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SHORT COMMUNICATION

The use of cubic spline and far-side boundary condition for the collocation solution of a transient convection-diffusion problem

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Abstract−Cubic spline collocation method with the far-side boundary condition has been proposed as a numerical method for the convection-dominant convection-diffusion problem. It has been shown that the proposed method can give highly accurate result for very large Peclet number problems by effectively suppressing the undesired ripple that is commonly observed in ordinary orthogonal collocation method.

Key words: Convection-diffusion Problem, Boundary Condition, Cubic Spline, Numerical Solution

INTRODUCTION

A variety of numerical methods have been presented for the solution of transient convection-diffusion problems. The governing equation given by a second-order partial differential equation (PDE) is solved numerically using two different types of techniques. In the method of lines (MOL) [1], the space dimensions are discretized by a method such as finite difference method (FDM), finite element method (FEM), orthogonal collocation method (OCM), and others to obtain a set of ordinary differential equations (ODE's) in time. Alternatively, both the space and time dimensions are discretized to obtain a set of nonlinear algebraic equations. The numerical solution by the MOL can be stiff with time due to the diffusion terms and steep in the spatial direction due to convection [2]. It might produce spurious oscillations in a convection dominant case due to the difficulty of chasing the steep profile. In this respect, discovering a successful numerical technique for the convection-dominant problem has been considered one of the challenging research subjects [3]. Special high-resolution FDM's such as essentially non-oscillatory and total variation diminishing have been suggested and applied to the convection-dominant problems [4,5]. Also the spline collocation method has been proposed by Soliman [6] for a static convection-diffusion problem. The collocation method which is classified as a method of weighted residuals [7] has several important advantages over the other discretization methods for simple geometry cases. It can provide an accurate solution with a small number of collocation points, gives continuous solutions, and easily handles general boundary conditions while still being simple to program [8]. In addition, the collocation method generates a low-order ODE model which can be conveniently used for real-time control and optimization. In spite of these advantages, it is prone to generate spurious oscillations in the solution for the convection-dominant case.

The aim of the present study is to propose the cubic spline collocation method (CSCM) and a new numerical boundary condition (BC) named far-side BC to improve the performance of the reduced-order ODE model for a convection-dominant transient convection-diffusion system. In the CSCM, the interpolation function is given as a concatenation of piecewise cubic polynomials defined over each subdomain such that the adjacent polynomials satisfy some smoothness conditions, called cubic spline conditions, at the connecting points. Hence, the CSCM provides a much smoother solution by using multiple cubic splines than the OCM, which approximates a true profile by a single high-order polynomial. The far-side BC is a finite approximation of the zero-slope condition at infinity, which is valid for many convection-diffusion problems. This BC can be easily adopted in the CSCM. The effectiveness of the proposed methods is demonstrated through numerical study.

TRANSIENT DIFFUSION-CONVECTION PROBLEM

We consider the following PDE describing the transient behavior of solute concentration in a one-dimensional adsorption system such as simulated moving bed (SMB) process:

$$\varepsilon\frac{\partial y}{\partial \hat{t}}+(1-\varepsilon)\frac{\partial q}{\partial \hat{t}}+\varepsilon u\frac{\partial y}{\partial \hat{z}}-\varepsilon D\frac{\partial^2 y}{\partial \hat{z}^2}=0 \tag{1}$$

where y and q represent the solute concentrations in the bulk and adsorbent phases, respectively; ε and D denote the overall void fraction of the bed and the diffusion coefficient, respectively; u represents the linear velocity of the moving phase. Let us assume that y and q are partitioned according to the following linear adsorption isotherm:

$$q=Hy \tag{2}$$

Substituting Eq. (2) into Eq. (1) and rearranging Eq. (1) using the dimensionless space coordinates, $z\triangleq\hat{z}/L$, where L is the column length, and dimensionless time $t\triangleq\dfrac{\varepsilon D/L^2}{\varepsilon+(1-\varepsilon)H}\hat{t}$ give

$$\frac{\partial y}{\partial t}+P_e\frac{\partial y}{\partial z}-\frac{\partial^2 y}{\partial z^2}=0 \tag{3}$$

where $P_e\triangleq uL/D$ denote the Peclet number. The initial and boundary conditions for this problem are usually given as

$$y(0, z)=y_I(z) \tag{4}$$

$$y(t, 0)=y_0(t) \tag{5}$$

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$$\frac{\partial y(t,1)}{\partial z}=0 \tag{6}$$

The BC in Eq. (6) needs more contemplation. Nevertheless, it is generally taken under the assumption that the column is sufficiently long irrespective of the reality.

CUBIC SPLINE COLLOCATION AND FAR-SIDE BOUNDARY CONDITION

1. Cubic Spline Collocation

The idea of the collocation method is to approximate the PDE solution using a parameterized interpolation function $\bar{y}(z;\ \theta(t))$ such that the residual of Eq. (3) obtained by substituting y(t, z) with the interpolation function vanishes at pre-specified collocation points. In the ordinary OCM, a polynomial in z is used for the interpolation function and the collocation points are chosen as the zeros of an orthogonal polynomial. In the OCM, the degree of the interpolation polynomial increases with the number of collocation points. This may result in undesirable ripples in the resulting approximate solution. The CSCM is same as the OCM except that the cubic spline function is used as the interpolation function. The cubic spline func- tion is a concatenation of piece-wise cubic poly- nomials whose derivatives from the zeroth to the second-order are continuous at the nod- al points where adjacent two piece-wise cubic polynomials are con- nected. If the domain [0, 1] is divided into n intervals and the cor- responding nodes are defined as $z_0=0$, $z_1, \ldots, z_{n-1}$, $z_n=1$, the cubic spline is described as follows:

$$\bar{y}(z;\ 0)\triangleq\sum_{k=0}^{n-1}\theta_k p_k(z)S_k(z) \tag{7}$$

where $S_k(z)=1$ over $[z_k, z_{k+1}]$ and 0 otherwise; $p_k(z)$ denotes a cubic polynomial that satisfies

$$p_{i-1}(z_i)=p_i(z_i),\ p_{i-1}^{(1)}(z_i)=p_i^{(1)}(z_i),\ p_{i-1}^{(2)}(z_i)=p_i^{(2)}(z_i),$$
$$i=1,\ \ldots,\ n-1 \tag{8}$$

where the superscript $^{(j)}$ denotes the j^{th}-order derivative. Since the degree of the piecewise polynomials is limited to three and strong smoothness conditions are imposed at each node, the cubic spline is inherently smooth and ripple is suppressed though not completely eliminated.

Each cubic polynomial has four coefficients. Therefore, when there are n intervals, we have 4n coefficients to determine. The above spline condition specifies 3(n−1) relations for the coefficients. Collocation condition at the n–1 internal points and the BC at two boundary points provide n+1 conditions. Hence, two more conditions are needed to uniquely determine the cubic polynomials. In this study, we introduced the following conditions:

$$p_0^{(2)}(z_0=0)=p_{n-1}^{(2)}(z_n=1)=0 \tag{9}$$

The collocation points may be chosen differently from the nodal points for the cubic spline. In this study, both points were taken to be same.

After some straightforward manipulations, the interpolation function can be parameterized with the output at the collocation points as follows [9]:

$$\bar{y}(z)=\mathbf{M}(z)^T\mathbf{Y} \tag{10}$$

where $\mathbf{M}(z)$ is an (n+1)×1 vector and $\mathbf{Y}$ represents $[y(t, z_0)\ y(t, z_1) \ldots y(t, z_n)\ ]^T$. From the above relation, we have

$$\frac{\partial \mathbf{Y}}{\partial z}=\begin{bmatrix}\mathbf{M}^{(1)}(z_0)^T\\ \vdots \\ \mathbf{M}^{(1)}(z_n)^T\end{bmatrix}\mathbf{Y}\triangleq\bar{\mathbf{A}}\bar{\mathbf{y}},\ \frac{\partial^2 \mathbf{Y}}{\partial z^2}=\begin{bmatrix}\mathbf{M}^{(2)}(z_0)^T\\ \vdots \\ \mathbf{M}^{(2)}(z_n)^T\end{bmatrix}\mathbf{Y}\triangleq\bar{\mathbf{B}}\mathbf{Y} \tag{11}$$

The requirement that the residual is zero at the collocation points leads Eq. (3) to

$$0=\frac{\partial \mathbf{Y}}{\partial t}+P_e\frac{\partial \mathbf{Y}}{\partial z}-\frac{\partial^2 \mathbf{Y}}{\partial z^2}\rightarrow\frac{d\mathbf{Y}}{dt}=(-P_e\bar{\mathbf{A}}+\bar{\mathbf{B}})\mathbf{Y}=\bar{\mathbf{D}}\mathbf{Y} \tag{12}$$

Indeed, the above ODE holds only at the internal points (from z_1 to z_{n-1}) while the boundary conditions hold on the boundaries. After the boundary conditions are applied, Eq. (12) is reduced to

$$\frac{d\mathbf{y}}{dt}=\mathbf{D}\mathbf{y}+\mathbf{b}y_0(t),\ \mathbf{y}=\begin{bmatrix}y(t,z_1)\\ \vdots \\ y(t,z_{n-1})\end{bmatrix} \tag{13}$$

2. Far-side Boundary Condition

In most convection-diffusion problems, the BC in Eq. (6) is valid only when the column is long enough or the concerned process is specially designed for the condition to be enforced. Nevertheless, the condition has been exclusively adopted for this type of problems even when the column is not sufficiently long. As shall be seen later, application of Eq. (6) compels the profile of y to be flat at z=1 and may induce undesirable ripples in the inner region. In fact, a finite-length column can be considered as a cut of an infinite-length column. Hence, the physically more correct BC for most convection-diffusion problems is

$$0=\left.\frac{\partial y(t,z)}{\partial z}\right|_{z\to\infty}\approx\frac{\partial y(t,z_L)}{\partial z}\ \text{ for a sufficiently large } z_L \tag{14}$$

For finite difference/element/volume methods, Eq. (14) increases complexity since the region, $(1, z_L)$ should be discretized, too. However, the collocation method has no problem in adopting the above condition. For the CSCM, we have

$$\frac{\partial \bar{y}(t,z_L)}{\partial z}=\mathbf{M}(z_L)^T\mathbf{Y}=0 \tag{15}$$

RESULTS AND DISCUSSION

In Fig. 1, responses of y(t, z) by the regular OCM and CSCM, and the CSCM with the far-side BC to a step change in $y_0(t)$ are compared for $P_e=75$. For such a high Peclet number, the true solution represents a simple plug flow profile with minor axial dispersion effect. Hence the solution cannot contain any ripples as far as the BC at z=0 doesn't changes sinusoidally. The set of ODE's from the collocation approximation was solved using the Runge-Kutta 4^{th}-order method (in MATLAB). All the results in the figures were obtained with n=7. For the regular OCM and CSCM, however, $z_n=1$ is chosen as a boundary while for the CSCM with the far-side BC, $z_n=z_L=10$ was taken as a boundary. As given in the figure, the OCM uses the zeros of the n^{th}-order Legendre polynomial as the collocation points whereas the CSCM's use the equi-distance points

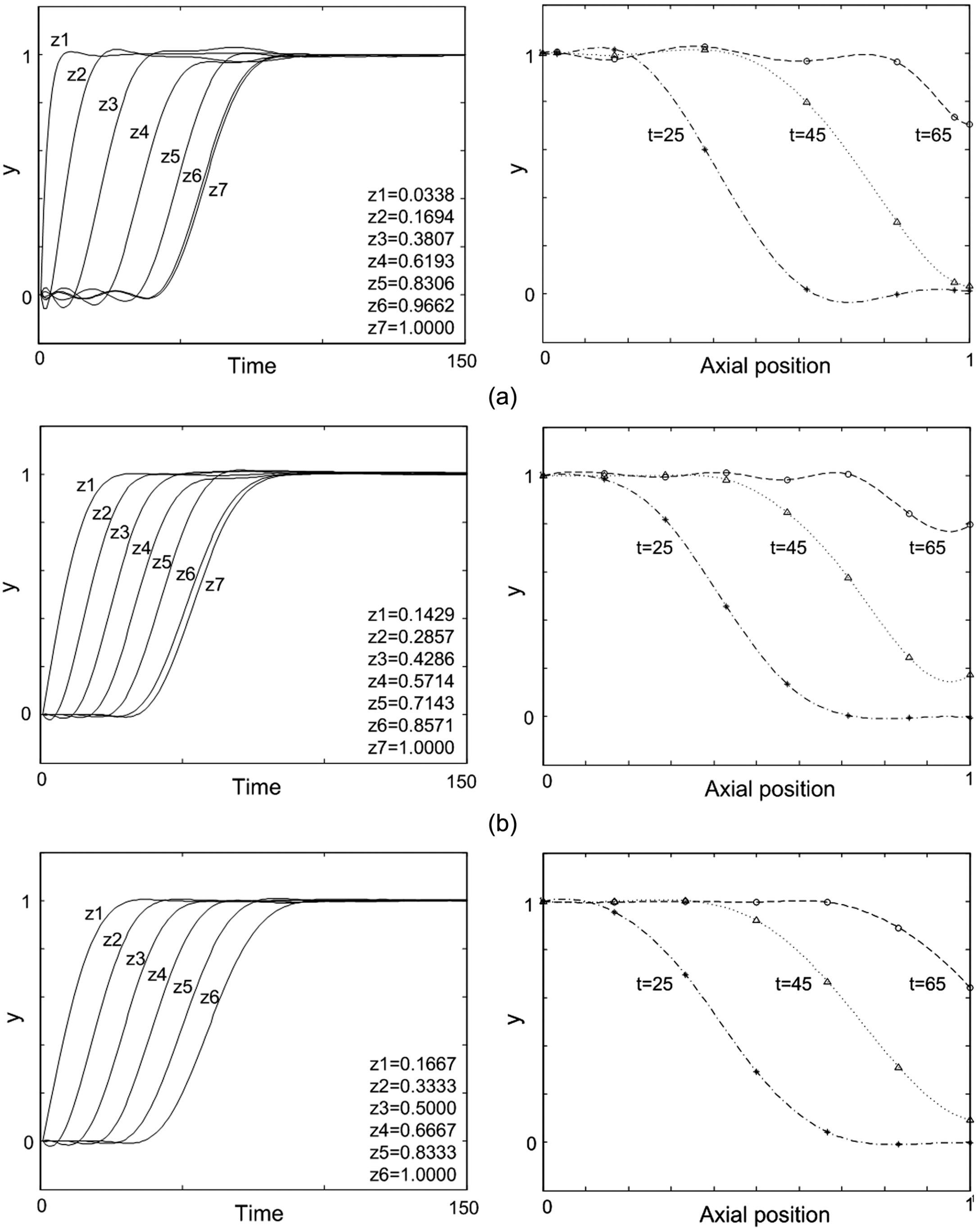

Fig. 1. Response of y(t) to a step change in $y_0(t)$ when $y_I(z)$=0 and P_e=75; (a) OCM (b) CSCM with traditional BC in (6) (c) CSCM with far-side BC in (14).

over [0, 1] with or without z_L as collocation points. The CSCM show better profiles than the OCM with unrealistic ripples effectively suppressed though not completely. Comparison of the axial profiles shows that the inherent smoothness of the cubic splines yields such a result. It can be seen that the far-side BC enhances the performance of the numerical model even more.

In Fig. 2, performance of the three different approximations are compared for P_e=225. It lucidly shows the merits from the CSCM with the far-side BC. Although **y** oscillates all through the time by the very high Peclet number, the CSCM with the far-side BC could produce most physically correct profiles among the three approximations.

Existence of oscillatory modes can be determined by the complex eigenvalues in **D** in Eq. (13). In Table 1, we present the range of P_e that gives non-oscillatory stable solution when n=5 and 15, respectively. It can be seen that the CSCM can stand severer convection-dominant problems without oscillation than the OCM. An interesting result is that the choice of BC does not show any con-

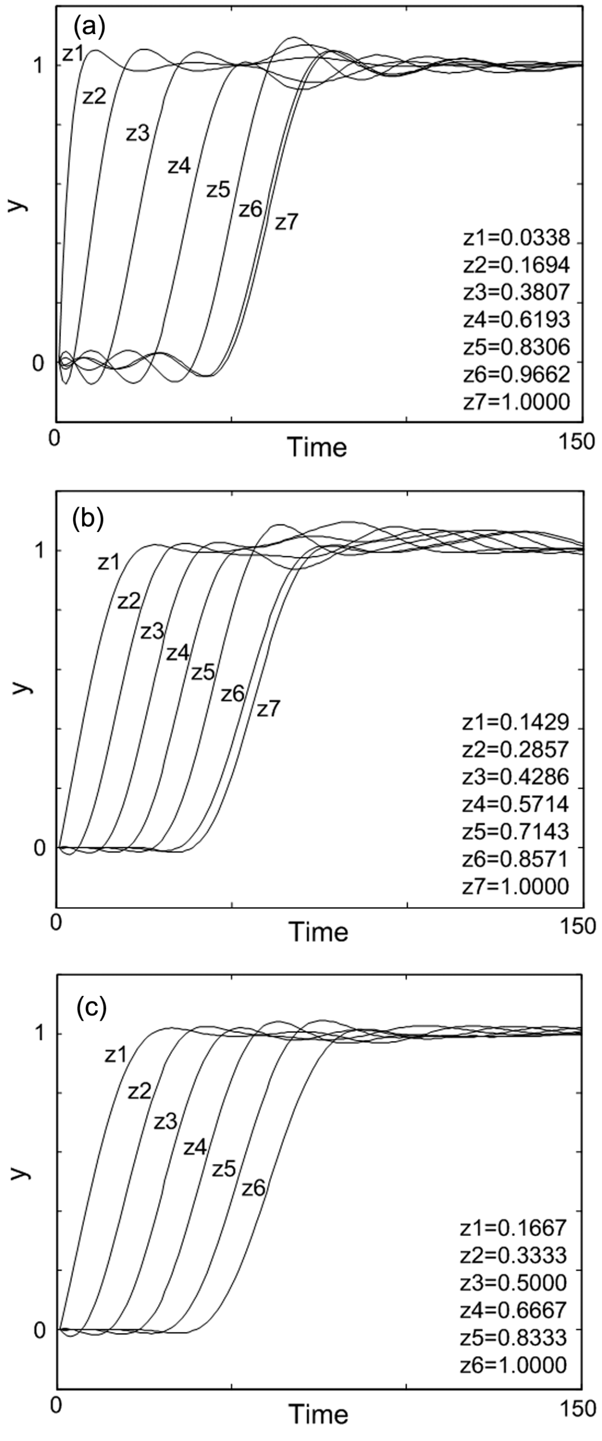

Fig. 2. Response of y(t) to a step change in $y_0(t)$ when $y_I(z)=0$ and $P_e=225$; (a) OCM (b) CSCM with traditional BC in (6) (c) CSCM with far-side BC in (14).

spicuous effect on the suppression of oscillation. However, numerical study has revealed that although the complex eigenvalues begin to appear with the almost same P_e values, the oscillation develops more slowly with the far-side BC than with the traditional BC.

An additional interesting result is that the CSCM with the far-side BC gives numerically stable solution for very large number of collocation points. With MATLAB coding, the OCM starts to produce numerically unstable results from n=29 whereas the CSCM gives stable results for any number of collocation points we have tested. Fig. 3 shows the result with n=200 by the CSCM with the BC at z_L=10 when P_e=7500.

Finally, to find how accurately can the proposed CSCM with far-side BC approximate the true solution, we considered the following steady state problem:

$$P_e\frac{\partial y}{\partial z}-\frac{\partial^2 y}{\partial z^2}-ky=0 \text{ with } y(0)=1,\ \left.\frac{\partial y}{\partial z}\right|_{z=\infty}=0 \qquad (16)$$

Table 1. Range of P_e that gives non-oscillatory stable profile

	OCM with (6)	CSCM with (6)	CSCM with (14)
n=5	$P_e \le 7.23$	$P_e \le 18.00$	$P_e \le 18.00$
n=15	$P_e \le 11.15$	$P_e \le 45.24$	$P_e \le 45.30$

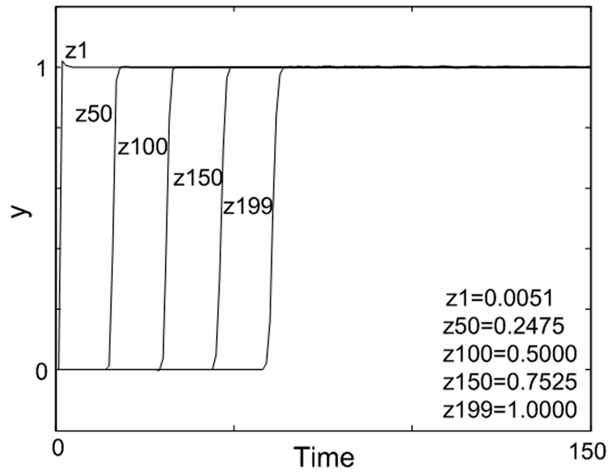

Fig. 3. Response of y(t) to a step change in $y_0(t)$ for the case of P_e= 7500 when the CSCM with the far-side BC with n=200 is used.

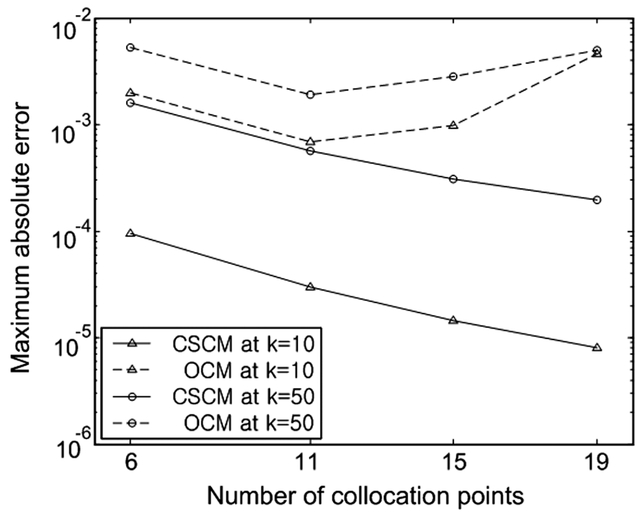

Fig. 4. Maximum absolute errors of approximate solutions by the CSCM with far-side BC and the OCM compared with the analytic solution to $P_e(\partial y/\partial z)-(\partial^2 y/\partial z^2)-ky=0$ with P_e=75.

In Fig. 4, the maximum absolute errors of the approximate solutions are compared with the analytic solution $y(z)=\exp\left(\frac{P_e-\sqrt{P_e^2+4k}}{2}z\right)$. The approximate solutions were obtained by the CSCM with far-side BC and the normal OCM for P_e=75 and k=10 and 50. As can be observed, the CSCM yields much smaller error than the OCM and, in addition, decreases the error monotonically with increasing the number of collocation points while the OCM does not.

CONCLUSIONS

In this paper, a cubic spline collocation method with the far-side boundary condition has been proposed for numerical solution of convection-dominant convection-diffusion problem. Numerical study with a one-dimensional adsorption system shows that the proposed method represents the very steep concentration profile of the concerned system more correctly by effectively suppressing the unrealistic oscillation. The proposed method is useful not only in obtaining numerical solutions but also in deriving a reliable reduced-order model that can be used for real-time optimization and/or control of a convection-dominant convection-diffusion system such as simulated moving bed process.

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