.28**			**0.00**		**0.01**			**0.01**		**0.02**

Table 2. Comparison of numerical solution of dimensionless concentration of methanol $u(y)$ with the analytical solutions by TSM and AGM methods for different values of φ when $\beta = 3$.

	$\varphi = 0.1$					$\varphi = 1$					$\varphi = 5$				
y	**NUM**	**TSM Eq.(8)**	**Err % of TSM**	**AGM Eq.(16)**	**Err % of AGM**	**NUM**	**TSM Eq.(8)**	**Err % of TSM**	**AGM Eq.(16)**	**Err % of AGM**	**NUM**	**TSM Eq.(8)**	**Err % of TSM**	**AGM Eq.(16)**	**Err % of AGM**
0.0	1.0000	1.0000	0.00	1.0000	0.00	1.0000	1.0000	0.00	1.0000	0.00	1.0000	1.0000	0.00	1.0000	0.00
0.2	0.9550	0.9955	4.07	0.9955	4.07	0.9557	0.9560	0.03	0.9587	0.31	0.6579	0.6579	0.00	0.755	12.86

0.4	0.9920	0.9920	0.00	0.9921	0.01	0.9215	0.9220	0.05	0.927	0.59	0.4309	0.4309	0.00	0.5861	26.48
0.6	0.9895	0.9895	0.00	0.9896	0.01	0.8972	0.8978	0.07	0.9046	0.82	0.2892	0.2892	0.00	0.4764	39.29
0.8	0.9881	0.9880	0.01	0.9881	0.00	0.8829	0.8832	0.03	0.8913	0.94	0.2122	0.2122	0.00	0.4147	48.83
1.0	0.9875	0.9875	0.00	0.9876	0.01	0.8784	0.8784	0.00	0.8868	0.95	0.1878	0.1878	0.00	0.3948	52.43
Average			**0.68**		**0.68**			**0.03**		**0.60**			**0.00**		**29.98**

Table 3. Comparison of numerical solution of dimensionless concentration of α-pinene v$(y)$with the analytical solutions by TSM and AGM methods for fixed values of $\alpha = 2$, $\varphi_1 = 1$ and different values of β_1

$\beta_1 = 1$						$\beta_1 = 5$					$\beta_1 = 10$				
y	**NUM**	**TSM Eq.(9)**	**Err % of TSM**	**AGM Eq.(17)**	**Err % of AGM**	**NUM**	**TSM Eq.(9)**	**Err % of TSM**	**AGM Eq.(17)**	**Err % of AGM**	**NUM**	**TSM Eq.(9)**	**Err % of TSM**	**AGM Eq.(17)**	**Err % of AGM**
0.0	1.0000	1.0000	0.00	1.0000	0.00	1.0000	1.0000	0.00	1.0000	0.00	1.0000	1.0000	0.00	1.0000	0.00
0.2	0.8502	0.8515	0.15	0.8667	1.90	0.9403	0.9413	0.11	0.9464	0.64	0.9672	0.9675	0.03	0.9693	0.22
0.4	0.7380	0.7399	0.26	0.7682	3.93	0.8951	0.8958	0.08	0.9055	1.15	0.9418	0.9422	0.04	0.9456	0.40
0.6	0.6604	0.6623	0.29	0.7006	5.74	0.8627	0.8634	0.08	0.8766	1.59	0.9237	0.9244	0.08	0.9289	0.56
0.8	0.6154	0.6167	0.21	0.6611	6.91	0.8436	0.8440	0.05	0.8594	1.84	0.9131	0.9134	0.03	0.9188	0.62
1.0	0.6015	0.6016	0.02	0.648	7.18	0.8377	0.8376	0.01	0.8537	1.87	0.9098	0.9098	0.00	0.9155	0.62
Average			**0.15**		**4.28**			0.05		**1.18**			**0.03**		**0.40**

Table 4. Comparison of numerical solution of dimensionless concentration of α-pinene v$(y)$with the analytical solutions by TSM and AGM methods for fixed values of $\beta_1 = 4, \alpha = 2$ and different values of φ_1 .

$\varphi_1 = 0.1$						$\varphi_1 = 1$					$\varphi_1 = 5$				
β_1	**NUM**	**TSM Eq.(9)**	**Err % of TSM**	**AGM Eq.(17)**	**Err % of AGM**	**NUM**	**TSM Eq.(9)**	**Err % of TSM**	**AGM Eq.(17)**	**Err % of AGM**	**NUM**	**TSM Eq.(9)**	**Err % of TSM**	**AGM Eq.(17)**	**Err % of AGM**
0.0	1.0000	1.0000	0.00	1.0000	0.00	1.0000	1.0000	0.00	1.0000	0.00	1.0000	1.0000	0.00	1.0000	0.00
0.2	0.9928	0.9928	0.00	0.9928	0.00	0.9297	0.9302	0.05	0.937	0.78	0.7163	0.7160	0.04	0.7856	8.82
0.4	0.9871	0.9872	0.01	0.9874	0.03	0.8755	0.8762	0.08	0.8891	1.53	0.5082	0.5080	0.04	0.6345	19.91
0.6	0.9832	0.9833	0.01	0.9835	0.03	0.8371	0.8379	0.10	0.8553	2.13	0.3684	0.3682	0.05	0.5345	31.08
0.8	0.9808	0.9809	0.01	0.9811	0.03	0.8145	0.8149	0.05	0.8353	2.49	0.2895	0.2893	0.07	0.4776	39.38
1.0	0.9801	0.9801	0.00	0.9803	0.02	0.8074	0.8073	0.01	0.8287	2.57	0.2656	0.2656	0.00	0.4591	42.15
Average			**0.01**		**0.02**			**0.05**		**1.58**			**0.03**		**23.56**

Table 5. Comparison of numerical solution of dimensionless concentration of methanol $u(y)$with the analytical solutions by TSM, AGM and previous result (ADM) for different values of φ when $\beta = 3$.

	$\varphi = 1$							$\varphi = 5$						
y	**NUM**	**TSM Eq.(8)**	**Err % of TSM**	**AGM Eq.(16)**	**Err % of AGM**	**ADM Eq.(23)**	**Err % of ADM**	**NUM**	**TSM Eq.(8)**	**Err % of TSM**	**AGM Eq.(16)**	**Err % of AGM**	**ADM Eq.(23)**	**Err % of ADM**
0.0	1.0000	1.0000	0.00	1.0000	0.00	1.0000	0.00	1.0000	1.0000	0.00	1.0000	0.00	1.0000	0.00
0.2	0.9557	0.9560	0.03	0.9587	0.31	0.9550	0.07	0.6579	0.6579	0.00	0.755	12.86	0.7750	15.11
0.4	0.9215	0.9220	0.05	0.927	0.59	0.9200	0.16	0.4309	0.4309	0.00	0.5861	26.48	0.6000	28.18

0.6	0.8972	0.8978	0.07	0.9046	0.82	0.8950	0.25	0.2892	0.2892	0.00	0.4764	39.29	0.4750	39.12
0.8	0.8829	0.8832	0.03	0.8913	0.94	0.8800	0.33	0.2122	0.2122	0.00	0.4147	48.83	0.4000	46.95
1.0	0.8784	0.8784	0.00	0.8868	0.95	0.8750	0.39	0.1878	0.1878	0.00	0.3948	52.43	0.3750	49.92
Average			**0.03**		**0.60**		**0.20**			**0.00**		**29.98**		**29.88**

Table 6. Comparison of numerical solution of dimensionless concentration of α-pinene $v(y)$with the analytical solutions by TSM, AGM and previous result (ADM) for fixed values of $\alpha = 2\,,\ \varphi_1 = 1\ and$ different values of β_1

y	$\beta_1 = 1$							$\beta_1 = 5$						
	NUM	**TSM Eq.(9)**	**Err % of TSM**	**AGM Eq.(17)**	**Err % of AGM**	**ADM Eq.(24)**	**Err % of ADM**	**NUM**	**TSM Eq.(9)**	**Err % of TSM**	**AGM Eq.(17)**	**Err % of AGM**	**ADM Eq.(24)**	**Err % of ADM**
0.0	1.0000	1.0000	0.00	1.0000	0.00	1.0000	0.00	1.0000	1.0000	0.00	1.0000	0.00	1.0000	0.00
0.2	0.8502	0.8515	0.15	0.8667	1.90	0.8200	3.68	0.9403	0.9413	0.11	0.9464	0.64	0.94	0.03
0.4	0.7380	0.7399	0.26	0.7682	3.93	0.6800	8.53	0.8951	0.8958	0.08	0.9055	1.15	0.8933	0.20
0.6	0.6604	0.6623	0.29	0.7006	5.74	0.5800	13.86	0.8627	0.8634	0.08	0.8766	1.59	0.86	0.31
0.8	0.6154	0.6167	0.21	0.6611	6.91	0.5200	18.35	0.8436	0.8440	0.05	0.8594	1.84	0.84	0.43
1.0	0.6015	0.6016	0.00	0.648	7.18	0.5000	20.30	0.8377	0.8376	0.01	0.8537	1.87	0.8333	0.53
Average			**0.15**		**4.28**		**10.79**			**0.05**		**1.18**		**0.25**

6. CONCLUSIONS

Two approximate semi-analytical methods for solving reaction-diffusion problems in biofiltration of volatile organic compounds were discussed. Analytical expressions for the concentration of methanol and α-pinene profiles in the air stream and biofilm phase for all parameters are obtained using Taylor series and Akbari-Ganji's methods. The effects of the parameter on the concentration profiles were discussed. This model is also validated using simulation results. With sufficient precision, the proposed approximate approach can be used to a variety of multicomponent reactions in different catalyst geometries.

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APPENDIX-A. APPROXIMATE ANALYTICAL SOLUTION OF EQ. (5) USING TAYLOR SERIES

The dimensionless mass balance equation in biofilm base is given as follows:

$$\frac{d^2u}{dy^2} = \varphi\left(\frac{u}{1+\beta u}\right) \tag{A1}$$

$$\frac{d^2v}{dy^2} = \alpha\varphi_1\left(\frac{v}{1+\beta_1 v}\right) \tag{A2}$$

The boundary conditions are

$$u = 1, v = 1 \text{ at } y = 0 \quad \text{(A3)}$$

$$\frac{du}{dy} = \frac{dv}{dy} = 0 \quad \text{at } y = 1 \quad \text{(A4)}$$

The solution of the equations (A1) and (A2) using Taylors series can written as follows**:**

$$u(y) = \sum_{i=0}^{\infty} \frac{d^i u}{dy^i} \frac{(y-1)^i}{i!}\bigg|_{y=1} \quad = u(1) + \frac{(y-1)}{1!}\frac{du}{dy}\bigg|_{y=1} + \frac{(y-1)^2}{2!}\frac{d^2u}{dy^2}\bigg|_{y=1} + \frac{(y-1)^3}{3!}\frac{d^3u}{dy^3}\bigg|_{y=1} + \cdots \quad \text{(A5)}$$

$$v(y) = \sum_{i=0}^{\infty} \frac{d^i v}{dy^i} \frac{(y-1)^i}{i!}\bigg|_{y=1} \quad = \alpha\left(v(1) + \frac{(y-1)}{1!}\frac{dv}{dy}\bigg|_{y=1} + \frac{(y-1)^2}{2!}\frac{d^2v}{dy^2}\bigg|_{y=1} + \frac{(y-1)^3}{3!}\frac{d^3v}{dy^3}\bigg|_{y=1} + \cdots\right) \quad \text{(A6)}$$

From the boundary condition Eq. (A4), we have

$$u'(1) = 0 \quad \text{(A7)}$$

and Eq. (A1) can be rewritten as follows:

$$[yu''(y) + n\,u'(y)](1 + \beta u(y)) - y\,\varphi u(y) = 0 \quad \text{(A8)}$$

Using the boundary conditions we get

$$u_1(1) = u''(1) = \frac{\varphi\,u(1)}{(1+\beta\,u(1))}\frac{1}{2!} \quad \text{(A9)}$$

Continuing this process, we get

$$u_2(1) = u'''(1) = \frac{-n\ \varphi\,u(1)}{(1+\beta\,u(1))}\frac{1}{3!} \quad \text{(A10)}$$

$$u_3(1) = u''''(1) = \frac{\varphi\,u(1)\,(\varphi-(n^2+2n)(1+\beta\,u(1))^2)}{(1+\beta\,u(1))^3}\frac{1}{4!} \quad \text{(A11)}$$

The Taylor series solution of Eq. (A1) and (A2) are given in the form

$$u(y) = u(1) + u_1(1)(y-1)^2 + u_2(1)(y-1)^3 + u_3(1)(y-1)^4 \quad \text{(A12)}$$

$$v(y) = v(1) + v_1(1)(y-1)^2 + v_2(1)(y-1)^3 + v_3(1)(y-1)^4 \quad \text{(A13)}$$

where

$$u_1(1) = \frac{\varphi\,u(1)}{(1+\beta\,u(1))}\frac{1}{2!},\ u_2(1) = \frac{-n\ \varphi\,u(1)}{(1+\beta\,u(1))}\frac{1}{3!},\ u_3(1) = \frac{\varphi\,u(1)\,(\varphi-(n^2+2n)(1+\beta\,u(1))^2)}{(1+\beta\,u(1))^3}\frac{1}{4!} \quad \text{(A14)}$$

$$v_1(1) = \frac{\alpha\varphi_1\,v(1)}{(1+\beta_1\,v(1))}\frac{1}{2!},\ v_2(1) = \frac{(\alpha\varphi_1)^2\,v(1)}{(1+\beta_1\,v(1))^3}\frac{1}{4!},\ v_3(1) = \frac{(\alpha\varphi_1)^3\,v(1)\,(1+\beta_1\,v(1)-7\,v(1))}{(1+\beta_1\,v(1))^5}\frac{1}{6!} \quad \text{(A15)}$$

From boundary condition (A3), we get

$$u(0) = u(1) + u_1(1)(-1)^2 + u_2(1)(-1)^3 + u_3(1)(-1)^4 \quad \text{(A16)}$$

$$v(0) = v(1) + v_1(1)(-1)^2 + v_2(1)(-1)^3 + v_3(1)(-1)^4 \quad \text{(A17)}$$

where $u(1)$ and $v(1)$ can be obtained from boundary condition (). Now Eqs. (A16) and (A17) can be used in the boundary condition

$$1 = u(1) + u_1(1) - u_2(1) + u_3(1) + \cdots \quad \text{(A18)}$$

$$1 = v(1) + v_1(1) - v_2(1) + v_3(1) + \ldots \quad \text{(A19)}$$

From Eq.(A14), (A15), we can obtain the value of $u(1)$ and $v(1)$.

APPENDIX-B. ANALYTICAL EXPRESION OF CONCENTRATION OF SUBSTRATE USING THE AKBARI-GANJI'S METHOD

The AGM begins by assuming the solution to Eq. (A1) is in the form of the hyperbolic function:

$$u(y) = B_1 \cosh(my) + B_2 \sinh(my) \tag{B1}$$

Substituting boundary conditions (A2)-(A4) in Eq. (B1) gives

$$B_1 = 1,\ B_2 = -\tanh m \tag{B2}$$

$$u(y) = \cosh(my) - \tanh m \sinh(my) \tag{B3}$$

From Eq. (B3) and (B1) at y=1, we obtain

$$m = \pm\sqrt{\varphi\left(\frac{1}{(1+\beta)}\right)} \tag{B4}$$

Therefore, a derived analytical expression of the concentration is given by

$$u(y) = \cosh\left(\sqrt{\varphi\left(\frac{1}{(1+\beta)}\right)}\, y\right) - \tanh m \sinh\left(\sqrt{\varphi\left(\frac{1}{(1+\beta)}\right)}\, y\right) \tag{B5}$$

NOMENCLATURE:

Symbols	**Definitions**	**Units**
A_s	Biofilm surface area per unit volume of the biofilters	m^2/m^3
C_m	Concentration of methanol in the air stream	g/m^3
C_{mi}	Concentration of methanol in the inlet air stream	g/m^3
C_p	Concentration of α- pinene in the air stream	g/m^3
C_{pi}	Concentration of α- pinene in the inlet air stream	g/m^3
D_{em}	Effective diffusivity of methanol in the biofilm	m^2/h
D_{ep}	Effective diffusivity of α- pinene in the biofilm	m^2/h
h	Dimension along the height of the biofilters	m
H	Total height of the biofilters	m
K_i	Inhibition Constant for α- pinene in the presence of methanol	g/m^3

K_m	Half saturation constant of methanol in Monod kinetics obtained from differential biofilters experiments	g/m^3
K_p	Half saturation constant of α- pinene in Monod kinetics	g/m^3
m_m	Air/ biofilm partition coefficient for methanol, dimensionless	- None
m_p	Air/ biofilm partition coefficient for α-pinene, dimensionless	None
S_m	Concentration of methanol in the biofilm	g/m^3
S_p	Concentration of α- pinene in the biofilm	g/m^3
U_g	Superficial velocity of air through the biofilters	m/s
X	Dry cell density of the biofilm	kg/m^3
Y	Organic carbon content of the biofilm	g/g
Y_m	Biomass yield coefficient for methanol	$kg/$ $cell/kg\ methanol$
Y_p	Biomass yield coefficient for α- pinene	$kg/cell/kg\ \alpha$-pinene
$S_m = \dfrac{C_m}{m_m} = S_{im}$	Initial concentration of methanol in the biofilm	g/m^3
$S_p = \dfrac{C_p}{m_p} = S_{ip}$	Initial concentration of α- pinene in the biofilm	g/m^3
L	Linear operator	$-$
Greek Letters		
α	Coefficient of for the effect of methanol on α-pinene biodegradation, dimensionless	$-$
δ	Biofilm thickness	m
$\mu_{\max(m)}$	Maximum specific growth rate for methanol biodegradation	h^{-1}
$\mu_{\max(p)}$	Maximum specific growth rate for α- pinene biodegradation	h^{-1}

ρ_b	Density of the biofilm	kg/m^3
Dimensionless Parameters:		
$\beta = \frac{S_{im}}{K_m}$	Dimensionless constant of methanol in Monod kinetics obtained from differential biofilters experiments	$-$
$\varphi = \frac{X\mu_{\max(m)}}{Y_m}\frac{\delta^2}{D_{em}K_m}$	Dimensionless parameter	$-$
$y = \frac{x}{\delta}$	Dimensionless coordinate in dry cell density of the biofilm	$-$
$u = \frac{S_m}{S_{im}}$	Dimensionless concentration of methanol in the biofilm	$-$
$\beta_1 = \frac{S_{ip}}{K_p}$	Dimensionless concentration of α- pinene in Monod kinetics obtained from bench-scale biofiltration results	$-$
$\varphi_1 = \frac{\alpha X\mu_{\max(m)}}{Y_m}\frac{\delta^2}{D_{em}K_m}$	Dimensionless parameter	$-$
$v = \frac{S_p}{S_{ip}}$	Dimensionless concentration of α- pinene in the biofilm	$-$
$A = \frac{H\ A_s\, D_{em}\, S_{im}}{U_g\, \delta\, C_{im}}$	Dimensionless parameter	$-$
$A_1 = \frac{H\ A_s\, D_{ep}\, S_{ip}}{U_g\, \delta\, C_{ip}}$	Dimensionless parameter	$-$
$a = \frac{C_m}{C_{im}}$	Dimensionless concentration of methanol in the air stream	$-$
$b = \frac{C_p}{C_{ip}}$	Dimensionless concentration of α- pinene in the air stream	$-$
C_{im}^*	Initial (before treatment) concentration of methanol	$-$
C_{imf}^* C_{ip}^*	Final (before treatment) concentration of methanol Initial (before treatment) concentration of α-pinene	$-$ $-$

C^*_{ipf}	Final (before treatment) concentration of α-pinene	$-$
$h^* = \frac{h}{H}$	Dimensionless along the height of the biofilters	$-$

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