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A novel numerical technique for adiabatic tubular chemical reactor problems

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Abstract

We proposed a novel technique to obtain highly accurate solution to the problem of an irreversible exothermic chemical reaction occurring in an adiabatic tubular chemical reactor. The study also delves into the convergence behavior and error analysis of this technique. Furthermore, we investigate the approximation of the steady-state temperature of the reaction under various scenarios involving the Peclet and Damkohler numbers, and the dimensionless adiabatic temperature rise. To validate our findings, we compare our results with those obtained using several other established methods, including the Taylor and B-Spline Wavelet Methods, Adomian Method, Shooting Method, Contraction Mapping Principle, Sinc-Galerkin Method, and Chebyshev Finite Difference Method. These comparisons affirm that our proposed technique yields solutions that are not only accurate but also stable and efficient when applied to the specified model.

Subject Classification: *34B15, 65L10, 65L12.*

Keywords: *Chemical reactor, Chebyshev polynomials, Numerical approach, Mathematical modelling.*

1. Introduction

A representation of a non-reversible heat-generating chemical reaction occurring in an adiabatic tubular chemical reactor is presented [1]. This problem can be modelled by the following equation [2] as,

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

Here, the steady state temperature of the reaction is denoted by $y(x)$ and the Peclet and Damkohler numbers are denoted by λ and μ, respectively and the dimensionless increase in adiabatic temperature is represented by β. The existence of the numerical solutions to this problem is studied by [2-4] for a specific range. Recently, many numerical methods are developed to solve this type of equations [5-13].

We introduce an innovative numerical technique to address the problem of solving an irreversible exothermic chemical reaction in a chemical reactor that operates adiabatically in a tubular configuration. The present method is based on Chebyshev Finite Difference Method (CFDM) [13-18], demonstrates C^1 smoothness at the boundaries of each partition akin to splines [19-22], in contrast to CFDM and composite CFDM [23]. The error analysis and convergence of the presented numerical method are discussed. The approximation of the equilibrium temperature of the reaction is depicted for various parameter variations including λ, μ, and β. The numerical results are compared with Taylor Wavelet Method (TWM) [9], B-Spline Wavelet Method (BSWM) [10], Adomian Method (ADM) [11], Shooting Method (SM) [11], Contraction Mapping Principle (CMP) [11], Sinc-Galerkin Method (SGM) [12], Chebyshev Finite Difference Method (CFDM) [13]. The outcomes confirm that the present method has great advantages in terms of accuracy and efficiency.

The article is organized as follows: Smooth Composite CFDM is introduced in Section 2. Section 3 is reserved for the analysis of convergence and error. In Section 4, the results of real life experiments are given comparatively with other methods and the conclusions are discussed in Section 5.

2. Proposed Method

The polynomial approximation can be expressed as,

$$y(x) \cong {\sum_{n=0}^{N}}' a_n T_n(x) \tag{2}$$

where the sign (ʹ) indicates that the first and last terms are subjected to halving and the order of polynomial is denoted by N.

The first kind of Chebyshev polynomials is given as

$$T_m(x) = \cos(m\cos^{-1}(x)), \quad \forall m \geq 0, \qquad x \in [-1,1]. \tag{3}$$

The coefficients a_m can be obtained as

$$a_m = \frac{2}{N}\sum_{i=0}^{N}{}' y(x_i)T_m(x_i). \tag{4}$$

The Composite CFDM is based on splitting of the domain into the M – subdomains with $h = \frac{(b-a)}{M}$. The collocation points are chosen as the extreme values of Chebyshev polynomials, $x_l = \cos(\frac{\pi l}{N}), \quad l = 0,1,\ldots,N$ and they are transferred to the j^{th} subdomain, i.e., $\left[a + \frac{(b-a)j}{M}, a + \frac{(b-a)(j+1)}{M}\right]$ by

$$t_{lj} = \frac{(b-a)}{2M}\left(1 + x_l + 2j\right), \quad j = 0,\ldots,M-1. \tag{5}$$

The computed solution within the i^{th} subdomain is termed as

$$y_i(x) \cong \sum_{m=0}^{N}{}' a_{im}T_m(x), \tag{6}$$

and

$$a_{im} = \frac{2}{N}\sum_{j=0}^{N}{}' y_i(x_j)T_m(x_j). \tag{7}$$

m^{th} order derivative at the nodes x_k can be found as

$$y_i^{(m)}(x_k) = \sum_{j=0}^{N} d_{k,j}^{(m)}\, y_i(x_j), \tag{8}$$

where

$$d_{k,j}^{(m)} = \frac{2}{N}\sum_{n=0}^{N}{}' T_n(x_j)T_n^{(m)}(x_k) \tag{9}$$

and open form of $d_{k,j}^{(m)}$ is given as [24]

$$d_{k,j}^{(m)} = \frac{4q_j}{N}\sum_{n=\lceil m\rceil}^{N}\sum_{i=0}^{N}\sum_{l=0}^{n}\frac{nq_n}{c_i}\frac{(-1)^{n-l}(n+l-1)!\,\Gamma(l-m+\frac{1}{2})}{\Gamma(l+\frac{1}{2})\,(n-l)!\,\Gamma(l-m-i+1)\,\Gamma(l-m+i+1)}T_n(x_j)\;T_i(x_k),$$
$$k,j = 0,1,\ldots,N, \quad i = 1,2,\ldots,N-1. \tag{10}$$

To satisfy smoothness,

$$y_{i+1}^{(r)}(x_N) = y_i^{(r)}(x_0), \qquad r = 0,\ldots,\lfloor m-1\rfloor. \tag{11}$$

must be satisfied. The present approach simplifies the given problem by transforming it into a system comprising (N + 1) algebraic equations with (N + 1) unknowns for each subregion. Consequently, integrating the approximation polynomials yields the general solution, $P_N(x) \in C^{\lfloor m-1 \rfloor}[a,b]$.

3. Examination of Convergence and Error

This section is dedicated to analyzing the convergence and errors of the proposed technique.

Theorem 4.1. (Convergence)

Let $\left|y_i^{(n)}(x)\right| \le C_i$ and $y_i(x) \in L_w^2(-1,1)$. Then, converges to the $y_i(x)$ uniformly when $N \to \infty$. Thus, the convergence of $y(x) = \bigcup_{i=1}^{M} y_i(x)$ is satisfied for the whole range.

Proof: Considering the orthogonality, we get

$$\int_{-1}^{1} T_m(x) y_i(x) w(x) dx = \int_{-1}^{1} \sum_{n=0}^{\infty}{}' T_m(x) a_{in} T_n(x) w(x) dx \tag{12}$$

and then

$$a_{im} = \frac{2}{c_m \pi} \int_0^{\pi} y_i(\cos\theta) \cos m\theta d\theta. \tag{13}$$

Applying the integration by parts n-times gives

$$a_{im} = \frac{1}{\pi c_m 2^{n-2}} \int_0^{\pi} y_i^{(n)}(\cos\theta) \sum_{k=1}^{n+1} \left(\left(-1\right)^{n+k+1} \frac{\Gamma\left(m-k+1\right)}{\Gamma\left(m+n-k+2\right)} (m+n-2k+2) \times \binom{n}{n-k+1} \cos\left(\theta(m+n-2k+2)\right) \right) d\theta. \tag{14}$$

An upper limit for the eq. is acquired as

$$\begin{aligned} \left|a_{im}\right| &= \left| \frac{1}{\pi c_m 2^{n-2}} \int_0^{\pi} y_i^{(n)}(\cos\theta) \sum_{k=1}^{n+1} \left((-1)^{1+k+n} \frac{\Gamma(1-k+m)}{\Gamma(2-k+n+m)} (2-2k+n+m) \right.\right. \\ &\quad \left.\left. \times \binom{n}{1-k+n} \cos((2-2k+n+m)\theta) \right) d\theta \right| \\ &\le \frac{C_i}{c_m} \frac{1}{\pi 2^{n-2}} \int_0^{\pi} \left| \sum_{k=1}^{n+1} \left((-1)^{1+k+n} \frac{\Gamma(1-k+m)}{\Gamma(2-k+n+m)} (2-2k+n+m) \binom{n}{1-k+n} \right.\right. \\ &\quad \left.\left. \cos((2-2k+n+m)\theta) \right) \right| d\theta \\ &\le \frac{C_i}{c_m} \frac{1}{2^{n-2}} \frac{2^n}{\prod_{k=0}^{n-1}(2k+1-n+m)} \le \frac{4C_i}{\prod_{k=0}^{n-1}(2k+1-n+m) c_m} \quad \text{for} \quad m > n-1. \end{aligned} \tag{15}$$

$$\left|a_{im}\right| = \left|\frac{1}{\pi c_m 2^{n-2}}\int_0^{\pi} y_i^{(n)}(\cos\theta)\sum_{k=1}^{n+1}\left((-1)^{1+k+n}\frac{\Gamma(1-k+m)}{\Gamma(2-k+n+m)}(2-2k+n+m)\right.\right.$$
$$\left.\left.\times\binom{n}{1-k+n}\cos((2-2k+n+m)\theta)\right)d\theta\right|$$
$$\leq \frac{C_i}{c_m}\frac{1}{\pi 2^{n-2}}\int_0^{\pi}\left|\sum_{k=1}^{n+1}\left((-1)^{1+k+n}\frac{\Gamma(1-k+m)}{\Gamma(2-k+n+m)}(2-2k+n+m)\binom{n}{1-k+n}\right.\right.$$
$$\left.\left.\cos((2-2k+n+m)\theta)\right)\right|d\theta$$
$$\leq \frac{C_i}{c_m}\frac{1}{2^{n-2}}\frac{2^n}{\prod_{k=0}^{n-1}(2k+1-n+m)} \leq \frac{4C_i}{\prod_{k=0}^{n-1}(2k+1-n+m)c_m} \quad \text{for} \quad m > n-1.$$

Considering (15), a bound for the approximation is obtained as

$$\left|y_i(x)\right| \leq \left|a_{i0}\right| + \ldots + \left|a_{in-1}\right| + \sum_{m=n}^{\infty}\frac{4C_i}{\prod_{k=0}^{n-1}\left(m-n+2k+1\right)c_m} < \infty. \tag{16}$$

Consequently, the solution is bounded by

$$\left|y(x)\right| \leq \max_{1\leq i\leq M}\left|y_i(x)\right| \leq \max_{1\leq i\leq M}\left(\left|a_{i0}\right| + \ldots + \left|a_{in-1}\right| + \sum_{m=n}^{\infty}\frac{4C_i}{\prod_{k=0}^{n-1}\left(m-n+2k+1\right)c_m}\right)$$
$$\leq \left|\overline{a}_0\right| + \ldots + \left|\overline{a}_{n-1}\right| + \sum_{m=n}^{\infty}\left(\frac{4C}{\prod_{k=0}^{n-1}\left(m-n+2k+1\right)c_m}\right) < \infty,$$

where $C = \max_{1\leq i\leq M} C_i$ and $\overline{a}_j = \max_{1\leq i\leq M}\left|a_{ij}\right|$.

Theorem 4.2 (Round-off error)

The Round-off error of $d_{l,j}^{(m)}$ is given as

$$d_{l,j}^{(m)*} - d_{l,j}^{(m)} \leq 2\theta_j\left(\delta - \mathrm{O}\left(\frac{\delta}{N^2}\right)\right)\frac{2N^2+m}{(2m+1)!!}\prod_{r=1}^{m-1}(N^2-r^2), \tag{17}$$

where the exact and calculated values are denoted by $d_{l,j}^{(m)*}$ and $d_{l,j}^{(m)}$, respectively.

Proof: The relation between exact $\left(x_k^*\right)$ and computed values $\left(x_k\right)$ are given as $x_k^* = x_k + \delta_k$, where $\left|\delta_k\right|$ is a small error and $\delta = \max_k \left|\delta_k\right|$.

Then the error of the multiplication can be expressed as

$$\left|x_k^* x_m^* - x_k x_m\right| = \left(\delta_k + \delta_m\right) - O\left(\frac{\delta_k}{N^2}\right) - O\left(\frac{\delta_m}{N^2}\right) \le 2\delta - O\left(\frac{\delta}{N^2}\right) = 2\left(\delta - O\left(\frac{\delta}{N^2}\right)\right). \tag{18}$$

Thus,

$$\begin{aligned} d_{k,j}^{(m)*} - d_{k,j}^{(m)} &= \frac{\theta_j}{N}\sum_{n=0}^{N} \sum_{l=0(n+l+m)\text{ even}}^{n-m} \prod_{i=2-m}^{m-2} \left(n^2-(l+i)^2\right)\frac{\theta_n n}{c_l}\frac{1}{(m-1)!2^{(m-3)}}(-1)^{\left[\frac{kj}{N}\right]+\left[\frac{nl}{N}\right]} \\ &\times\left(\left(\delta_{nj-N\left[\frac{nj}{N}\right]} + \delta_{lk-N\left[\frac{lk}{N}\right]}\right) - \mathrm{O}\left(\frac{1}{N^2}\delta_{nj-N\left[\frac{nj}{N}\right]}\right) - \mathrm{O}\left(\frac{1}{N^2}\delta_{lk-N\left[\frac{lk}{N}\right]}\right)\right) \\ &\le \frac{\theta_j}{N}\left(\delta - \mathrm{O}\left(\frac{\delta}{N^2}\right)\right)\frac{4}{(2m-1)!!}\sum_{n=m}^{N}\theta_n \prod_{r=0}^{m-1}(n^2-r^2) \\ &\le 2\theta_j\left(\delta - \mathrm{O}\left(\frac{\delta}{N^2}\right)\right)\frac{2N^2+m}{(2m+1)!!}\prod_{r=1}^{m-1}(N^2-r^2). \end{aligned} \tag{19}$$

Theorem 4.3 (Truncation Error)

Assume that the numerical solution of $y_i(x)$ for i^{th} interval is defined by $P_N y_i = \sum_{n=0}^{N} a_{in} T_n$. The estimation of the truncation error is provided in reference [25] as,

$$N^{-m} C_i \left\|y_i\right\|_{H_w^{m,N}(-1,1)} \ge \left\|y_i - P_N y_i\right\|_{L_w^2(-1,1)}. \tag{20}$$

Proof: An isomorphism between the spaces $L_w^2(0,2\pi)$ and $L_w^2(-1,1)$ can be defined as

$$\left\|y_i^*\right\|^2_{L_w^2(0,2\pi)} = 2\left\|y_i\right\|^2_{L_w^2(-1,1)}. \tag{21}$$

Further, also maps $H_w^m(-1,1)$ into the $H_p^m(0,2\pi)$, where p represents periodicity. Thus, $y_i \in C^{m-1}[-1,1]$ can be extended to $y_i^* \in C^{m-1}(-\infty,\infty)$ due to the periodicity. We have

$$\left\|y_i^*\right\|_{H_w^m(0,2\pi)} \le C_i \left\|y_i\right\|^2_{H_w^m(-1,1)}. \tag{22}$$

Hence $y_i(x) = \sum_{n=0}^{\infty} a_{in} T_n(x)$ and $y_i^*(\theta) = \sum_{n=0}^{\infty} a_{in}\cos(k\theta)$, then $\left(P_N y_i\right)^* = P_N^* y_i^*$. Thus,

$$\left\|P_N y_i - y_i\right\|_{L^2_w(-1,1)} = \frac{\left\|P^*_N y^*_i - y^*_i\right\|_{L^2_w(0,2\pi)}}{\sqrt{2}} \leq \frac{C_i}{N^m}\left\|y_i^{*(m)}\right\|^2_{L^2_w(0,2\pi)}. \tag{23}$$

Finally, we obtain the following estimate

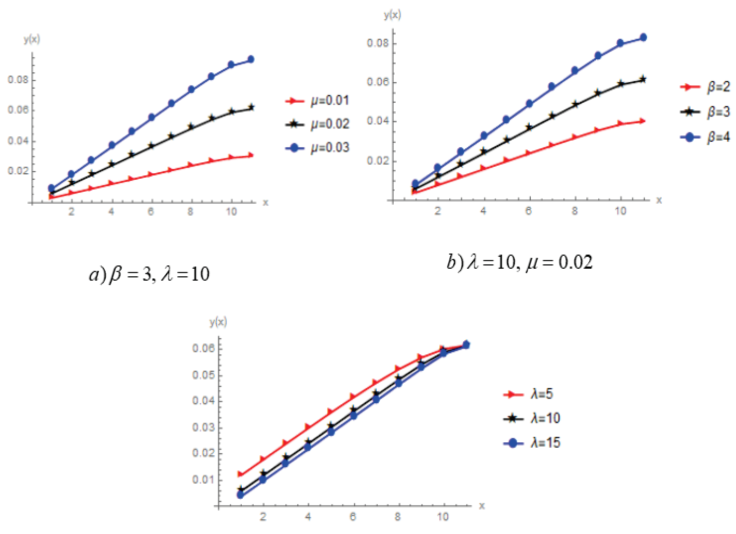
$$\left\|P_N y - y\right\|_{L^2_w(-1,1)} \leq \left\|\bigcup_{i=1}^{M}(P_N y_i - y_i)\right\|_{L^2_w(-1,1)}$$

$$\leq \max_{1\leq i\leq M}\frac{C_i}{N^m}\left\|y_i^{*(m)}\right\|^2_{L^2_w(0,2\pi)} \leq \frac{C}{N^m}\max_{1\leq i\leq M}\left\|y_i^{*(m)}\right\|^2_{L^2_w(0,2\pi)}. \tag{24}$$

4. The real life application of the present method

Adiabatic tubular chemical reactor problem is investigated by the Smooth Composite CFDM. In order to assess the precision and relevance of the proposed technique, the maximum absolute residual errors are established as,

$$ME_n = \max_{0\leq x\leq 1}\left|\bigcup_{n=1}^{M}\left(y_n''(x) - \lambda y_n'(x) + \lambda\mu\left(\beta - y_n(x)\right)e^{y_n(x)}\right)\right|. \tag{25}$$



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

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

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

Figure 1

The numerical outcomes obtained using the current method (N = 8, M = 4) are analyzed for the following scenarios: a) β = 3, λ = 10, with varying values of μ, b) μ = 0.02, λ = 10, with varying values of β and c) μ = 0.02, β = 3, with varying values of λ.

Figure 1 displays the numerical results obtained from the present technique with parameters set to $N = 8$, $M = 4$, across various combinations of β, λ, and μ. Table 1 provides a comparative analysis between the outcomes of the proposed technique and seven other methods (TWM [9], BSWM [10], ADM [11], SM [11], CMP [11], SGM [12], and CFDM [13]) specifically for $\beta = 3$, $\lambda = 10$ and $\mu = 0.02$. The comparison regarding ME_n values of the Smooth Composite CFDM is tabulated in Table 2, considering

Table 1

Comparative analysis of numerical outcomes for $\beta = 3$, $\lambda = 10$ and $\mu = 0.02$.

x	TWM [9]	BSWM [10]	ADM [11]	SM [11]	CMP [11]	SGM [12] $N = 20$	CFDM [13]	Present Method $N = 8$ $M = 4$
0	0.006048	0.006045	0.006048	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	0.018192
0.4	0.030424	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	0.042669
0.8	0.054371	0.054332	0.054371	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	0.061458

Table 2

Comparisons for the Smooth Composite CFDM across various values of N and M, with parameters set to $\beta = 3$, $\lambda = 10$ and $\mu = 0.02$.

N	$M = 1$	$M = 2$	$M = 4$	$M = 8$
2	5.32E–01	4.51E–01	3.49E–01	2.41E–01
3	3.85E–01	2.51E–01	1.29E–01	5.16E–02
4	2.44E–01	1.10E–01	3.31E–02	6.99E–03
5	1.34E–01	3.78E–02	6.22E–03	6.74E–04
6	6.34E–02	1.05E–02	9.12E–04	5.01E–05
7	2.60E–02	2.42E–03	1.09E–04	3.02E–06
8	9.37E–03	4.76E–04	1.09E–05	1.53E–07
9	2.98E–03	8.12E–05	9.54E–07	6.70E – 9
10	8.46E–04	1.22E–05	7.29E–08	2.55E–10

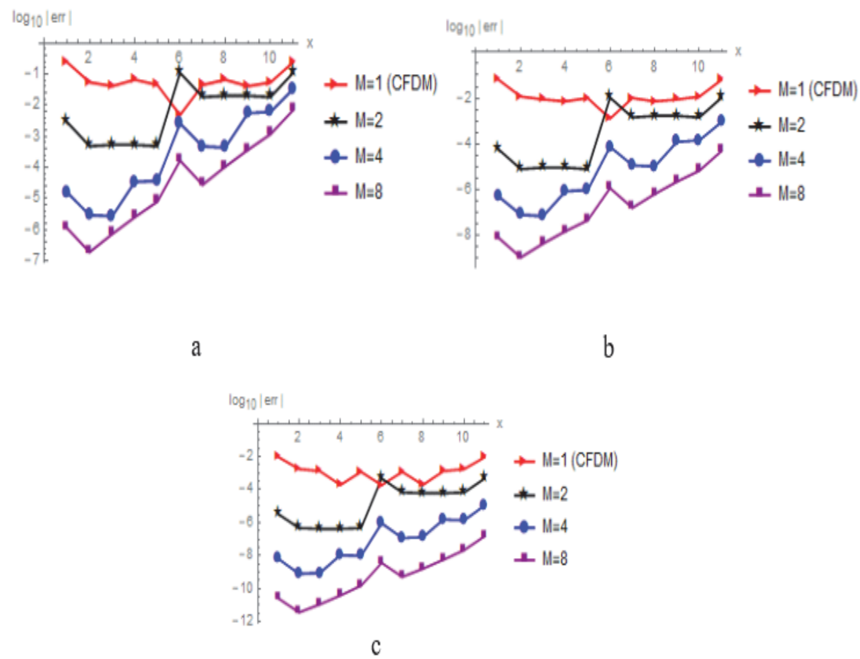


Figure 2

The ME_n for the different M values and $N = 4, 6, 8$ in (a), (b) and (c), respectively.

$\beta = 3$, $\lambda = 10$ and $\mu = 0.02$, along with different combinations of N and M. Lastly, Figure 2 showcases the absolute residual errors in $\log_{10}|err|$ for various combinations of N and M.

The results reveal that the error of the presented method decreases when the order of polynomials or the number of subintervals increases. Comparisons of the Smooth Composite CFDM with the seven mentioned techniques show that the present method gives effective, stable and accurate results.

6. Conclusions

We introduced a new approach, the Smooth Composite CFDM, for addressing the boundary value problem associated with an irreversible exothermic chemical reaction occurring in a tubular chemical reactor operating adiabatically. We also provided analyses on convergence and higher-order error estimation. Additionally, we investigated the approximation of the temperature of the reaction at equilibrium under various scenarios of Peclet and Damkohler numbers, as well as dimensionless adiabatic temperature rise. Comparative evaluations against existing approaches outlined in the existing literature showcase the effectiveness, stability, and accuracy of our proposed method. Taken together, these findings support the notion that our proposed model can be effectively tackled using the introduced numerical technique.

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