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An Efficient Computational Method Pertaining to Concentration Profiles of Methanol and Pinene in Bio-film Phase Arising in Biochemical Engineering

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Abstract : In this paper, a mathematical model for a mixture of a hydrophobic (α-pinene) and a hydrophilic (methanol) volatile organic compound is discussed. This model describes the system of diffusion equations containing a nonlinear term represents Michaelis-Menten kinetics. The analytical expressions for the concentration profiles of α-pinene and methanol in bio-film phase have been derived by the Legendre computational method (LCM). To The best our knowledge until there is no LCM solution is addressed for the model. The results obtained have been compared with the Adomian decomposition method (ADM) graphically. Excellent agreement between the two methods is noticed.
Keywords: Mathematical modelling; boundary value problem; Legendre computational method.

1. Introduction

The rise in air pollutants has necessitated the development of different cleansing methods of gaseous effluents. Among them, bio-filtration technique has gained popularity due to the use bio-films and is a widely implemented method. The bio-films are composed of immobilised naturally occurring microorganisms on a porous medium, such as a combination of different media of compost, soil, peat or synthetic substances. The pollutants get transferred from the vapour phase to the bio-film through the filter-bed so formed. The popularity of biological control processes stems from the advantages it provides, such as low operating cost and the low secondary pollution it causes. Also, bio-filters consume low power, making it ideal for power-starved countries. Research has been carried out [1] for developing mathematical models of biological processes in packed trickle-bed bio-filters. Hence, the bio-filter performance and biomass accumulation in the reactor has been studied and their relationship has been analysed.

In VOC bio-filtration, Moheseni et al. [2] developed a mathematical model for the removal of α-pinene and methanol. The exact analytical solution for the concentration of substrate in bio-film phase has been studied in [3, 4], in which the Adomian decomposition method (ADM) had been used. In this communication, the analytical solution has been derived using the Legendre Computational Method (LCM) and the results have

been compared with ADM. It shall help optimise the parameters on the performance of the bio-filters in the removal of compounds like α-pinene, which are hydrophobic in nature.

The IUPAC name for α-pinene is given as, 2, 6, 6-Trimethylbicyclohept-2-ene, and is an organic compound. It is flammable in nature and is an isomer of pinene, belonging to the terpene class. Methanol is also known as methyl alcohol and is the bi-product of destructive distillation of wood. It is also an organic compound.

Hariharan [5] introduced an efficient Legendre wavelet based approximation method for a few Newell-Whitehead and Allen-Cahn equations. Hariharan and Kannan [6] reviewed the wavelet solutions for the solutions of reaction-diffusion equations (RDEs) arising in science and engineering. Excellent references are there in [7-9].

The organisation of the paper is as follows: Firstly, the mathematical formulation of the model is discussed. Then, the Legendre's computational method is briefly explained. Thereafter, the equation is solved using the LCM and the simulation results are plotted. Finally the paper is concluded after a comparison of the ADM and LCM methods.

2. Dimensionless mass balance equation for bio-film phase

In reference [10], Mohseni et al., have discussed the non-linear differential equation for the removal of α-pinene and methanol in the bio-film at steady state. For the present discussion, the equation is converted to a dimensionless form.

$$\frac{d^2 S_m^*}{dX^{*2}} = P\left[\frac{S_m^*}{1 + bS_m^*}\right] \tag{1}$$

$$\frac{d^2 S_p^*}{dX^{*2}} = aP_1\left[\frac{S_p^*}{1 + b_1 S_p^*}\right] \tag{2}$$

The above equations have the following boundary conditions:

$$S_m^* = 1, S_p^* = 1 \; at \; X^* = 0 \tag{3}$$

$$\frac{dS_m^*}{dX^*} = \frac{dS_p^*}{dX^*} = 0 \; at \; X^* = 1 \tag{4}$$

Here, the variables defined are expressed as:

$$\mathbf{S_m^* = \frac{S_m}{S_{im}}; S_p^* = \frac{S_p}{S_{ip}}}$$

$$b = \frac{S_{im}}{k_m}\; ;\; b_1 = \frac{S_{ip}}{k_p}$$

$$P = \frac{X\mu_{m,m}}{y_m}\frac{d^2}{d_{em}k_m};\; P_1 = \frac{X\mu_{m,p}}{y_p}\frac{d^2}{d_{ep}k_p}$$

$$a = \frac{1}{\left(1 + \left({}^{c_m}/_{K_{mp}}\right)^2\right)};\; X^* = \frac{x}{d}$$

3. Properties of shifted Legendre polynomials

The Legendre polynomials $P_n(z)$, defined on the interval [-1,1], have the following properties [11]:

$$P_n(z) = (-1)^n P_n(z), \quad P_n(-1) = (-1)^n, \quad P_n(1) = 1 \tag{5}$$

It is well known that the weight function is ω (z) =1 and the weighted space $L^2_{\omega}(-1,1)$ is equipped with the following inner product and norm;

$$(u,v)=\int_{-1}^{1}u(z)v(z)\omega(z)dz, \quad \|u\|=(u,u)^{\frac{1}{2}}. \tag{6}$$

The set of Legendre polynomials forms a complete orthogonal system $L^2(-1,1)$ and;

$$\|P_n(z)\|^2=h_n=\frac{2}{2n+1}, \tag{7}$$

is obtained. In order to use these polynomials on the interval [0, L] the so-called shifted Legendre polynomials are defined by introducing the change of variable $z=\frac{2x}{L}-1$.

The shifted Legendre polynomials are defined as;

$$P_n^*(x)=P_n(\frac{2x}{L}-1) \text{ where } P_n^*(0)=(-1)^n, \tag{8}$$

The analytic form of the shifted Legendre polynomial $P_n^*(x)$ of degree n is given by;

$$P_n^*(x)=\sum_{k=0}^{n}(-1)^{n+k}\frac{(n+k)!}{(n-k)!(k!)^2L^k}x^k. \tag{9}$$

Let $\omega_L(x)=1,$ and the weighted space $L^2_{\omega_L}(0,L)$ is defined with the following inner product and norm;

$$(u,v)_{\omega_L}=\int_0^L u(x)\,v(x)\,\omega_L(x)\,dx, \quad \|u\|_{\omega_L}=(u,u)^{\frac{1}{2}}_{\omega_L}. \tag{10}$$

The set of the shifted Legendre polynomials forms a complete $L^2_{\omega_L}(0,L)$ orthogonal system and $\|P_n^*(x)\|^2_{\omega_L}=\frac{L}{2}h_n=\frac{L}{2n+1}$ is obtained. The function u(x) which is square integrable in [0,L], may be expressed in terms of shifted Legendre polynomials as;

$$u(x)=\sum_{i=0}^{\infty}c_i\ P_i^*(x), \tag{11}$$

where the coefficients c_i are given by:

$$c_i=\frac{1}{\|P_i^*(x)\|^2_{\omega_L}}\int_0^L u(x)\,P_i^*(x)\,\omega_L(x)\,dx, \qquad i=0,1,2,..... \tag{12}$$

3.1 Fundamental relations

It is suggested the solution $u(x)\in C^m[0,L]$ can be approximated in terms of the first (m+1) terms of shifted Legendre polynomials given by

$$u(x) = \sum_{i=0}^{m} c_i \, P_i^*(x). \qquad (13)$$

4. Method of solution using LCM

The solutions of the Eq. (1) and Eq. (2) subject to the boundary conditions Eq. (3) and Eq. (4) are obtained using the Legendre computational Method. The main idea of the proposed method is to convert the differential equation with boundary conditions into a system of algebraic equations. So the following operational matrices of derivatives are considered: For M=2, a system of 3 linear algebraic equations is obtained, two of them from the initial conditions and the other from the main equation using the collocation point $x_0 = 0.5$;

$$D = \begin{bmatrix} 0 & 0 & 0 \\ 2 & 0 & 0 \\ 0 & 6 & 0 \end{bmatrix} \qquad D' = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 12 & 0 & 0 \end{bmatrix}$$

5. Experimental Setup

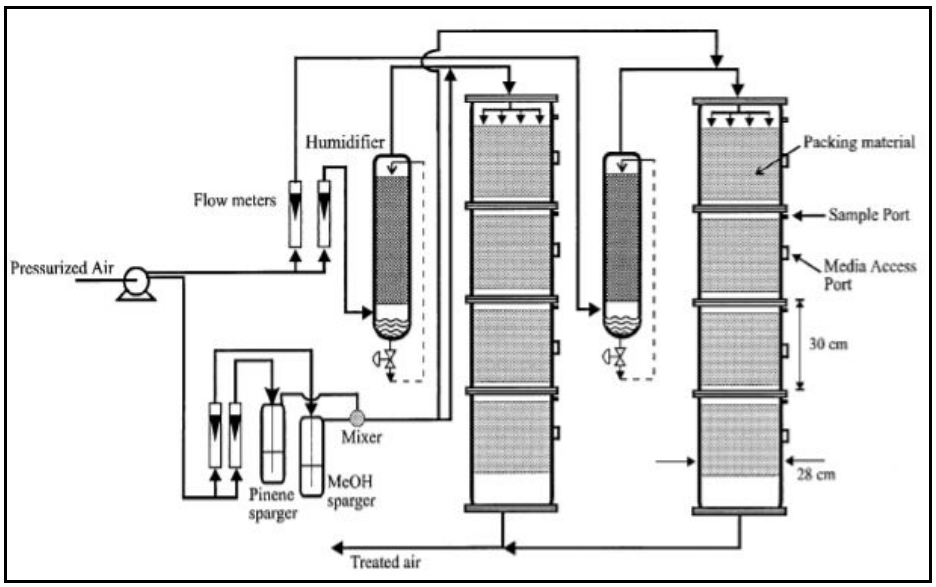

Fig. 1: Experimental setup for the bio-filtration of α-pinene and methanol [10].

Mohseni and Allen [10] performed an experiment for the bio-filtration process of α-pinene and methanol, the setup of which is shown in Fig.1. The various components used for this experiment are listed in the figure. The numerical results obtained by LCM are consistent with the experimental results found.

6. Numerical Simulation

The accuracy of the LCM solution is compared with the ADM solution for some finite number of terms. Following figures shown graphically represent this comparison. Based on the values of *b, P* and *a*, the results were obtained. Here *b* depends on the half saturation constant and initial concentration. The concentration of methanol decreases and reaches a constant level due to the maximum specific growth rate of methanol, *P*. The concentration of α-pinene is increased when the film thickness decreases.

Case 1: *P*=10 and *a*=1

The dimensionless concentration of α-pinene in the bio-film phase, S_D^* is plotted against the dimensionless distance, X*. In this case, the proposed LCM is applied with the values *P*=10 and *a*=1. Various values of *b* are considered. They are taken as *b=100*, *b=10* and *b*=5. It can be inferred from the Fig.2, that both the methods give very similar results. For larger M, the LCM results are closer to the experimental values. Our proposed results are compared with results obtained in [3]. In both the cases, it is observed that the curves

begin from S_p^* = 1 and gradually decrease, as the dimensionless distance increases. The curves show a steeper decrease as the value of *b* becomes smaller.

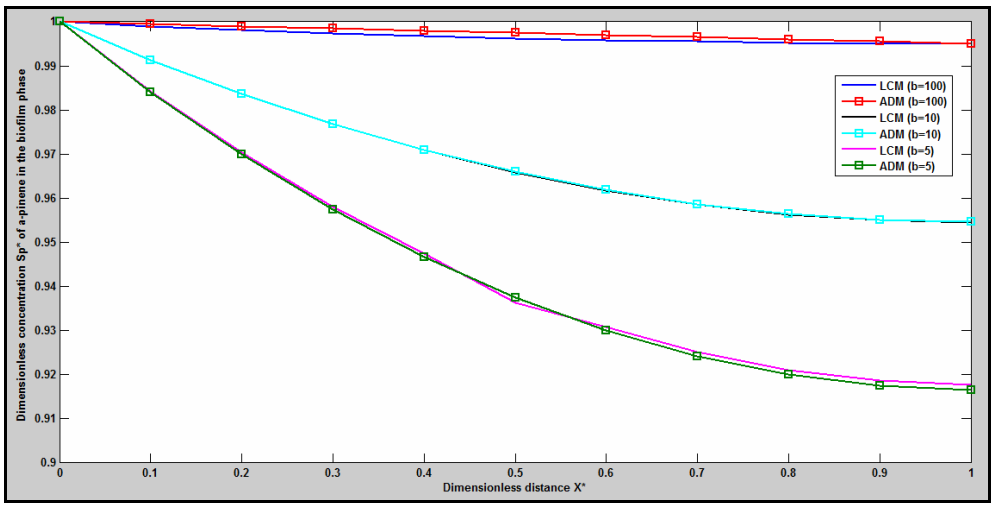

Fig.2: Comparison of S_p^* by ADM and LCM for *P*=10 and *a*=1

Case 2: b_1=10 and *a*=1

The dimensionless concentration of α-pinene in the bio-film phase, S_p^* is plotted against the dimensionless distance. In this case, the LCM is applied with the values b_1=10 and *a*=1. Various values of *P* are considered. They are taken as P=0.1, P=6 and P=8. It can be inferred from the Fig.3, that both the methods give very similar results.

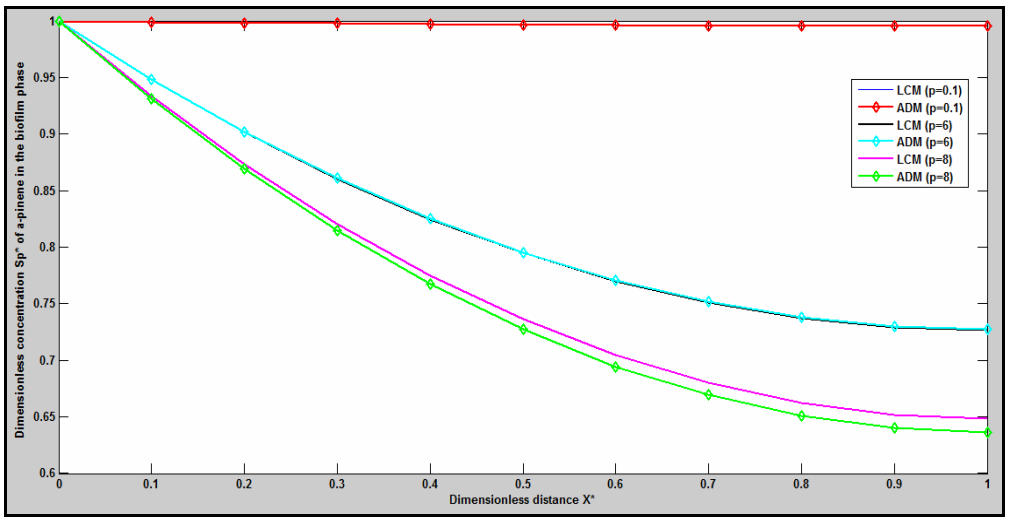

Fig.3: Comparison of S_p^* by ADM and LCM for b_1=10 and *a*=1

Our proposed results are compared with results obtained in [3]. Good agreement with the ADM is observed. In both the cases, it is observed that the curves begin from S_p^* = 1 and gradually decrease, as the dimensionless distance increases. The curves show a steeper decrease as the value of *P* becomes larger.

Case 3: *P*=10

The dimensionless concentration of methanol in the bio-film phase, S_m^* is plotted against the dimensionless distance, X*. In this case, the Legendre computational method is applied with the values *P*=10 and *a*=1. Various values of *b* are considered. They are taken as *b=100*, *b=10* and *b*=5.It can be inferred from the Fig.4, that both the methods give very similar results. Our proposed results are compared with results

obtained in [3]. In both the cases, it is observed that the curves begin from $S_p^{\bullet}$ = 1 and gradually decrease, as the dimensionless distance increases. The curves show a steeper decrease as the value of *b* becomes smaller.

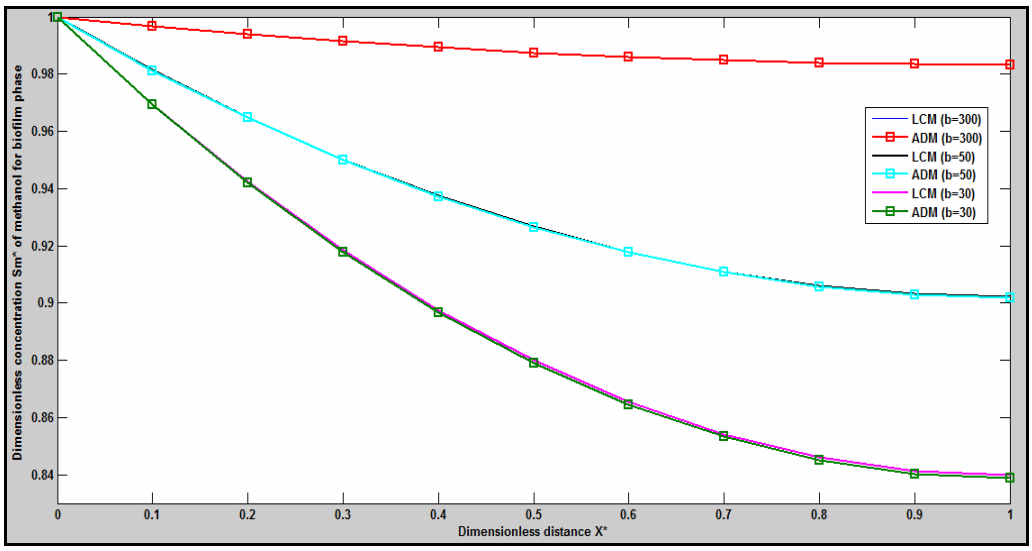

Fig.4: Comparison of $S_m^{\bullet}$ by ADM and LCM for *P*=10.

Case 4: *b*=1

The dimensionless concentration of methanol in the bio-film phase, $S_m^{\bullet}$ is plotted against the dimensionless distance. In this case, the Legendre computational method is applied with the values *b*=1. Various values of *P* are considered. They are taken as *P=0.1*, *P=6* and *P*=8. It can be inferred from the Fig.5, that both the methods give very similar results. Our proposed results are compared with results obtained in [3]. In both the cases, it is observed that the curves begin from $S_m^{\bullet}$ = 1 and gradually decrease, as the dimensionless distance increases. The curves show a steeper decrease as the value of *P* becomes larger.

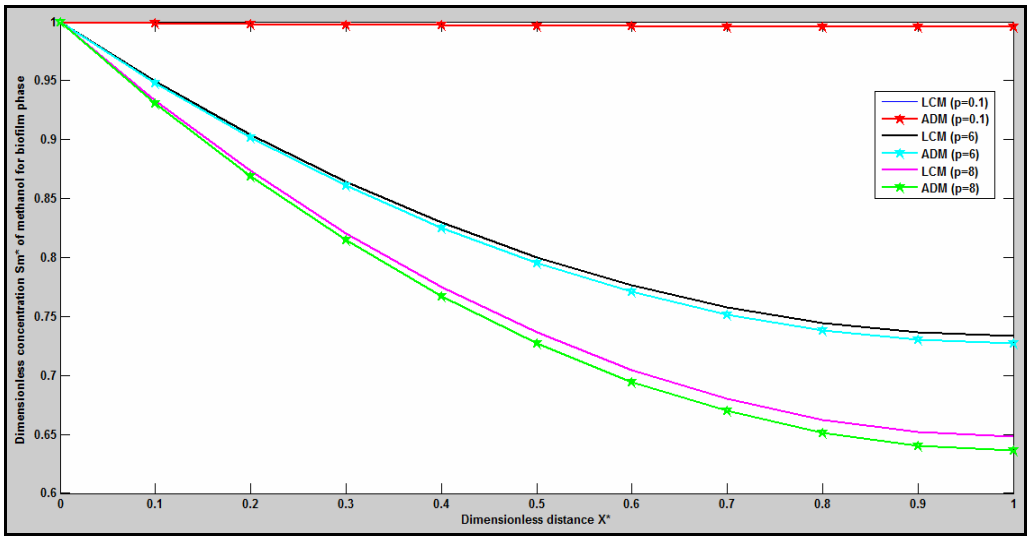

Fig.5: Comparison of $S_m^{\bullet}$ by ADM and LCM for *b*=1.

7. Conclusion and future scope

This paper presented the solution of concentrations of methanol and α-pinene in the bio-film phase using the Legendre computational method. The results were compared with the Adomian Decomposition Method and were validated with numerical simulation. The results were in agreement and therefore it provides a good understanding of the system and optimization of parameters in the bio-filtration model. It seems possible

to extend the removal of methanol and α-pinene in the bio-film model for non-steady state solution. Legendre and Chebyshev wavelet based methods for solving other types of nonlinear reaction-diffusion equations are presently on-going.

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Nomenclature:

a	:	Coefficient for the effect of methanol on α-pinene biodegradation
b	:	Dimensionless constant of methanol in Monod kinetics obtained from differential bio-filters experiments
b_1	:	Dimensionless constant of α-pinene in Monod kinetics obtained from differential bio-filters experiments
c_m	:	Concentration of methanol in air-stream (in g/m^3)
d	:	Bio-film thickness (in m)
d_{em}	:	Effective diffusivity of methanol in the bio-film (in m^2/h)
d_{ep}	:	Effective diffusivity of α-pinene in the bio-film (in m^2/h)
k_m	:	Half saturation constant of methanol in Monod kinetics obtained from differential bio-filters experiments (in g/m^3)
k_p	:	Half saturation constant of α-pinene in Monod kinetics (in g/m^3)
k_{mp}	:	Inhibition constant for α-pinene in the presence of methanol (in g/m^3)
P	:	Dimensionless parameter for methanol
P_1	:	Dimensionless parameter for α-pinene
S_m	:	Concentration of methanol in bio-film (in g/m^3)
S_p	:	Dimensionless concentration of α-pinene in bio-film (in g/m^3)
$S_m^{\bullet}$	:	Dimensionless concentration of methanol in bio-film
$S_p^{\bullet}$	:	Concentration of α-pinene in bio-film
S_{im}	:	Initial concentration of methanol in bio-film (in g/m^3)
S_{ip}	:	Initial concentration of α-pinene in bio-film (in g/m^3)
X	:	Dry cell density of the bio-film
X^*	:	Dimensionless coordinate in dry cell density of the bio-film
y_m	:	Biomass yield coefficient of methanol (in *kg cell kg* methanol)
y_p	:	Biomass yield coefficient of α-pinene (in kg/cell/kg α-pinene)
$\mu_{m,m}$	:	Maximum specific growth rate for methanol biodegradation (in h^{-1})
$\mu_{m,p}$	:	Maximum specific growth rate for α-pinene biodegradation (in h^{-1})

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