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An Efficient Wavelet Analysis Method to Film–Pore Diffusion Model Arising in Mathematical Chemistry

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Abstract In this paper, we have established an efficient Legendre wavelet based approximation method to solve film–pore diffusion model arising in engineering. Film–pore diffusion model is widely used to determine study the kinetics of adsorption systems. The use of Legendre wavelet based approximation method is found to be accurate, simple, fast, flexible, convenient, and computationally attractive. It is shown that film–pore diffusion model satisfactorily describe kinetics of methylene blue adsorption onto the three low-cost adsorbents, Guava, teak and gulmohar plant leaf powders, used in this study.

Keywords Methylene blue · Adsorption kinetics · Film–pore diffusion model · Low-cost adsorbents · Legendre wavelet method

Introduction

In recent years, adsorption mechanism has been established to be one of the highly efficient methods for removal of colors, odors, and organic and inorganic pollutants emanating from various industrial processes. Large amounts of dyes are used by textile industry and a significant portion of these dyes are not consumed in the process and therefore let out with the effluent. As the cost of commercial adsorbents is too high, interest for using low-cost adsorbents for removal of dyes from textile effluents is continuously growing. A recent survey indicates that, in India, on an average fresh water consumed and effluent generated per kg of finished textile are 175 and 125 L, respectively (Ponnusami et al. 2010). The presence of dyes in aqueous effluents is highly objectionable as this affects the photosynthetic activity in receiving water body by reducing/preventing light penetration. As the dyes are recalcitrant in nature it is difficult to treat them in conventional biological treatment plant (Ponnusami et al. 2007, Ponnusami et al. 2009). Various researchers have worked on biological degradation of dyes. But, very often, the metabolic intermediates are found to be more toxic than the original compound (Cheung et al. 2001). Therefore, identification of low-cost adsorbents is given more attention by the researchers recently as commercial adsorbents like activated carbon are too costly. Few recent studies investigating application of low-cost adsorbents are: jackfruit peel (Hameed 2009), pine apple stem (Hameed et al 2009), phoenix tree leaves (Han et al. 2011), pomelo peel (Hameed et al. 2008), shells of bittim (Aydin and Baysal 2006), orange peel (Khaled et al. 2009), broad been peels (Hameed and El-Khaiary 2008) etc.

In our previous reports, we have established the feasibility and adsorption of MB onto three plant leaf powders namely guava leaf powder (GLP), teak leaf powder (TLP), and gulmohar leaf powder (GUL) (Ponnusami et al. 2010). Film–pore diffusion model (FPDM) was employed successfully to describe the kinetics of methylene blue adsorption onto GLP, TLP, and GUL. Diffusion based kinetic models are too complex and require rigorous solution methods. For many of the diffusion models, pure analytical solution is not possible. In our previous paper, we had employed method of lines to solve film–pore diffusion model and had shown that Film–pore model could describe the kinetics of adsorption of MB onto GLP, TLP, and GUL (Ponnusami et al. 2010). In this work, we have proposed a wavelet based approximation method to film–pore diffusion model.

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There is a growing interest in using various wavelets to study problems, of greater computational complexity. Among the wavelet transform families, the Haar and Legendre wavelets deserve much attention. The basic idea of Legendre wavelet method (LWM) is to convert the PDEs to a system of algebraic equations by the operational matrices of integral or derivative. The main goal is to show how wavelets and multi-resolution analysis can be applied for improving the method in terms of easy implementability and achieving the rapidity of its convergence. Yin et al. (2012) introduced the Laplace Legendre wavelets method for solving Lane–Emden-type differential Equations. Recently, Hariharan and Kannan (2014) reviewed the Haar wavelets for solving differential and integral equations arising in science and engineering. Wavelet method for solving ODEs and PDEs is well documented in the literature (Chen and Hsiao 1997; Hsiao 2007; Shi et al. 2010, Fazal-I-Haq et al. 2010; Wu 2009; Zhi and Cao 2012; Geng et al. 2011; Lepik 2005, 2007a, b; Hariharan and Kannan (2010a, b, c); Hariharan (2010; Porter and McKay 2001; Ho and McKay 1998; Yin et al 2012; Hariharan et al. 2012).

Hariharan and Kannan (2010a, b, c) and Hariharan (2010) had introduced the diffusion equation, convection–diffusion equation, Reaction–diffusion equation, Nonlinear parabolic equations, fractional Klein–Gordon equations, Sine–Gordon equations and Fisher's equation by the Haar wavelet method.

In this work, we have applied a LWM for the numerical solution of the film–pore diffusion model equation.

Materials and Methods

Detailed development of FPDM is described earlier by McKay and co-workers (2001, 1998). Solution of FPDM by method of lines is described in our previous paper (Ponnusami et al. 2010). In the present paper, development of LWM is described in detailed, and the results are compared with our previous solution.

Legendre Wavelets Preliminaries (Yin et al. 2012)

Wavelets

Wavelets are the family of functions which are derived from the family of scaling function $\{\emptyset_{j,k}: k \in Z\}$ where:

$$\emptyset(x) = \sum_k a_k \emptyset \leq (2x - k) \tag{1}$$

For the continuous wavelets, the following equation can be represented:

$$\Psi_{a,b}(x) = |a|^{\frac{-1}{2}} \Psi\left(\frac{x-b}{a}\right) \quad a, \ b \in R, \ a \neq 0, \tag{2}$$

where a and b are dilation and translation parameters, respectively, such that $\Psi(x)$ is a single wavelet function.

The discrete values are put for a and b in the initial form of the continuous wavelets, i.e.,

$$a = a_0^{-j}, \quad a_0 > 1, b_0 > 1, \tag{3}$$

$$b = kb_0 a_0^{-j}, \quad j, k \in Z. \tag{4}$$

Then, a family of discrete wavelets can be constructed as follows:

$$\Psi_{j,k} = |a_0|^{\frac{1}{2}} \Psi\left(2^j x - k\right), \tag{5}$$

So, $\Psi_{j,k}(x)$ constitutes an orthonormal basis in L^2 (R), where $\Psi(x)$ is a single function.

Legendre Wavelets

The Legendre wavelets are defined by

$$\Psi_{nm}(t) = \begin{cases} \sqrt{m+\frac{1}{2}} 2^{\frac{k}{2}} L_m\left(2^k t - \hat{n}\right), & \text{for } \frac{\hat{n}-1}{2^k} \leq t \leq \frac{\hat{n}+1}{2^k}, \\ 0, & \text{otherwise} \end{cases} \tag{6}$$

where $m = 0, 1, 2, \ldots, M-1$ and $n = 0, 1, 2, \ldots, 2^{k-1}$. The coefficient $\sqrt{m+\frac{1}{2}}$ is for orthonormality, then, the wavelets $\Psi_{k,m}(x)$ form an orthonormal basis for $L^2[0,1]$. In the above formulation of Legendre wavelets, the Legendre polynomials are in the following way:

$$p_0 = 1,$$

$$p_1 = x,$$

$$p_{m+1}(x) = \frac{2m+1}{m+1} x p_m(x) - \frac{m}{m+1} p_{m-1}(x). \tag{7}$$

and $\{p_{m+1}(x)\}$ are the orthogonal functions of order m, which is named the well-known shifted Legendre polynomials on the interval [0,1]. Note that, in the general form of Legendre wavelets, the dilation parameter is $a = 2^{-k}$ and the translation parameter is $b = n\ 2^k$.

Block-Pulse Functions (BPFs) (Yin et al. 2012)

The block-pulse functions form a complete set of orthogonal functions which defined on the interval [0, b) by

$$b_i(t) = \begin{cases} 1, & \frac{i-1}{m} b \leq t < \frac{i}{m} b, \\ 0, & \text{elsewhere} \end{cases} \tag{8}$$

for $i = 1, 2,\ldots, m$. It is also known that for any absolutely integrable function $f(t)$ on [0,b) can be expanded in block-pulse functions:

$$f(t) \cong \xi^T B_m(t) \tag{9}$$

$$\xi^T = [f_1, f_2, \ldots, f_m], B_m(t) = [b_1(t), b_2(t), \ldots, b_m(t)] \tag{10}$$

where f_i are the coefficients of the block-pulse function, given by

$$f_i = \frac{m}{b}\int_0^b f(t) b_i(t) \mathrm{d}t \tag{11}$$

Remark 1 Let A and B are two matrices of m x m, then $A \otimes B = \left(a_{ij} \times b_{ij}\right)_{mm}$.

Lemma 1 Assuming $f(t)$ and $g(t)$ are two absolutely integrable functions, which can be expanded in block-pulse function as $f(t) = FB(t)$ and $g(t) = GB(t)$, respectively, then we have

$$f(t)g(t) = FB(t)B^T(t)G^T = HB(t), \tag{12}$$

where $H = F \otimes G$.

Approximating the Nonlinear Term (Yin et al. 2012)

The Legendre wavelets can be expanded into m-set of block-pulse Functions as

$$\Psi(t) = \emptyset_{m\times m} B_m(t) \tag{13}$$

Taking the collocation points as following

$$t_i = \frac{i - 1/2}{2^{k-1}M}, \quad i = 1,\ 2,\ \ldots,\ 2^{(k-1)}M \tag{14}$$

The m-square Legendre matrix $\emptyset_{m\times m}$ is defined as

$$\emptyset_{mm} \cong [\Psi(t_1)\Psi(t_2)\ldots\Psi(t_{2^{k-1}M})] \tag{15}$$

The operational matrix of product of Legendre wavelets can be obtained by using the properties of BPFs, let $f(x, t)$ and $g(x, t)$ are two absolutely integrable functions, which can be expanded by Legendre wavelets as $f(x,t) = \Psi^T(x)F\Psi(t)$ and $g(x,t) = \Psi^T(x)G\Psi(t)$, respectively. Then

$$f(x,t) = \Psi^T(x)F\Psi(t) = B^T(x)\emptyset_{mm}^T F \emptyset_{mm} B(t), \tag{16}$$

$$g(x,t) = \Psi^T(x)G\Psi(t) = B^T(x)\emptyset_{mm}^T G \emptyset_{mm} B(t), \tag{17}$$

and

$$F_b = \emptyset_{mm}^T F \emptyset_{mm}, G_b = \emptyset_{mm}^T G \emptyset_{mm}, H_b = F_b \otimes G_b.$$

Then,

$$f(x,t)g(x,t) = B^T H_b B(t),$$

$$= B^T(x)\emptyset_{mm}^T inv\left(\emptyset_{mm}^T\right) H_b inv\left(inv\left(\emptyset_{mm}^T\right) H_b inv(\emptyset_{mm})\right)\emptyset_{mm} B(t)$$

$$= \Psi^T(x) H \Psi(t) \tag{18}$$

where $\mathrm{H} = inv(\emptyset_{mm}^T) H_b inv((\emptyset_{mm}))$

Function Approximation (Yin et al. 2012)

A given function $f(x)$ with the domain [0,1] can be approximated by:

$$f(x) = \Sigma_{k=1}^{\infty}\Sigma_{m=0}^{\infty} c_{k,m}\Psi_{k,m}(x) = C^T.\Psi(x). \tag{19}$$

Here C and Ψ are the matrices of size $(2^{j-1}\ M \times 1)$.

$$C = \left[c_{1,0}, c_{1,1}, \ldots c_{1,M-1}, c_{2,0}, c_{2,1}, \ldots c_{2,M-1}, \ldots c_{2,1}^{j-1}, \ldots c_{2,M-1}^{j-1}\right]^T \tag{20}$$

$$\Psi(x) = [\Psi_{1,0}, \Psi_{1,1}, \Psi_{2,0}, \Psi_{2,1}, \ldots \Psi_{2,M-1}, \ldots \Psi_{2^{j-1},M-1}] \tag{21}$$

Method of Solution

Consider the equation (Hariharan et al. 2012)

$$\dot{\bar{C}}_i(Z,\tau) = A(\bar{C}_i)\left[\overline{C_i}'' + \left(\frac{1}{Z}\right)\overline{C_i}'\right] \tag{22}$$

$$\left.\begin{array}{l} C_i(z,0) = e^{-z} \\ C_i(z,1) = e^{-z-0.09} \\ C_i(0,\tau) = e^{-0.09\tau} \\ C_i(1,\tau) = e^{-1-0.09\tau} \end{array}\right\} \tag{23}$$

We solve Eq. (22) by applying the LWM

$$\overline{C_i}''(z,\tau) = C^T P_\tau \Psi(z,\tau) + \overline{C_i}''(z,0) \tag{24}$$

$$\overline{C_i}'(z,\tau) = C^T P_\tau P_z[\Psi(z,\tau) - P_z\Psi(1,\tau)] + g_1(z,\tau) \tag{25}$$

$$\dot{\overline{C_i}}(z,\tau) = C^T P_z^2[\Psi(z,\tau) - z\Psi(1,\tau)] + g_2(z,\tau) \tag{26}$$

$$\begin{aligned} \overline{C_i}(z,\tau) = {} & C^T P_\tau P_z^2[\Psi(z,\tau) - z\Psi(1,\tau)] + \overline{C_i}(z,0) \\ & - \overline{C_i}(0,0) \\ & + z\left[\overline{C_i}(1,\tau) - \overline{C_i}(1,0) + \overline{C_i}(0,0) - \overline{C_i}(0,\tau)\right] \\ & + \overline{C_i}(0,\tau) \end{aligned} \tag{27}$$

in which

$$g_1(z,\tau) = \dot{\overline{C}}_i(z,0) - \overline{C_i}(1,0) - \overline{C_i}(0,\tau) + C_i(1,\tau) + 1$$

and,

$$g_2(z,\tau) = z\left[\bar{C}_i(1,\tau) - C_i'(0,\tau)\right] + C_i'(0,\tau)$$

Table 1 Comparison between LWM and method of lines (MOL) by obtaining the mass transfer coefficients using film–pore diffusion model adsorption of MB onto GLP and $k = 2$ and $M = 3$, $t = 10$ s

Temperature (K)	C_0 (mgdm^{-3})	k_f (ms^{-1})		D_{eff} (m^{2}s^{-1})		Error	
		MOL (M)	LWM (L)	MOL (M)	LWM (L)	E_M	E_L
303	50	1.00×10^{-6}	4.23×10^{-6}	1.74×10^{-13}	1.24×10^{-14}	1.197	0.038
	100					0.140	0.029
	150					0.935	0.283
	200					1.610	1.541
313	50	1.71×10^{-6}	6.35×10^{-6}	6.46×10^{-13}	7.32×10^{-14}	1.462	1.312
	100					1.120	0.653
	150					1.267	0.120
	200					7.570	3.626
323	50	4.27×10^{-6}	4.01×10^{-6}	3.11×10^{-13}	5.31×10^{-13}	0.856	0.192
	100					0.160	0.001
	150					2.168	1.127
	200					3.164	1.002

E_M error by method of lines, E_L error by LWM

Substitute the Eqs. (24)–(26) into Eq. (22), we get

$$C^T P_z^2[\Psi(z,\tau) - z\Psi(1,\tau)] + g_2(z,\tau) = A(\overline{C_i})\left[\left(C^T P_\tau \Psi(z,\tau) + \overline{C_i}''(z,0)\right) + \frac{1}{z}\left(C^T P_\tau P_z[\Psi(z,\tau) - P_z\Psi(1,\tau)] + g_1(z,\tau)\right)\right] \quad (28)$$

From formula (28) the wavelet coefficients C^T can be calculated successfully

Here $A(\overline{C_i})$ are constants (linear) and $\epsilon = 0.5$, $\rho = 500$.

Table 1 gives a comparison of Legendre wavelet (LW) solutions and method of lines. It is evident that LW solutions are better than that of the method of lines. Value of absolute error decreased when k was increased. The results show that combining with wavelet matrix, the method in this paper can be effectively used in numerical calculus for constant coefficient differential equations, and that the method is feasible. We can see that the numerical solutions are in good agreement with exact solution. The power of the manageable method is thus confirmed.

All the numerical experiments presented in this section were computed in double precision with some MATLAB codes on a personal computer System with Processor Intel(R) Core$^{(TM)}$ 2 Duo CPU T5470 at 1.60 GHz (2CPUs) and 1 GB RAM.

Conclusion

In the present paper, FPDM model equations had been solved by the LWM It was found that the model could predict the concentration decay curve for all adsorption of methylene blue onto TLP, GUL, and GLP excellently with a small deviation during initial period. In comparison with existing numerical schemes used to solve the nonlinear parabolic equations, the scheme in this paper is an improvement over other methods in terms of accuracy. It is worth mentioning that LW solution provides excellent results even for small values of k. For larger values of k, we can obtain the results closer to the real values.

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