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On comparison of OCFE using Hermite basis with analytic and MATLAB 'pdepe' solver for axial dispersion model

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ABSTRACT: Trial function expansions are widely used in solving boundary value problems. The expansion coefficients are typically determined by variational principles or by weighted-residual methods, the latter being more widely applicable. These methods are attractive because of compactness of the results, as compared with the finite difference solutions. In the present paper, the numerical results are obtained for the solution of two point boundary value problems of mathematical model related to diffusion-dispersion during flow through multi-particle system. The method of orthogonal collocation of finite elements using the Hermite basis is applied on axial domain of the system of partial differential equations. Numerical results then obtained are compared with earlier works through analytical methods, and MATLAB 'pdepe' solver. The results are found comparable with analytic ones and even good, than the 'pdepe' solver.

I. INTRODUCTION

The need of paper & pulp industry to achieve its target production and also to have less environment load can be best matched with planned research on mathematical models. Modeling of any system can be done using the techniques like process modeling, physical modeling & statistical modeling. The mathematical models describing the pulp washing process are based on axial dispersion and particle diffusion. These models are established in terms of transport equations using basic mass transfer relation like diffusion equation and material balance equations. An additional term is used to account for the accumulation (or depletion) capacity of material sorbed by the particles. The transport equations together with adsorption-desorption isotherms and appropriate boundary and initial conditions describe the equilibrium between the concentration of the solute in the liquor and concentration of the solute on the fibers. These models characterize the performance of equipment in terms of various input parameters such as interstitial velocity, longitudinal dispersion coefficient, mass transfer coefficient and porosity of the packed bed.

A lot of literature is available on the subject of longitudinal dispersion in porous media. Pulp washing models based on axial dispersion and particle diffusion along with adsorption isotherms for sodium and lignin are fairly established. For pulp washing operation [1-17] has studied models based on the concepts of particle diffusion and axial dispersion. Investigators have followed linear, finite rate and Langmuir adsorption isotherms besides different boundary and initial conditions.

These models were solved analytically [3,6,7,9-15,17] and numerically by methods, such as finite-difference method [8], orthogonal collocation method [4,5], orthogonal collocation on finite elements [2], Petrov Galerkin method [1] and MATLAB 'pdepe' solver [16]. Due to the complexity of analytic solution one has to take the recourse of approximation techniques. The finite difference method requires strict selection of step size for the stability of the solution. Nevertheless, the accuracy of numerical solution is not so high. Orthogonal collocation method does not give good results when nature of equations is stiff; The discretization of even a few PDEs by the MOL can lead to an extremely large system of ODEs, the numerical solution of which may have severe cost and storage implications.

Through this paper, an attempt is made to provide more accurate numerical solutions of the pulp washing models. To validate the solution technique, the model is solved and compared with results of earlier work of Brenner [3] and Singh [16]. The results show fairly good accuracy. The numerical results obtained are much more accurate than the other previous workers.

II. DESCRIPTION OF THE DIFFUSION MODEL

The diffusion models involve parameters such as longitudinal dispersion coefficient and mass transfer coefficients. Physical models proposed by various investigators can be classified based on mass transfer principles of two types (i) differential contact models (macroscopic) and the (ii) dispersion models (macroscopic).

Brenner [3] studied the washing of filter cake based on the phenomena of longitudinal mixing and assumed it to be governed by the equation:

$$D\frac{\partial^2 C}{\partial X^2} = U\frac{\partial C}{\partial X} + \frac{\partial C}{\partial T} \qquad \ldots(1)$$

where T is the time from commencement of the displacement, X is the distance from the point of introduction of the displacing fluid, $C = C(X,T)$ is the solute concentration, D is the axial dispersion coefficient and U is the average interstitial velocity of the fluid, *i.e.*, $U = Q/A\varepsilon$. The thickness of the bed is L and the initial solute concentration is denoted by C_0, (assumed constant throughout the bed). In addition $C_e = C_e(1,T)$ is the solute concentration of the fluid exiting from bed.

At the inlet to the bed, the boundary condition is given by

$$UC - D_L\frac{\partial C}{\partial X} = UC_s \quad \text{at } X = 0 \quad \ldots(2)$$

This condition is imposed by the requirement that there is no loss of solute from the bed through the plane at which the displacing fluid is introduced.

At the bed exit, in order to avoid the unacceptable conclusion that the solute concentration passes through a maximum (or minimum) in the interior of the medium, it is necessary to impose the boundary condition

$$\frac{\partial C}{\partial X} = 0 \qquad \text{at } X = L \qquad \ldots(3)$$

Initially it is assumed that the bulk fluid concentration is equal to the inlet solute concentration, *i.e.*,

$$C(X,0) = C_0 \qquad \text{for all } X \qquad \ldots(4)$$

III. ORTHOGONAL COLLOCATION ON FINITE ELEMENTS USING HERMITE BASIS

The Hermite cubic interpolant of function f relative to partition $a = x_0 < x_1 < \ldots < x_n = b$ is a function s that satisfies:

i. on each subinterval $[x_j, x_{j+1}]$, where j=0,1,2,...,n-1, and s coincides with a cubic polynomial $s_j(x)$,
ii. s interpolates f and f' at $x_0, x_1, \ldots, x_n$,
iii. s is continues on [a, b],
iv. s' is continues on [a, b].

The Hermite cubic Interpolation of f and its first derivative at $x = x_j$ requires

$$s_j(x_j) = f(x_j) \text{ and } s'_j(x_j) = f'(x_j)$$

Combining the continuity of s and s' at $x = x_{j+1}$ with interpolation of f and its first derivative at $x = x_{j+1}$, one gets:

$$s_j(x_{j+1}) = s_{j+1}(x_{j+1}) = f(x_{j+1}) \text{ and}$$
$$s'_j(x_{j+1}) = s'_{j+1}(x_{j+1}) = f'(x_{j+1})$$

Hence, $s_j(x)$ is a third degree polynomial that interpolates both f and f' at $x = x_j$ and at $x = x_{j+1}$. Therefore $s_j(x)$ can be written down as:

$$s_j(x) = H_{1,j}(x)f(x_j) + H_{1,j+1}(x)f(x_{j+1}) + \hat{H}_{i,j}(x)f'(x_j) + \hat{H}_{i,j+1}(x)f'(x_{j+1})$$

where, $H_{1,j}(x) = \left[1 - 2\frac{x - x_j}{x_j - x_{j+1}}\right]\left(\frac{x - x_{j+1}}{x_j - x_{j+1}}\right)^2$, $H_{1,j+1}(x) = \left[1 - 2\frac{x - x_{j+1}}{x_{j+1} - x_j}\right]\left(\frac{x - x_j}{x_{j+1} - x_j}\right)^2$,

$$\hat{H}_{i,j}(x) = (x - x_j)\left(\frac{x - x_{j+1}}{x_j - x_{j+1}}\right)^2,$$

$$\hat{H}_{i,j+1}(x) = (x - x_{j+1})\left(\frac{x - x_j}{x_{j+1} - x_j}\right)^2.$$

In the method of orthogonal collocation on finite elements using Hermite basis, the axial domain ($0 \le x \le 1$) is divided into small sub domains called ‘elements’. The global variable x varies in the ℓ^{th} element, where $\ell = 1, 2, \ldots, ne$. The node points are set at $x_1, x_2, \ldots, x_{ne+1}$ as shown in Fig. 1. The boundary points 0 and 1 have been placed at $x_1 = 0$ and $x_{ne+1} = 1$. To apply the orthogonal collocation with in ℓ^{th} element, a variable $u = \frac{x - x_\ell}{x_{\ell+1} - x_\ell}$ is introduced in ℓ^{th} element in such a way that as x varies from x_ℓ to $x_{\ell+1}$, u varies from 0 to 1, as shown in Fig. 2.

Then the orthogonal collocation is applied within each element. The Hermite polynomials are C^1 continuous; therefore the trial function and its first derivative are automatically continuous at the nodal points or at the boundaries of the elements.

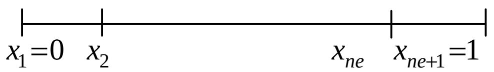

Fig. 1. Finite elements on global domain.

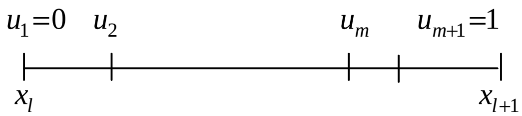

Fig. 2. Orthogonal collocation on local domain.

IV. SOLUTION OF MATHEMATICAL MODEL

The equations of the model given by equations (1-4) are initially put in the dimensionless form using following dimensionless variables:

$$c=\frac{C-C_s}{C_0-C_s};\; x=\frac{X}{L};\quad t=\frac{UT}{L};\quad P=\frac{UL}{D}$$

The mathematical equations in the dimensionless form can be rewritten as:

$$\frac{1}{P}\frac{\partial^2 c}{\partial x^2}=\frac{\partial c}{\partial x}+\frac{\partial c}{\partial t} \qquad \ldots(5)$$

The boundary conditions in dimensionless form are given below:

$$Pc-\frac{\partial c}{\partial x}=0 \qquad \text{at } x=0 \qquad \ldots(6)$$

$$\frac{\partial c}{\partial x}=0 \qquad \text{at } x=1 \qquad \ldots(7)$$

Now, to solve the system of two point boundary value problem given by equation (5) along with the boundary conditions given by (6) and (7), the method of orthogonal collocation on finite elements with Hermite basis is used. The approximate solution $c(x,t)$ is taken as:

$$c(x,t)=c(u,t)=\sum_{i=1}^{4}a_i(t)H_i(u)$$

where $a_i(t)$'s are the unknown parameters, yet to be determined. The Hermite basis functions are defined as follows:

$$H_1(u)=(1-u)^2(1+2u)$$

$$H_2(u)=u(1-u)^2 h_l$$

$$H_3(u)=u^2(3-2u)$$

$$H_4(u)=u^2(u-1)h_l$$

Within each element zeros $V_2=\frac{1}{2}(1-\frac{1}{\sqrt{2}})$ and $V_3=\frac{1}{2}(1+\frac{1}{\sqrt{2}})$ of shifted Chebyshev polynomial $T_2(x)=2(2x-1)^2-1,$ are used as collocation points. The end points of the elements are denoted by $V_1=0$ and $V_4=1$. The Chebyshev polynomials are used because these have the tendency to keep the error down to minimum at the corners.

After applying OCFE following discredited form of the model is obtained:

$$\sum_{i=1}^{4}H_i\frac{da_i^{(k)}}{dt}=\frac{1}{Ph_k^2}\sum_{i=1}^{4}a_i^{(k)}B_{ji}-\frac{1}{h_k}\sum_{i=1}^{4}a_i^{(k)}A_{ji} \qquad \ldots(8)$$

where $k=1,2$ and $j=2,3,4,5$. The discretized form of differential algebraic equation (DAEs) is solved with MATLAB 15s system solver software.

V. RESULTS AND DISCUSSION

The dimensionless model equation (8) of longitudinal mixing is solved with the method of orthogonal collocation on finite elements using Hermite basis. The results obtained from present study are compared, for P = 25, with the analytic results of Brenner [3] and those of Singh *et.al.* [16] using MATLAB 'pdepe' solver. The results are listed in Table 1. From Fig. 3 it can be seen that the Hermite basis results are matching upto t=0.6 with analytic results and then start deviating. A maximum deviation of 3.79% occurs, which is within the reasonable limits. The percentage error in case of 'pdepe' solver applied by Singh *et.al.* [16] is very large.

Table 1: Comparison for P = 25.

Time (t)	Analytic solution	pdepe solver	Hermite basis
0.0	1.0000	1.0000	1.0000
0.1	1.0000	1.0000	1.0000
0.2	1.0000	1.0000	1.0000
0.3	1.0000	1.0000	1.0000
0.4	1.0000	1.0000	1.0000
0.5	1.0000	0.9996	1.0000
0.6	0.9998	0.9954	0.9998
0.7	0.9935	0.9720	0.9931
0.8	0.9361	0.8950	0.9334
0.9	0.7521	0.7303	0.7460
1.0	0.4721	0.4901	0.4653
1.1	0.2273	0.2467	0.2222
1.2	0.0852	0.0776	0.0803
1.3	0.0259	0.0422	0.0251
1.4	0.0066	-0.0082	0.0064
1.5	0.0014	-0.0027	0.0014

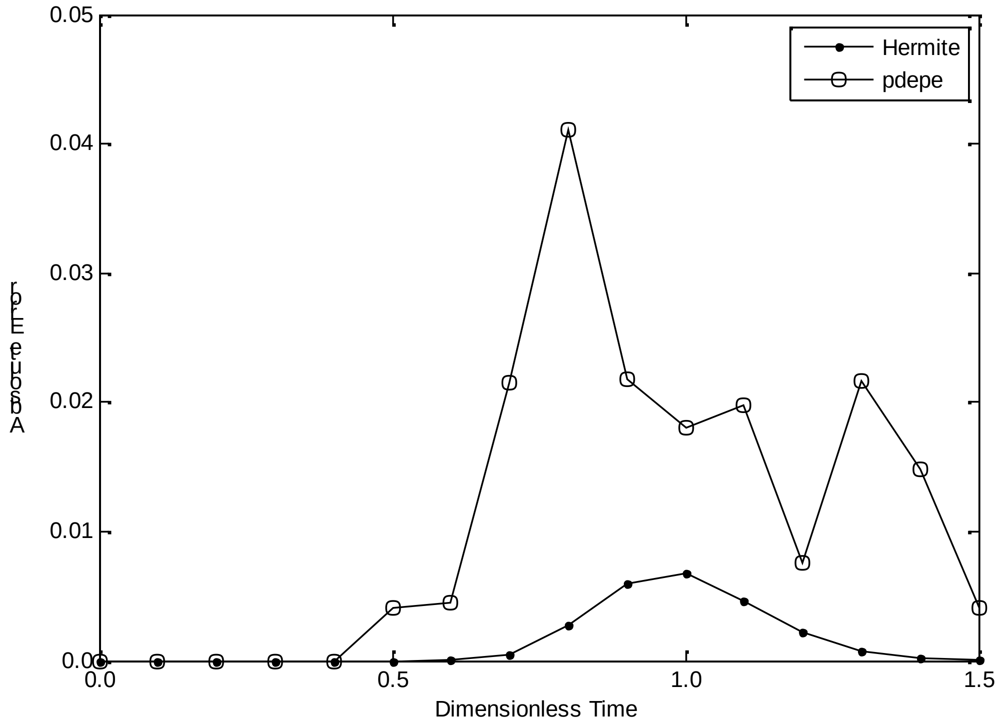

Fig. 3. Comparison of absolute error for Hermite basis and 'pdepe' solver.

VI. CONCLUSION

It can be concluded that the OCFE with Hermite basis can be applied to PDEs with ease and the results are quite comparable with the analytic ones. The present technique gives superior results than the inbuilt 'pdepe' solver of the MATLAB. For future work this technique can be extended to non linear problems for higher order Chebyshev polynomial, which will ultimately reduce the computational time.

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