

# The Analytical Expression of Steady-State Concentration of Mixture of Toluene and N- Propanol in the Biofilm: Akbari-Ganji's Method

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This paper discusses the biofiltration of toluene and propanol mixtures in a biofilter filled with a compost-woodchip combination. The base of the model is the mass transfer at the biofilm interface and chemical oxidation in the biofilm and gas phases. For all feasible experimental values of parameters, an approximate analytical expression of propanol and toluene concentration profiles in both phases has been determined using Akbari-Ganji's method. In addition, the numerical solution of the problem is provided in this paper using Matlab software. The obtained results are validated with the available numerical and previous results. The model presented here can be utilized to design purposes.

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**Keywords** Mathematical modelling; nonlinear equation; numerical simulations; toluene, *n*- propanol; Akbari-Ganji's method (AGM)

## 1. INTRODUCTION

In the petrochemical industry, *n*-propanol and Toluene are two of the most important chemicals found in air emissions. Propanol is hydrophilic and quickly biodegradable. Therefore, it should be easily removed in a biofilter, yet few investigations are reported on propanol removal in biofilters. On the other side, Toluene is more hydrophobic and will partition less favourably into biofilms, making it more difficult to remove in biofilters. Even though this condition frequently happens in industrial pollution, no research has been conducted on the biofiltration of propanol and toluene mixtures.

Only very few scientists have studied the solution of combinations of hydrophobic and hydrophilic VOCs. Initially developed to handle dilute odorous compounds, biofiltration technology has rapidly made tremendous progress, and its use has been extended to the treatment of diverse VOCs. [1–5]. Biofiltration is an efficient and low-cost method of extracting dilute VOC vapours from waste air [6–8]. Many scientists presented the analytical expression for the particle concentration in the biofilter, which is highly valuable for improving the reaction parameter.

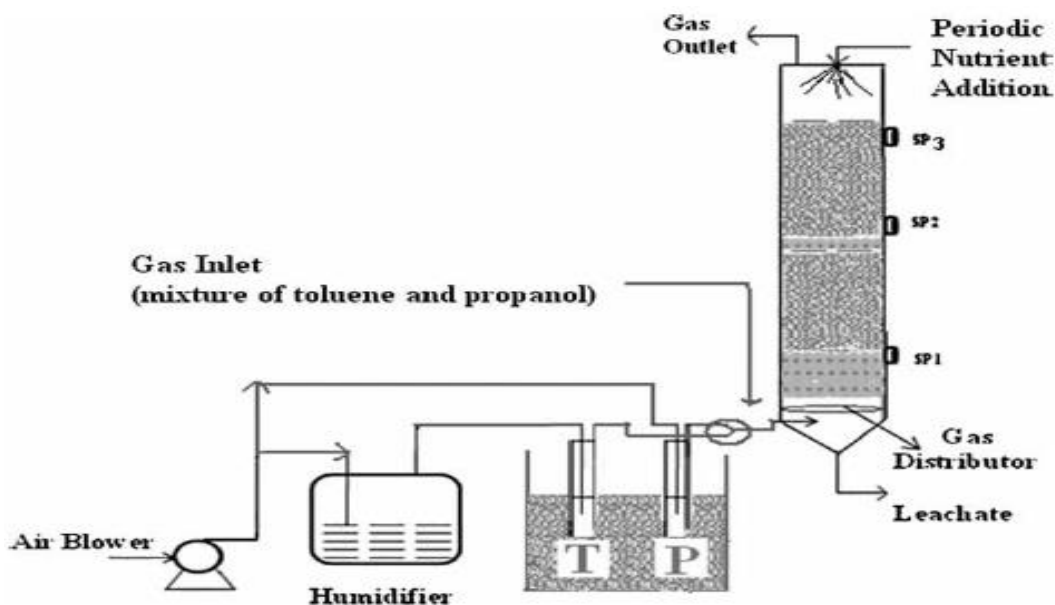
Dixit et al. [9] employed dynamic models to describe the elimination of VOCs in the biofilter by toluene and propanol mixtures. These dynamic models are derived from nonlinear differential equations in toluene and propanol. The Adomian decomposition approach [10] and the novel homotopy perturbation method [11] were used to derive the approximate analytical expressions of toluene and n-propanol concentration profiles in both bases. Saranya et al. [12] applied the homotopy perturbation approach and the hyperbolic function method to construct the approximate explicit solutions of n-butanol concentration profiles in the both phases for all possible parameter values. Veeramuni et al. [13] used the Adomian decomposition method (ADM) to solve the nonlinear differential equation of the toluene and propanol in the biofilter

For all possible experimental values of parameters, an approximate analytical expression of propane and toluene concentration profiles in the biofilm phase and gas phase has been derived using Akbari-Ganji's method in this communication. In moreover, this article presents a numerical solution to the problem using Matlab software.

## 2. MATHEMATICAL FORMULATION OF THE PROBLEM

A mathematical model was used to evaluate the function of the biofilter in removing toluene and n-propanol concentrations. Deshusses et al. [14] substantially modify the model, which specifies the critical processes during biofiltration, such as convection, absorption, diffusion, and biodegradation. The researchers used Monod-type kinetics with cross-inhibition effects of the substrate–pollutant mixture. The following assumptions are taken into account to derive the governing equations.

1. The air/biofilm partition coefficient represents the gas–biofilm interface equilibrium.
2. Since the biofilm only occurs on the external surfaces of the supporting particles, there is no biodegradation in the particles' interior pores.
3. The biofilm thickness is much bigger than the solid support size, so model equations are developed using planar biofilm geometry.
4. Now, at the air/biofilm interface, there is no gas-phase boundary layer. As a result, the gas-phase mass transfer resistance can be ignored.
5. The parameters of biomass, such as specific surface area, thickness, and kinetic coefficients, are equal all over the filter bed, and there is no excessive accumulation of biomass.
6. The only substrates that alter the biodegradation rate are toluene and n-propanol.



**Figure 1.** Schematic diagram for experiments involving mixtures of toluene and *n*-propanol [9].

### 2.1 Mass balance in the biofilm phase

The non-linear differential equations for removing a mixture of toluene and *n*-propanol in a biofilter are given in Table A [9]:

**Table A:** The mass balance equations and initial and boundary conditions

Equations	Initial and Boundary conditions
$\frac{\partial S_t}{\partial t} = D_{et} \frac{\partial^2 S_t}{\partial x^2} - \mu_{\max(t)} \frac{X}{Y_{x/s}} \frac{S_t(x)}{K_s + S_t(x) + \frac{(S_p(x))^2}{K_i}} \quad (1)$	$t = 0; 0 \leq x \leq \delta; S_t = S_p = 0 \quad (3)$
	$t < 0; x = 0; S_t = \frac{c_t}{m_t}; S_p = \frac{c_p}{m_p} \quad (4)$
$\frac{\partial S_p}{\partial t} = D_{ep} \frac{\partial^2 S_p}{\partial x^2} - \mu_{\max(p)} \frac{X}{Y_{x/s}} \frac{S_p(x)}{K_s + S_p(x)} \quad (2)$	$t < 0; x = \delta; \frac{\partial S_t}{\partial x} = \frac{\partial S_p}{\partial x} = 0 \quad (5)$

where  $S_t(x)$  and  $S_p(x)$  represent the concentration of the toluene and propanol in the biofilm, and  $D_{et}$  and  $D_{ep}$  denote the effective diffusivity of toluene and propanol in the biofilm,  $K_i$  is an inhibition constant,  $\mu_{\max(t)}$  and  $\mu_{\max(p)}$  are maximum specific rate during toluene and propanol biodegradation,  $X$  is the dry cell density of the biofilm,  $Y_{x/s}$  is the yield coefficient of biomass,  $K_s$  is the half saturation constant for toluene,  $m_t$  and  $m_p$  are the partition coefficient of the toluene and propanol in the biofilm and  $\delta$  denotes the biofilm thickness.

### 2.2 Mass balance in air phase

Table B describes the mass balance equation for the concentrations of toluene and propanol in the air phase.

**Table B:** The mass balance equation and boundary conditions

Equations	Boundary conditions
$\varepsilon \frac{\partial C_t}{\partial t} = U_g \frac{\partial C_t}{\partial h} - a_s D_{et} \left[ \frac{\partial S_t}{\partial x} \right]_{x=0} \quad (6)$	At $h = 0, C_t = C_{ti}$ and $C_p = C_{pi}$ (8)
$\varepsilon \frac{\partial C_p}{\partial t} = U_g \frac{\partial C_p}{\partial h} - a_s D_{ep} \left[ \frac{\partial S_p}{\partial x} \right]_{x=0} \quad (7)$	

where subscript ‘i’ denotes the concentration of the respective VOCs at the inlet of the biofilter,  $C_t$  and  $C_p$  are the concentration of the toluene and propanol in the air stream,  $\varepsilon$  is the bed porosity,  $a_s$  is the surface area of biofilm,  $H$  is the bed height in biofilter.

2.3 Dimensionless form of mass balance in the biofilm phase and air phase

When the following non-dimensional variables are introduced into Equations (1), (2), and (6), (7), they take on a dimensionless form:

$$\chi = \frac{x}{\delta}, U = \frac{S_t C_t}{m_t}, V = \frac{S_p C_p}{m_p}, \Phi_1 = \mu_{\max(t)} \frac{X \delta^2}{Y_{x/s} D_{et} K_s}, \Phi_2 = \mu_{\max(p)} \frac{X \delta^2}{Y_{x/s} D_{ep} K_s},$$

$$\beta_1 = \frac{C_t}{m_t K_s}, \beta_2 = \left( \frac{C_p}{m_p} \right)^2 \frac{1}{K_s K_i}, \beta_3 = \frac{C_p}{m_p K_s} \quad (9)$$

$$\eta = \frac{H a_s D_{et} S_t}{U_g \delta C_{ti}}, \eta_1 = \frac{H a_s D_{ep} S_p}{U_g \delta C_{pi}}, z = \frac{h}{H}, A = \frac{C_t}{C_{ti}}, \text{ and } B = \frac{C_p}{C_{pi}} \quad (10)$$

Using the above dimensionless variables, Eqs. (1), (2) and Eqs. (6), (7) reduces the following normalized form (Table-C).

**Table C:** Dimensionless form of mass balance equations in the biofilm phase and air phase

	Equations	Boundary conditions
Biofilm phase	$\frac{d^2 U(\chi)}{d \chi^2} = \frac{\Phi_1 U(\chi)}{1 + \beta_1 U(\chi) + \beta_2 (V(\chi))^2} \quad (11)$	$U(0) = 1, V(0) = 1 \quad (13)$ $\left. \frac{dU(\chi)}{d \chi} \right _{\chi=1} = 0, \left. \frac{dV(\chi)}{d \chi} \right _{\chi=1} = 0 \quad (14)$
	$\frac{d^2 V(\chi)}{d \chi^2} = \frac{\Phi_2 V(\chi)}{1 + \beta_3 V(\chi)} \quad (12)$	
Gas phase	$\frac{dA}{dz} = \eta \left[ \frac{dU(\chi)}{d \chi} \right]_{\chi=0} \quad (15)$	$A(z = 0) = \frac{C_t}{C_{ti}} \quad (17)$ $B(z = 0) = \frac{C_p}{C_{pi}} \quad (18)$
	$\frac{dB}{dz} = \eta_1 \left[ \frac{dV(\chi)}{d \chi} \right]_{\chi=0} \quad (16)$	

### 3. RESULTS AND DISCUSSION

#### 3.1 Approximate analytical expression of the concentrations using Akbari-Ganji's method.

Some asymptotic methods are employed to solve the nonlinear differential equations, such as the homotopy perturbation method [15-17], the Adomian decomposition method [18,19], variation iteration method [20,21], Taylor series method [22,23] and Akbari- Ganji's method [24-27]. As compared to solving linear differential equations, modelling nonlinear differential equations analytically are far more complex. In this regard, the Akbari-Ganji method (AGM) is an effective algebraic strategy for addressing such problems. The boundary and initial conditions are satisfied in the AGM by a solution function with unknown constant coefficients. Using AGM method, the following simple expression of concentration of toluene and propanol in biofilm and air phase can be obtained (Appendix-A).

**Table D:** Analytical expression of the concentrations

	Toluene	propanol
Biofilm phase	$U(\chi) = \frac{\cosh(m(1-\chi))}{\cosh m} \quad (19)$	$V(\chi) = \frac{\cosh(n(1-\chi))}{\cosh n} \quad (20)$
Gas phase	$A(z) = 1 - \eta z m \tanh m \quad (21)$	$B(z) = 1 - \eta_1 z n \tanh n \quad (22)$

Here m and n can be obtained from the following equations

$$m^2[1 + \beta_1 \operatorname{sech}(m) + \beta_2(\operatorname{sech}(n))^2] = \Phi_1 \quad \text{and} \quad n = \sqrt{\frac{\Phi_2}{1+\beta_3}} \quad (23)$$

#### 3.2. Previous analytical results

The Adomian decomposition approach was used to solve the non-linear differential equations in biofilter models analytically for various kinetics. Veeramuni et al. [13] solved Eqs. (11) and (12) with corresponding given boundary conditions using the Adomian decomposition method (ADM). They obtained that the analytical expressions for the concentration of toluene  $U(\chi)$  and propanol  $V(\chi)$  in biofilm as follows[13,28]:

$$U(\chi) = 1 + \frac{2 \Phi_1(b-3a)\chi}{3} + \Phi_1 a \chi^2 - \frac{b \Phi_1}{3} \chi^3 + \frac{a \Phi_1}{12} \chi^4 \quad (24)$$

$$V(\chi) = 1 + \frac{2 \Phi_2(d-3c)\chi}{3} + \Phi_2 c \chi^2 - \frac{d \Phi_2}{3} \chi^3 + \frac{c \Phi_2}{12} \chi^4 \quad (25)$$

$$\text{where } a = \frac{1}{2(1+\beta_1+\beta_2)}, b = 4 a^2(2 a \Phi_1(1 + \beta_1) - c \Phi_1\beta_1), c = \frac{1}{2(1+\beta_3)}, d = 4 c^3 \quad (26)$$

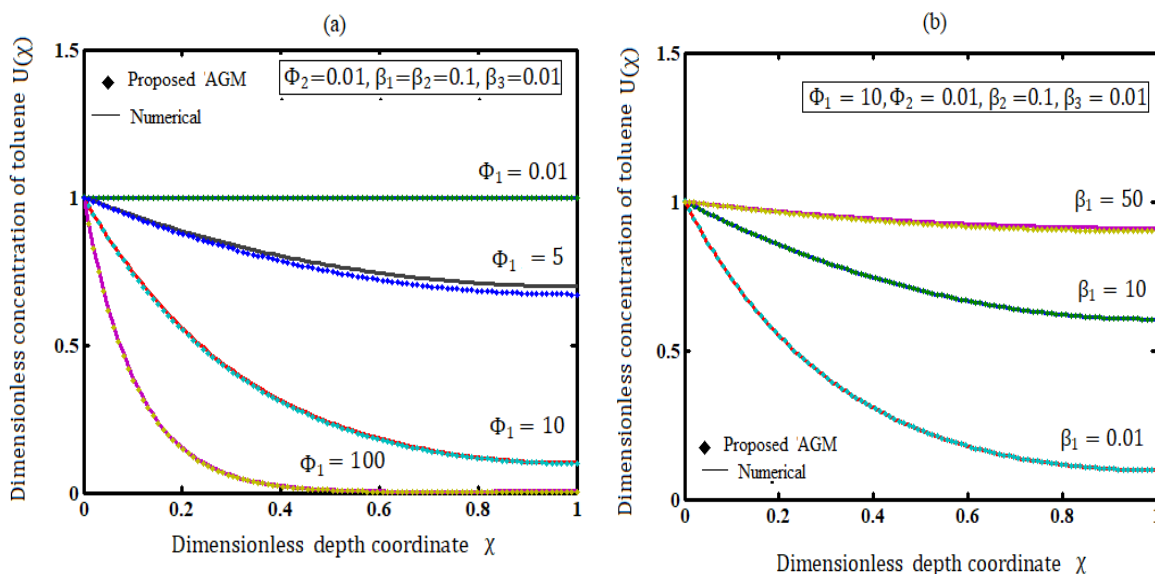
Sivasankari and Rajendran [28] derive the analytical expression of VOC and oxygen concentrations, as well as the appropriate effectiveness factor, for Monoid, Andrews, Interactive Monoid, and Andrews kinetics, for all parameter values.

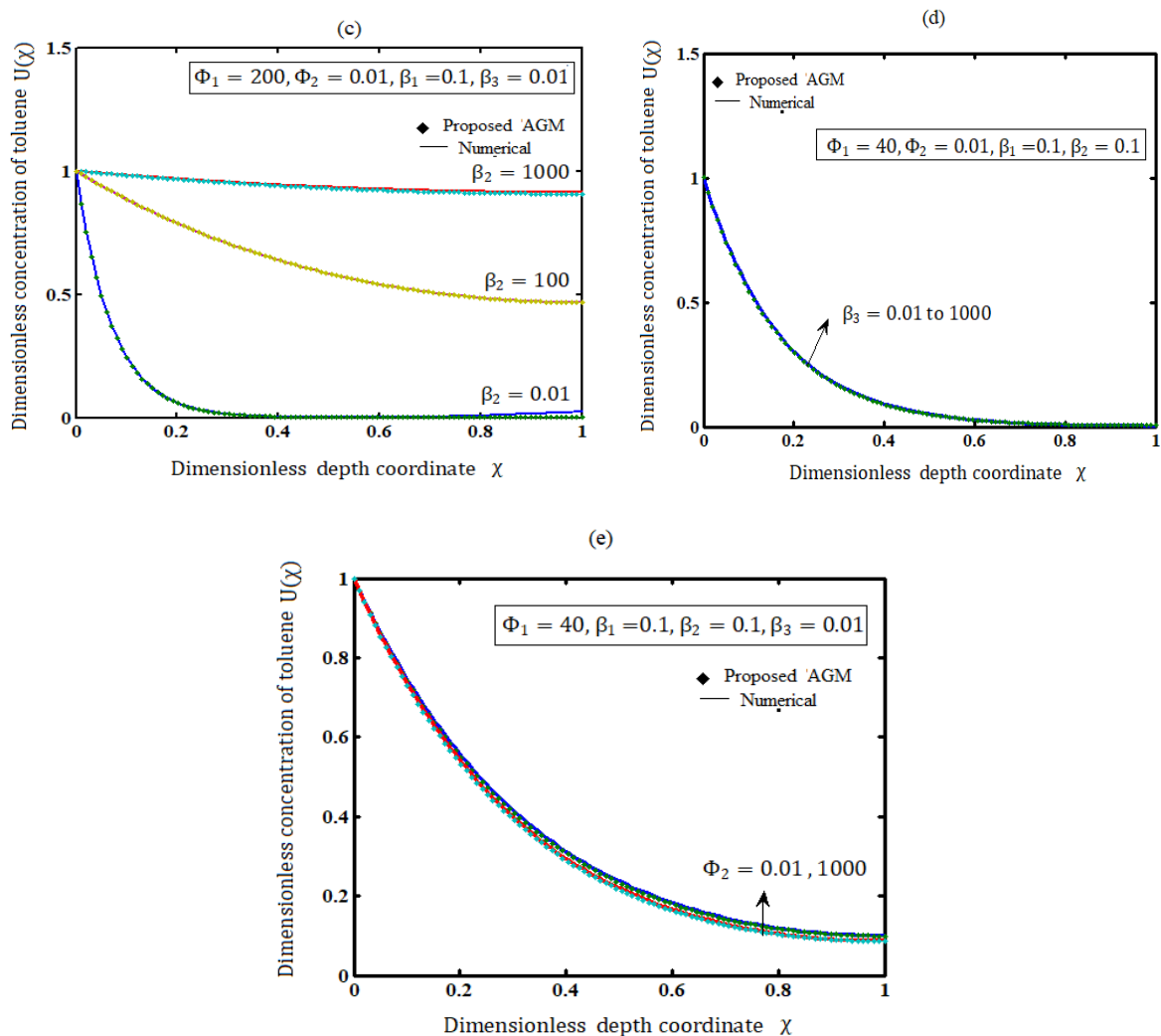
### 3.3 Numerical simulation

Numerically, the non-linear differential equations Eqs. (11) and (12) in the biofilm phase is solved for the boundary condition (Eqs (13) and (14)). The Matlab function bvp4c is used to solve this equation (see Appendix B). In Tables (1-2) and Figures 2 and 3, the analytical results for the concentration of the toluene and propanol in the biofilm phase were compared to simulation data and previously available analytical results (ADM). The maximum average error between our new analytical result (AGM method) and simulation result is 1% in toluene and 0.93% in propanol. But the previous analytical result (ADM method) has a maximum average error of 14% in toluene and 4 % in propanol.

### 3.4 Discussion

The simple closed-form of a novel analytical expression of the concentration of toluene and propanol in the biofilm is provided by equations (19) and (20). The concentrations of toluene and propanol in the air phase are described in simple new analytical expressions (21) and (22). The concentration of toluene profiles is shown in Figs. 2(a-e) for different values of  $\Phi_1$ ,  $\Phi_2$ ,  $\beta_1, \beta_2$  and  $\beta_3$ . An increase in  $\Phi_1$  or decrease in  $\beta_1, \beta_2$  leads to decrease in concentration of toluene. The variation of the parameters  $\Phi_2$  and  $\beta_3$  has no significant effect on the concentration of toluene. Also, the toluene concentration is uniform when  $\Phi_1 \leq 0.01$  or  $\beta_2 \geq 50, \beta_3 \geq 100$ .

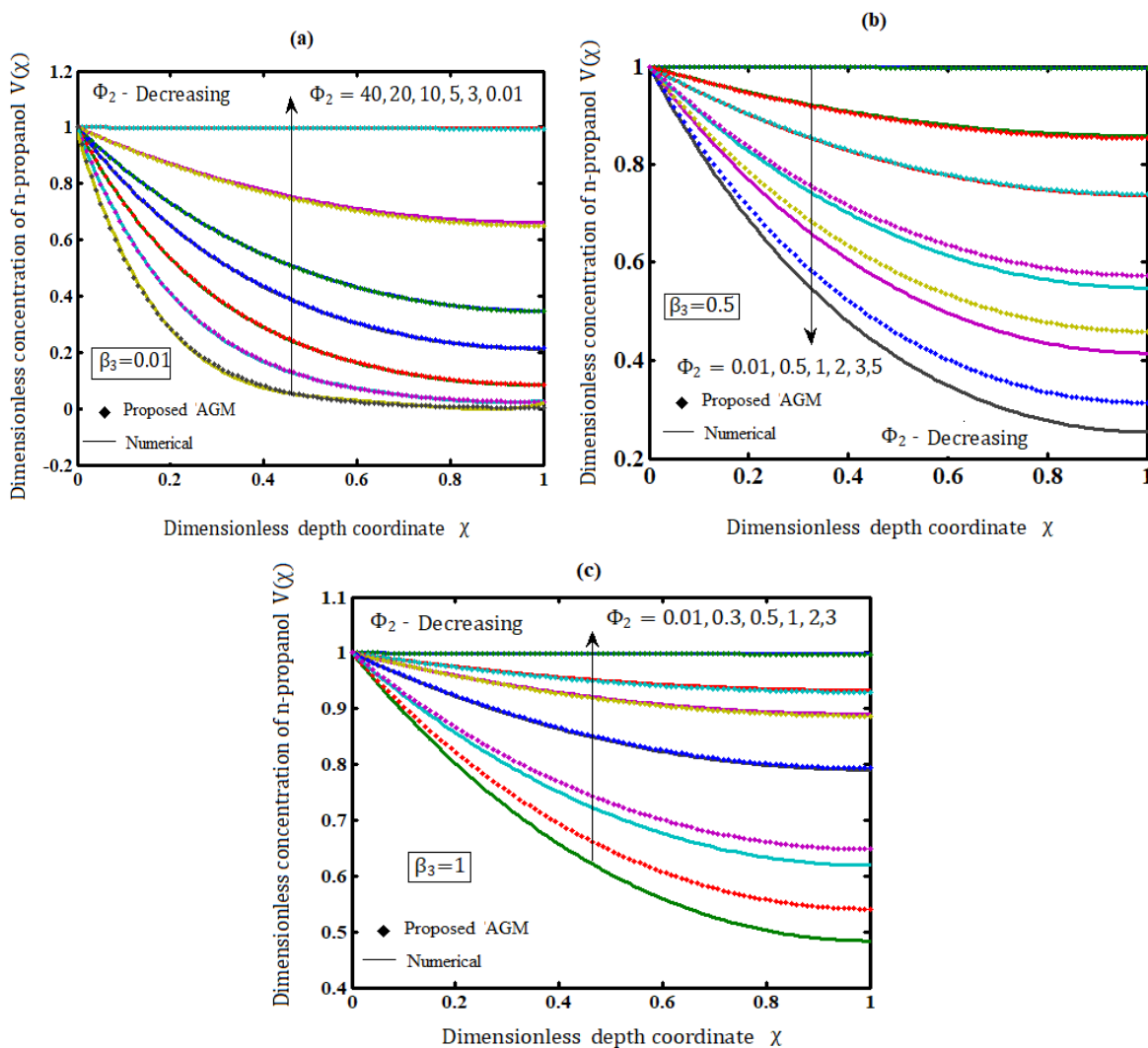




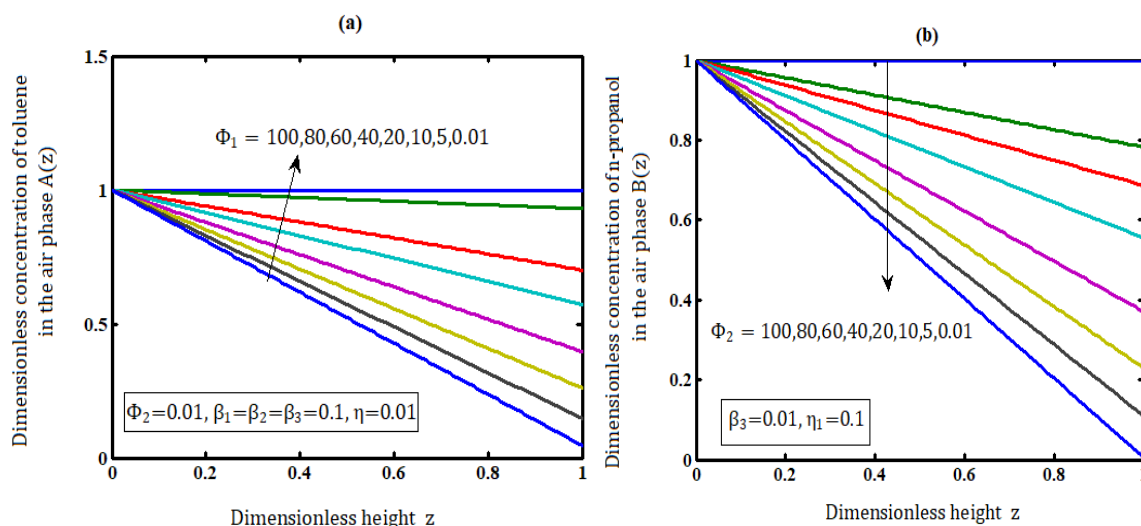
**Figure 2.** Comparison of analytical expression (Eq. (19)) of concentration of toluene  $U(\chi)$  with simulation result for various values for dimensionless parameter  $\Phi_1, \Phi_2, \beta_1, \beta_2,$  and  $\beta_3$ .

The concentration of propanol is shown in Figure 3 for various values of the parameters. It is evident that an increase in  $\Phi_2$ , concentration of toluene  $V(\chi)$  also decreases.

Fig. 4a depicts the concentration profiles in air phase for different values of parameter. Clearly as  $\Phi_1$  increases the value of toluene  $A(z)$  tends to decrease rapidly. Fig. 4b represents the propanol profile for different values of the  $\Phi_2$ . It is evident that an increase in concentration of propanol  $B(z)$  in the air phase also  $\Phi_2$  increases. The concentration in air phase is uniform when  $\Phi_1 \leq 0.01$  and  $\Phi_2 \geq 100$ .



**Figure 3.** Comparison of analytical expression (Eq. (20)) of concentration of propanol  $V(\chi)$  with simulation result for various values for dimensionless parameter  $\beta_3$ .



**Figure 4.** (a) Dimensionless concentration of toluene  $A(z)$  in the air phase versus dimensionless height  $z$  using Eq. (21). (b) Dimensionless concentration of propanol  $B(z)$  in the air phase versus dimensionless height  $z$  using Eq. (22).



### 4. CONCLUSIONS

In this paper, the nonlinear differential equation of the toluene and propanol in the biofilter has been solved analytically. Akbari-Ganji's methods are used to derive explicit solutions for the concentrations of toluene and propanol in the bio-film and gas-phase for all parameters. The numerical simulation data and earlier Adomian decomposition results are compared to the analytical results. These new analytical results contribute to a good understanding of the system and optimising the biofiltration model's parameters.

**Table 1.** Comparison between numerical and analytical results for dimensionless concentration of toluene  $U(\chi)$  for various values of parameter  $\Phi_1$  when  $\Phi_2 = 0.01, \beta_1 = \beta_2 = \beta_3 = 0.1$ .

$\chi$	$\Phi_1 = 0.01$					$\Phi_1 = 0.5$					$\Phi_1 = 1$				
	Num.	Concentration of Toluene $U(\chi)$		Error (%)		Num.	Concentration of Toluene $U(\chi)$		Error (%)		Num.	Concentration of Toluene $U(\chi)$		Error (%)	
		This Work AGM Eq. (19)	ADM [13] Eq. (24)	This Work AGM Eq. (19)	ADM [13] Eq. (24)		This Work AGM Eq. (19)	ADM [13] Eq. (24)	This Work AGM Eq. (19)	ADM [13] Eq. (24)		This Work AGM Eq. (19)	ADM [13] Eq. (24)	This Work AGM Eq. (19)	ADM [13] Eq. (24)
0	1.0000	1.0000	1.0000	0.0000	0.0000	1.0000	1.0000	1.0000	0.0000	0.0000	1.0000	1.0000	1.0000	0.0000	0.0000
0.2	0.9985	0.9984	0.9984	0.0100	0.0100	0.9327	0.9294	0.9425	0.3538	1.0507	0.8792	0.8754	0.9334	0.4322	6.1647
0.4	0.9974	0.9972	0.9971	0.0200	0.0301	0.8823	0.8759	0.9007	0.7254	2.0855	0.7904	0.7833	0.8923	0.8983	12.892
0.6	0.9966	0.9962	0.9961	0.0400	0.0502	0.8474	0.8386	0.8729	1.0385	3.0092	0.7298	0.7201	0.8669	1.3291	18.786
0.8	0.9961	0.9957	0.9952	0.0402	0.0903	0.8270	0.8168	0.8577	1.2333	3.7122	0.6950	0.6836	0.8488	1.6403	22.129
1	0.9960	0.9955	0.9959	0.0502	0.0100	0.8208	0.8101	0.8548	1.3036	4.1423	0.6843	0.6724	0.8320	1.7390	21.584
	Average error (%)			0.0267	0.0318	Average error (%)			0.7758	2.3333	Average error (%)			1.0065	13.593

**Table 2.** Comparison between numerical and analytical results for dimensionless concentration of propanol  $V(\chi)$  for various values of parameter  $\Phi_2$  when  $\beta_3 = 0.01$ .

$\chi$	$\Phi_2 = 0.01$					$\Phi_2 = 0.5$					$\Phi_2 = 1$				
	Num.	concentration of propanol $V(\chi)$		Error (%)		Num.	concentration of propanol $V(\chi)$		Error (%)		Num.	concentration of propanol $V(\chi)$		Error (%)	
		This Work AGM Eq. (20)	ADM [13] Eq. (25)	This Work AGM Eq. (20)	ADM [13] Eq. (25)		This Work AGM Eq. (20)	ADM [13] Eq. (25)	This Work AGM Eq. (20)	ADM [13] Eq. (25)		This Work AGM Eq. (20)	ADM [13] Eq. (25)	This Work AGM Eq. (20)	ADM [13] Eq. (25)
0	1.0000	1.0000	1.0000	0.0000	0.0000	1.0000	1.0000	1.0000	0.0000	0.0000	1.0000	1.0000	1.0000	0.0000	0.0000
0.2	0.9983	0.9982	0.9988	0.0100	0.0500	0.9269	0.9236	0.9421	0.3560	1.6399	0.8699	0.8666	0.8843	0.3793	1.6554
0.4	0.9971	0.9968	0.9980	0.0300	0.0903	0.8722	0.8659	0.9010	0.7223	3.3020	0.7747	0.7683	0.8019	0.8261	3.5110
0.6	0.9962	0.9958	0.9975	0.0401	0.1305	0.8344	0.8257	0.8737	1.0427	4.7100	0.7099	0.7011	0.7474	1.2396	5.2824
0.8	0.9957	0.9953	0.9972	0.0402	0.1506	0.8124	0.8022	0.8584	1.2555	5.6622	0.6727	0.6624	0.7169	1.5311	6.5705
1	0.9955	0.9951	0.9971	0.0402	0.1607	0.8057	0.7950	0.8540	1.3280	5.9948	0.6613	0.6505	0.7080	1.6331	7.0618
	Average error (%)			0.0267	0.0970	Average error (%)			0.7840	3.5515	Average error (%)			0.9349	4.0135

## NOMENCLATURE:

Symbols	Meanings	Units
$a_s$	Surface area of biofilm in the biofilter per unit volume	$m^{-1}$
$A$	Dimensionless concentration of toluene in air stream	None
$B$	Dimensionless concentration of propanol in air stream	None
$C_t, C_p$	Concentration of toluene and propanol in the air stream	$g\ m^{-3}$
$C_{ti}, C_{pi}$	Concentration of toluene and propanol in the inlet air stream	$g\ m^{-3}$
$D_{et}, D_{ep}$	Effective diffusivity of toluene and propanol in the biofilm	$m^2\ h^{-1}$
$h$	Dimension along the height of the biofilters	$m$
$H$	Total height of the biofilter packing	$m$
$K_t, K_p$	Monod kinetics for toluene and propanol in half saturation constant	$g\ m^{-3}$
$K_i$	Monod kinetics in inhibition constant	$g\ m^{-3}$
$m_t, m_p$	Dimensionless partition coefficient for toluene and propanol in air/biofilm	None
$S_t, S_p$	Concentration of toluene and propanol in the biofilm	$g\ m^{-3}$
$U_g$	Superficial velocity of air through the biofilter	$m\ s^{-1}$
$U, V$	Dimensionless concentration of toluene and propanol in the biofilm	None
$x$	Depth coordinate in the biofilm	$m$
$\chi$	Dimensionless depth coordinate in the biofilm	None
$X$	Biofilm dry cell density	$kg\ m^{-3}$
$Y_{x/s}$	Biomass yield coefficient	None
$z$	Dimensionless height	None
$\Phi_1, \Phi_2, \beta_1, \beta_2, \beta_3, \eta$ and $\eta_1$	Dimensionless constant	None
<i>Greek letters</i>		
$\varepsilon$	Dimensionless porosity of the filter bed	None
$\mu_{max}$	Maximum specific growth rate of toluene degraders	$h^{-1}$
$\delta$	Biofilm thickness	$m$

APPENDIX A.

ANALYTICAL SOLUTION NONLINEAR EQUATIONS (11) AND (12) USING AGM.

The trail solutions for Eqs. (11) and (12) using the Akbari- Ganji approach are taken as follows:

$$U(\chi) = A_0 \cosh(m \chi) + B_0 \sinh(m \chi) \tag{A1}$$

$$V(\chi) = A_1 \cosh(n \chi) + B_1 \sinh(n \chi) \tag{A2}$$

where  $A_0, A_1, B_0, B_1, m$  and  $n$  are constants. Using the boundary conditions (13) and (14), we obtain the constant

$$A_0 = 1, B_0 = -\text{Tanh}(m), \quad A_1 = 1, \quad B_1 = -\text{Tanh}(n) \tag{A3}$$

Now Eq. (A3) reduces to

$$U(\chi) = \frac{\cosh(m(1-\chi))}{\cosh m}, \tag{A4}$$

$$V(\chi) = \frac{\cosh(n(1-\chi))}{\cosh n} \tag{A5}$$

This constant can be obtained as follows: Eqs. (11) and (12) can be rewritten as

$$f(\chi) = \left(1 + \beta_1 U(\chi) + \beta_2 (V(\chi))^2\right) \frac{d^2 U(\chi)}{d \chi^2} - \Phi_1 U(\chi) = 0 \tag{A6}$$

$$g(\chi) = \left(1 + \beta_3 V(\chi)\right) \frac{\partial^2 V(\chi)}{\partial \chi^2} - \Phi_2 V(\chi) = 0 \tag{A7}$$

By substituting Eqs. ((A4) and (A5)) into Eqs. ((A6) and (A7)), we obtain

$$f(\chi)|_{\chi=1} = \left(1 + \frac{\beta_1}{\cosh(m)} + \frac{\beta_2}{(\cosh(n))^2}\right) \frac{m^2}{\cosh(m)} = \Phi_1 \frac{1}{\cosh(m)} \tag{A7}$$

$$g(\chi)|_{\chi=0} = (1 + \beta_3)n^2 = \Phi_2 \tag{A8}$$

From the above equation we get

$$m^2[1 + \beta_1 \text{sech}(m) + \beta_2 (\text{sech}(n))^2] = \Phi_1 \tag{A9}$$

$$n = \sqrt{\frac{\Phi_2}{1+\beta_3}} \tag{A10}$$

Substitute Eqs. ((A9) and (A10)) into Eqs. ((A4) and (A5)) gives the following analytical expression of concentration of toluene  $U(\chi)$  and propanol  $V(\chi)$  in biofilm for all dimensionless parameters  $\Phi_1, \Phi_2, \beta_1, \beta_2$  and  $\beta_3$ .

$$U(\chi) = \frac{\cosh(m(1-\chi))}{\cosh m} \tag{A11}$$

$$V(\chi) = \frac{\cosh\left(\sqrt{\frac{\Phi_2}{1+\beta_3}}(1-\chi)\right)}{\cosh \sqrt{\frac{\Phi_2}{1+\beta_3}}} \tag{A12}$$

Also solving Eqs(16) and (17)using the analytical expression of concentration of toluene  $U(\chi)$  and propanol  $V(\chi)$  in air phase for all dimensionless parameters  $\Phi_1, \Phi_2, \beta_1, \beta_2, \beta_3, \eta$  and  $\eta_1$ .

$$A(z) = \frac{C_t(z)}{C_{ti}} = 1 - \eta z m \tanh (m) \tag{A13}$$

$$B(z) = \frac{c_p(z)}{c_{pi}} = 1 - \eta_1 z \sqrt{\frac{\Phi_2}{1+\beta_3}} \tanh \sqrt{\frac{\Phi_2}{1+\beta_3}} \quad (\text{A14})$$

## APPENDIX B.

## MATLAB CODE FOR NUMERICAL SOLUTION OF THE NON-LINEAR EQS. (11) AND (12)

```

function pdex4
m = 0;
x = linspace(0,1);
t=linspace(0,1);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u1 = sol(:,:,1);
u2 = sol(:,:,2);
%-----
figure
plot(x,u1(end,:))
title('u1(x,t)')
xlabel('Distance x')
ylabel('u1(x,1)')
%-----
figure
plot(x,u2(end,:))
title('u2(x,t)')
xlabel('Distance x')
ylabel('u2(x,2)')
%-----
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c=[1;1];
f=[1;1].*DuDx;
p1=1;p2=1;beta1=1;beta2=1;beta3=0.01;
F1=-p1*u(1)./(1+beta1*u(1)+beta2*u(2)^2);
F2=-p2*u(2)./(1+beta3*u(2));
s=[F1; F2];
% -----
function u0 = pdex4ic(t) %create an initial conditions
u0 = [1;1];
% -----
function [pl,ql,pr,qr]=pdex4bc(xl,ul,xr,ur,t) %create a boundary conditions
pl = [ul(1)-1;ul(2)-1];
ql = [0;0];
pr = [0;0];
qr = [1;1]

```

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