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An Effective Numerical Technique for Boundary Value Problems Arising from an Adiabatic Tubular Chemical Reactor Theory

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Abstract
Mathematical models for an adiabatic tubular chemical reactor which forms an irreversible exothermic reaction are investigated by an efficient numerical technique, Fibonacci Collocation method. The reaction's steady-state temperature is calculated for several values of three parameters, namely, Peclet and Damkohler numbers and the dimensionless adiabatic temperature increment. When the generated outcomes are compared with the other numerical approaches, it has been sighted that the presented method produces reliable results for this type of problems.

1. Introduction

It is presented a model for an irreversible exothermic reaction produced by an adiabatic tubular chemical reactor [1]. This model can be turned into a BVP of second order [2], as shown below,

$$\begin{cases} y''(x)-\lambda y'(x)+\lambda\mu\left(\beta-y(x)\right)e^{y(x)}=0 \\ y'(0)-\lambda y(0)=0, \quad y'(1)=0, \end{cases} \tag{1}$$

where y is the reaction's steady-state temperature, λ is Peclet number, μ is the Damkohler number and β is the adiabatic temperature increase with no dimensions. The existence of the numerical solutions to (1) for a specific range has been demonstrated by the authors [2]-[3]. In recent years, this equation has been dealt with many numerical methods [4]-[11].

In this study, the problem (1) is solved by Fibonacci collocation method [12]-[15]. Numerical illustrations are carried out to validate the accuracy of the proposed numerical scheme. The reaction's steady-state temperature is calculated for several values of λ, μ and β. The obtained numerical outcomes are compared with the well-known numerical approaches and it has been shown that the results reflect the adequacy of the method and give high accuracy.

The outline of the paper is as follows: In Section 2, Fibonacci collocation method is presented. Section 3 is devoted to the applications of the method for the Adiabatic Tubular Chemical Reactor problem. The conclusions are given in Section 4.

2. Fibonacci Collocation Method

The approach to a function can be suggested with the help of Fibonacci polynomials [16]-[17] as,

$$y(x)\cong y_N(x)=\sum_{n=1}^{N+1} c_n\, F_n(x) \tag{2}$$

where N indicates the approximation polynomial's order. Fibonacci polynomials are identified as

$$F_n(x)=\sum_{k=0}^{n} F(n,k)x^k \tag{3}$$

here, $F(n,k)=\begin{pmatrix} n+k-1 \\ 2 \\ k \end{pmatrix}$. The recurrence relationship is,

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$$\begin{aligned} F_1 &= 1, \\ F_2 &= x, \\ &\vdots \\ F_n(x) &= x\,F_{n-1}(x) + F_{n-2}(x) \quad n \geq 3. \end{aligned} \tag{4}$$

(2) can be expressed as a matrix form,

$$y_N(x) = \mathbf{F.C} \tag{5}$$

where $\mathbf{F}(x) = \begin{bmatrix} F_1(x) & F_2(x) & \cdots & F_{N+1}(x) \end{bmatrix}$ and $\mathbf{C} = \begin{bmatrix} c_1 & c_2 & \cdots & c_{N+1} \end{bmatrix}$. Also, Fibonacci polynomials can also be written as a matrix form,

$$\mathbf{F} = \mathbf{PM} \tag{6}$$

and,

$$\mathbf{M} = \begin{pmatrix} 1 & 0 & 1 & 0 & 1 & 0 & 1 & \cdots \\ 0 & 1 & 0 & 2 & 0 & 3 & 0 & \cdots \\ 0 & 0 & 1 & 0 & 3 & 0 & 6 & \cdots \\ 0 & 0 & 0 & 1 & 0 & 4 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 1 & 0 & 5 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \tag{7}$$

$$\mathbf{P}(x) = \begin{bmatrix} 1 & x & \cdots & x^N \end{bmatrix}.$$

With the help of (5) and (6), the derivatives of $y_N(x)$ can be given as,

$$y_N^{(k)}(x) = \mathbf{P}^{(k)}(x)\mathbf{MC} = \mathbf{P}(x)\mathbf{B}^k\mathbf{MC} \tag{8}$$

Here, $\mathbf{B}^0$ is identity matrix of size $(N+1)$ and

$$\mathbf{B} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 4 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & 5 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & N \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}. \tag{9}$$

When the collocation points are taken as $x_j = \frac{j}{N}$, $j = 0,1,...,N$, the value of $y_N^{(k)}(x_j)$ can be defined as,

$$y_N^{(k)}(x_j) = \mathbf{P}^{(k)}(x_j)\mathbf{MC} = \mathbf{P}(x_j)\mathbf{B}^k\mathbf{MC} \tag{10}$$

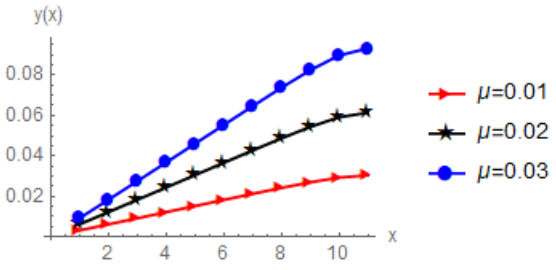
By using (10) in the problem (1), given BVP is transformed into $(N+1)$ algebraic equations. Any suitable root finding method can be used to find $(N+1)$ unknowns of the approximation polynomials.

3. Applications of the Fibonacci Collocation Method for the Adiabatic Tubular Chemical Reactor Problem

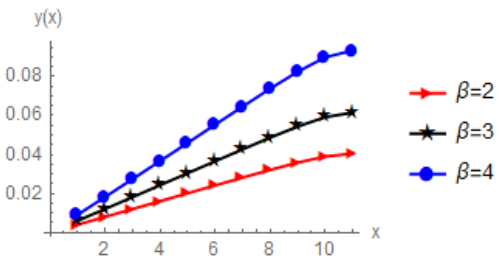
The Fibonacci collocation method is applied to the Adiabatic Tubular Chemical Reactor problem in this section. To indicate the accuracy and applicability of the present method, the maximum absolute residual errors are calculated, which is defined by,

$$ME_N = \max_{0 \leq x \leq 1} \left| \begin{matrix} y_N''(x) - \lambda y_N'(x) \\ +\lambda\mu\left(\beta - y_N(x)\right)e^{y_N(x)} \end{matrix} \right| \tag{11}$$

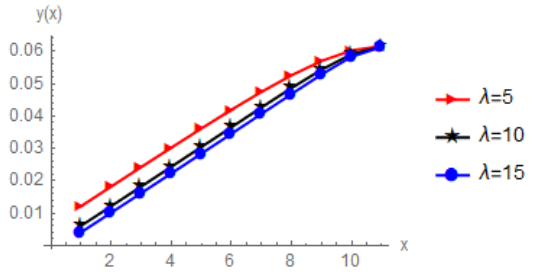
The numerical results of the method ($N = 12$) for different values of β, λ and μ are given in Figure 1 and the comparisons of the numerical results of the presented method (for $N = 13$) with Taylor Wavelet Method (TWM), B-Spline Wavelet, Adomian Method (ADM), Shooting Method, the contraction mapping principle (CMP), Sinc-Galerkin Method, Chebyshev Finite Difference Method (CFDM) for $\lambda = 10, \beta = 3, \mu = 0.02$ are given in Table 1. Besides, absolute residual errors in logarithm base 10 ($\log_{10}|err|$) are given in Figure 2 for the different values of N.



a) $\beta = 3, \lambda = 10$



b) $\lambda = 10, \mu = 0.02$



c) $\beta = 3,\ \mu = 0.02$

Figure 1. The numerical outcomes of the present method ($N = 12$) for a) $\beta = 3, \lambda = 10$ and different values of μ, b) $\lambda = 10,\ \mu = 0.02$ and different values of β and c) $\beta = 3,\ \mu = 0.02$ and different values of λ.

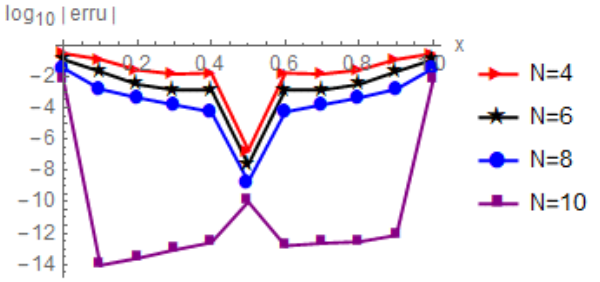


Figure 2. The absolute errors in the logarithm base 10 ($\log_{10}|err|$) different numbers of polynomial degrees (N).

Table 1. The comparison of the numerical outcomes for $\lambda = 10,\ \beta = 3,\ \mu = 0.02$.

x	TWM	B-Spline Wavelet	ADM	Shooting	CFDM	Sinc-Galerkin $N = 20$	Present Method $N = 13$
0	0.006048	0.006045	0.006048	0.006048	0.006048	0.006048	0.006048
0.2	0.018192	0.018194	0.018192	0.018192	0.018192	0.018192	0.018192
0.4	0.030424	0.030424	0.030424	0.030424	0.030424	0.030424	0.030424
0.6	0.042669	0.042675	0.042669	0.042669	0.042669	0.042669	0.042669
0.8	0.054332	0.054332	0.054371	0.054371	0.054371	0.054371	0.054371
1	0.061458	0.062030	0.061458	0.061458	0.061458	0.061458	0.061458

4. Conclusion and Suggestions

The boundary value problem arising from an adiabatic tubular chemical Reactor Theory is solved by an effective and robust technique, Fibonacci collocation method. From numerical results, it can be observed that the this problem is influenced by λ, μ and β. The numerical results reveal that the presented technique achieves high accuracy. Moreover, the presented numerical scheme is capable of solving this type of models.

Statement of Research and Publication Ethics

The study is complied with research and publication ethics

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