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Model order reduction of hyperbolic systems using method of characteristics and differential transform

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Abstract: Convection dominated systems described by first order hyperbolic PDE models are common in chemical engineering. Use of such PDEs in model based control requires a large number of states for its representation and consequently requires significant computational effort. Recently, Sudhakar et al. (2013a,b) have proposed to use method of characteristics (MOC) to obtain reduced order models for such systems and have demonstrated its use in model based control. The implementation of MOC requires the use of repeated solution of initial and boundary value problem. In this work we propose to use differential transform technique to obtain approximate analytical solution for these problems, which result in significant reduction in computational effort. The technique is demonstrated in two case studies involving fixed bed reactor and plug flow reactor. The comparison of dynamic response and the computational load from using DT and numerical integration of the resulting differential equations indicates the effectiveness of using DT in MOC.

Keywords: Hyperbolic PDE, Differential transform, Method of characteristics

1. INTRODUCTION

There are several convection dominated chemical engineering systems which are described by first order hyperbolic PDEs. Use of these PDEs in model based controller design is complicated. For example, distributed controller using feedback linearization approach is designed for hyperbolic PDEs by Christofides and Daoutidis (1998, 1996). The other general approach followed is to obtain a reduced order model for PDEs and design a model based controller based on the reduced order model. However, the resulting approximations are very high dimensional. Recently, Sudhakar et al. (2013a,b) have proposed to use method of characteristic (MOC) for hyperbolic PDEs to obtain lower order model and such lower order model reasonably approximates the higher order solution. Although there are works related to the use of MOC for hyperbolic PDEs (Knuppel et al., 2010; Mohammadi et al., 2010; Fuxman et al., 2007; Shang et al., 2004; Choi, 2007; Choi and Lee, 2005), the approximation proposed by Sudhakar et al. (2013a,b) results in model of significantly lower order. In the application of MOC, initial and boundary value problems are solved repeatedly over smaller intervals. The differential equations for such problems are same over all the intervals but with different initial and boundary conditions in each interval. This requires the initial and boundary value problems to be solved for each interval which increases the computational load significantly.

The use of analytical solutions of differential equations with simple substitution of initial and boundary conditions in each interval could potentially solve the problem with significantly lower computational load. However, the nonlinearity of the differential equations makes it difficult to obtain analytical solutions. An alternative is to use power series solutions. Differential transform (DT) is a technique based on the Taylor series expansion and this finds an approximate analytical solution in series form (Finkel, 2012). The main advantage of this technique is that the coefficient of the Taylor series can be obtained recursively and this results in significantly lower computational load. DT has been used in solving ODEs/BVPs resulting from optimal control problems (Huang et al., 2009; Sudhakar et al., 2012).

The main limitation of DT is that the radius of convergence of the resulting series solution is small. Hence it is difficult to obtain series solution using DT to nonlinear differential equations with larger domain length. However, in the case of MOC, the resulting differential equations are solved over only smaller interval and hence DT is a potentially attractive solution technique. In this contribution, we propose to use DT in the application of MOC for two case studies involving fixed bed reactor and plug flow reactor. The efficiency of the method is illustrated by comparing with the solution obtained using numerical integration in a dynamic simulation.

2. METHOD OF CHARACTERISTICS

MOC is a well-known technique for solving first order hyperbolic PDEs. The PDEs are solved by identifying certain directions called characteristic directions by relating the two independent variables z and t. The advantage is that the state variable can be obtained by integrating appropriate ODEs along these directions. The characteristic lines span the t-z space, and the accuracy of the solution depends on the density of such characteristic lines. The slopes of the characteristic lines depend on the value of the coefficient of the spatial derivative in hyperbolic PDEs. The number of characteristic lines with distinct slopes depends on the number of such distinct coefficient of the spatial derivative. Consider the following first order hyperbolic PDE,

$$\frac{\partial}{\partial t}\begin{bmatrix}\Phi_1\\ \Phi_2\end{bmatrix} = -\begin{bmatrix}\psi_1 & 0\\ 0 & \psi_2\end{bmatrix}\frac{\partial}{\partial z}\begin{bmatrix}\Phi_1\\ \Phi_2\end{bmatrix} + \begin{bmatrix}f_1(\Phi_1,\Phi_2)\\ f_2(\Phi_1,\Phi_2)\end{bmatrix} \quad (1)$$

In the above Eq. 1, Let, $\psi_1 \neq \psi_2$ and then we have characteristic lines with two slopes. Let $z_a(t; z^0, t^0)$ and $z_b(t; z^0, t^0)$ represents the characteristic lines in t-z plane starting from a point (z^0, t^0). Then the equation of the characteristic line $z_a(t; z^0, t^0)$ and the equation for the dependent variable along this line are as follows:

$$\frac{dz_a}{dt}(t; z^0, t^0) = \psi_1 \quad (2)$$

$$\frac{d\Phi_1}{dt}(t, z_a(t; z^0, t^0)) = f_1(\Phi_1, \Phi_2) \quad (3)$$

Similarly equations for the other characteristic line $z_b(t; z^0, t^0)$ are as follows:

$$\frac{dz_b}{dt}(t; z^0, t^0) = \psi_2 \quad (4)$$

$$\frac{d\Phi_2}{dt}(t, z_b(t; z^0, t^0)) = f_2(\Phi_1, \Phi_2) \quad (5)$$

Fig. 1 shows these characteristic lines starting from two points (z_0, t_0) and (z_1, t_0). Since only Φ_1 varies along $z_a(t)$ and only Φ_2 varies along $z_b(t)$, both the variables will be obtained only at the intersection points of these characteristic lines and one such point is shown in Fig. 1 as (z_p, t_p). The solution of Eq. 3 requires the simultaneous variation of Φ_1 and Φ_2 along the characteristic line $z_a(t; z_0, t_0)$ for the evaluation of the function f_1. Since $z_a(t; z_0, t_0)$ represents the variation of only Φ_1 starting from the point (z_0, t_0), the value of Φ_2 needs to be approximated. Similarly, the solution of Eq. 5 requires the simultaneous variation of Φ_1 and Φ_2 along the characteristic line $z_b(t; z_1, t_0)$ for the function f_2 and hence the value of Φ_1 needs to be approximated.

In the approximation proposed in our earlier work (Sudhakar et al., 2013a,b), we allow variation in f_1 and f_2 which improves the solution accuracy and results in significantly lower number of characteristic lines. In this, the value of Φ_2 along the line $z_a(t; z_0, t_0)$ is approximated from the other line $z_b(t; z_0, t_0)$. The arrow lines show the direction of approximation involved. Similarly the value of Φ_1 along $z_b(t; z_1, t_0)$ is approximated from the other line $z_a(t; z_1, t_0)$. This approximation involves only initial value problems along the characteristic lines and is referred to as MOC-1 in this paper. The equation solved along $z_a(t; z_0, t_0)$ is given by,

$$\begin{bmatrix}\frac{d\Phi_1}{dt}(t, z_a(t; z_0, t_0))\\ \frac{d\Phi_2}{dt}(t, z_a(t; z_0, t_0))\end{bmatrix} \approx \begin{bmatrix}f_1(\Phi_1,\Phi_2)\\ (\frac{\psi_1}{\psi_2})f_2(\Phi_1,\Phi_2)\end{bmatrix} \quad (6)$$

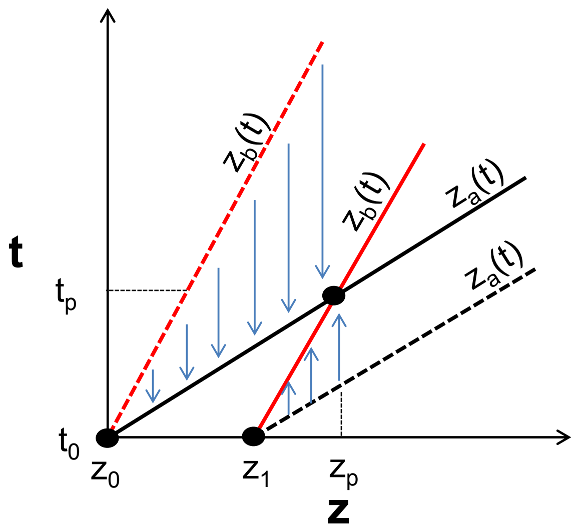

Fig. 1. Schematic figure showing characteristic lines starting from two different points in t-z plane

Equation solved along $z_b(t; z_1, t_0)$ is given by,

$$\begin{bmatrix}\frac{d\Phi_1}{dt}(t, z_b(t; z_1, t_0))\\ \frac{d\Phi_2}{dt}(t, z_b(t; z_1, t_0))\end{bmatrix} \approx \begin{bmatrix}(\frac{\psi_2}{\psi_1})f_1(\Phi_1,\Phi_2)\\ f_2(\Phi_1,\Phi_2)\end{bmatrix} \quad (7)$$

As an alternative, one could solve for Φ_1 at (z_p, t_p) as before by solving initial value problems along $z_a(t; z_0, t_0)$, and based on the values of Φ_1 at (z_p, t_p) and Φ_2 at (z_1, t_0), one could solve a two point boundary value problem to obtain Φ_2 at (z_p, t_p). This technique reduces the approximation along one of the characteristic lines (here $z_b(t; z_1, t_0)$) and hence improves the solution accuracy. This approximation involving initial value problem and boundary value problem is referred to as MOC-2 in this paper.

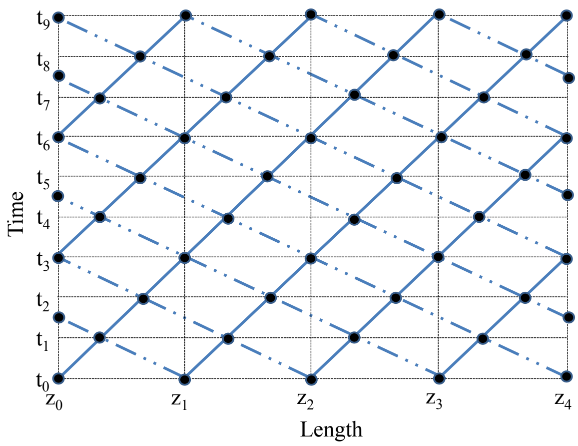

Fig. 2. Schematic figure showing characteristic lines with many intersection points

Now consider the schematic Fig. 2 which represents the characteristic lines (having positive and negative slopes) in the t-z plane with intersection points denoted by '•'. They ' also represent the points where the characteristic lines start. The differential equation solved along these lines takes the initial and boundary condition on these points. Thus in both the approximations (MOC-1 and

MOC-2), the differential equations need to be solved for each characteristic line and need to be restarted from every intersection point where a new initial condition is generated.

3. DIFFERENTIAL TRANSFORM

As in other transform methods, differential transform (DT) converts the original system of differential equations to a different domain. The equations are relatively easier to solve in the transformed domain. The solution to the original differential equations is obtained by inversion. For example, consider the following nonlinear ODE:

$$\frac{dy}{dt} = f(y);\; y(0) = y_o \tag{8}$$

The above differential equation in t domain is converted to algebraic equation in the alternate k domain by the application of DT. The algebraic equation is solved and the inverse transform is used to recover the solution $y(t)$.

Definition 1 (Chen and Ho, 1996) :
If $y(t)$ is a continuously differentiable function, then its DT is given by the following equation,

$$Y(k) = \frac{D^k}{k!}\left(\frac{d^k y(t)}{dt^k}\right)_{t=t_0} \quad \text{where } k = 0, 1, 2, ...\infty \tag{9}$$

where D is the domain length and $Y(k)$ is called k^{th} spectrum of $y(t)$, spectrum or the DT of the function $y(t)$. Application of this definition to (8) results in the following set of algebraic equations:

$$(k+1)Y(k+1) = F(k);\; Y(0) = y_o \tag{10}$$

here $F(k)$ and $Y(k)$ represent the DT of $f(y)$ and $y(t)$ respectively, k represents the order of the derivative of a function. The higher order derivatives of a functions are obtained recursively from the above equation. Use of transform method such as above is expected to provide an alternate way to deal with the solution of nonlinear differential problems. Inverse DT is used which converts the equation from the k domain back to original variables in t domain.

Definition 2 (Chen and Ho, 1996) :
The inverse DT is given by the following equation

$$y(t) = \sum_{k=0}^{\infty}\left(\frac{t-t_0}{D}\right)^k Y(k) \tag{11}$$

In the definition of DT, the index k runs from 0 to ∞. However, in practice k runs from 0 to N, where N is a finite value which represents the number of terms in the Taylor series representation of a function. Further a larger domain length D will require more number of terms in Taylor series for convergence. So it is advantageous to split the domain into several smaller sub-domains with independent Taylor series representation for each of the sub-domain involved.

$$D = \sum_{i=1}^{n} d_i \tag{12}$$

where n is the number of sub-domains. The number of such sub-domain is lower when the domain length D is small. In the application of MOC, the domain length is smaller which result in smaller number of sub-domains (n) with smaller number of Taylor series (N) term in each domain.

Table 1. k-domain expressions used for the case studies in this paper are based on recurrence relations (Finkel, 2012)

Functions $u(t)$	Spectrum $U(k)$
$u(0)$	$U(0) = u(0)$
$u(t) \pm v(t)$	$U(k) \pm V(k)$
$\lambda u(t)$	$\lambda U(k)$
$\frac{d^m u(t)}{dt}$	$\frac{(k+m)!}{k!}U(k+m)$
$u(t)v(t)$	$\sum_{i=0}^{k} U(i)V(k-i)$
$y(t) = u(t)^m$	$Y(0) = U(0)^m$ $Y(k) = \frac{1}{kU(0)}\sum_{j=1}^{k}([(m+1)j-k]$ $U(j)Y(k-j))$ for $k > 0$
$y(t) = e^{u(t)}$	$Y(k) = \frac{1}{k}\sum_{j=1}^{k} jU(j)Y(k-j)$ $Y(0) = e^{U(0)}$

3.1 Pade approximation

Pade approximation is a rational approximation which has higher radius of convergence and requires lesser terms compared to Taylor series expansion. Use of this approximation in DT would accelerate the rate of convergence of series solution in each domain and would result in reduced computational load in the implementation of DT. There are several studies in the literature which have used Pade approximation along with series solution techniques such as DT, Adomian decomposition etc. Wazwaz (1999, 2001) have used Adomian decomposition method along with Pade approximation to get converged results.

4. APPLICATION OF DT TO MOC

As mentioned previously in the section, application of MOC to first order hyperbolic PDE results in the solution of nonlinear ODE along each corresponding characteristic line. This involves repeated solution of ODE for every intersection point and is computationally demanding. DT can provide alternative way to obtain the solution of ODE. We illustrate the application of DT to MOC for two case studies through dynamic simulation of fixed bed reactor and plug flow reactor.

4.1 Application of DT based MOC to adiabatic fixed bed reactor - Dynamic simulation

The mathematical model of adiabatic fixed bed reactor which has characteristic lines with two positive slopes governed by $\psi_1 = \frac{v}{\epsilon}$ and $\psi_2 = v$ (Sudhakar et al. (2013a)) is given by,

$$\frac{\partial C_A}{\partial t} = -\frac{v}{\epsilon}\frac{\partial C_A}{\partial z} - \frac{\rho_b r_A}{\epsilon} \tag{13}$$

$$\frac{\partial C_B}{\partial t} = -\frac{v}{\epsilon}\frac{\partial C_B}{\partial z} - \frac{\rho_b\big(r_B - r_A\big)}{\epsilon} \tag{14}$$

$$\frac{\partial T}{\partial t} = -v\frac{\partial T}{\partial z} + \frac{\rho_b}{\rho C_p}(\Delta H_{r_A} r_A + \Delta H_{r_B} r_B); \tag{15}$$

For this system, the application of MOC results in solving differential equations for each characteristic line. Consider the equation solved along one of the characteristic lines as given by the Eq. 16

$$\frac{d}{dt}\begin{bmatrix} C_A \\ C_B \\ T \end{bmatrix} = \begin{bmatrix} -\dfrac{\rho_b r_A}{\epsilon} \\ -\dfrac{\rho_b(r_B - r_A)}{\epsilon} \\ \dfrac{\rho_b}{\rho C_p \epsilon}(\Delta H_{r_A} r_A + \Delta H_{r_B} r_B) \end{bmatrix} \tag{16}$$

with the nonlinear reaction term is given by

$$r_A = k_1 e^{\frac{-E_1}{RT}} C_A^{n_1} \tag{17}$$

$$r_B = k_2 e^{\frac{-E_2}{RT}} C_B \tag{18}$$

Let $y_1(t) = C_A(t)$, $y_2(t) = C_B(t)$, $y_3(t) = T(t)$, $r_A(t)$ and $r_B(t)$ be variables in time domain and $Y_1(k)$, $Y_2(k)$, $Y_3(k)$, $R_A(k)$ and $R_B(k)$ be the corresponding variables in the k-domain. Let us define the constants in the Eq. 16 as $a_1 = -\frac{\rho_b}{\epsilon}, a_2 = \frac{\rho_b}{\rho C_p \epsilon}$, $b_1 = k_1$, $b_2 = \frac{-E_1}{R}$, $b_3 = k_2$ and $b_4 = \frac{-E_2}{R}$. Application of DT to the Eq. 16 is given by the following equation

$$\begin{bmatrix} Y_1(k+1) \\ Y_2(k+1) \\ Y_3(k+1) \end{bmatrix} = \begin{bmatrix} (\dfrac{d}{k+1})a_1 R_1(k) \\ (\dfrac{d}{k+1})a_1(R_2(k) - R_1(k)) \\ (\dfrac{d}{k+1})a_2(\Delta H_{r_1} R_1(k) + \Delta H_{r_2} R_2(k)) \end{bmatrix} \tag{19}$$

with $Y_1(0) = y_1(0)$, $Y_2(0) = y_2(0)$, $Y_3(0) = y_3(0)$, $R_A(0) = b_1 e^{\frac{b_2}{Y_3(0)}} Y_1(0)^{n_1}$, $R_B(0) = b_3 e^{\frac{b_4}{Y_3(0)}} Y_2(0)$. The k-domain expression for nonlinear reaction term (r_A and r_B) is given by observing four types of nonlinearity in the Eq. 17 and Eq. 18 as given below. The k-domain expression for each of these nonlinearity is based on recurrence relation as in Finkel (2012).

- Inverse nonlinearity, $m_1 = \frac{1}{y_3}$

$$M_1(k) = -\frac{1}{y_3(0)} \sum_{j=1}^{k} Y_3(j) M_1(k-j) \tag{20}$$

with $M_1(0) = \frac{1}{y_3(0)}$

- Exponential nonlinearity, $m_2 = \exp(b_2 m_1)$ and $m_3 = \exp(b_4 m_1)$

$$\begin{bmatrix} M_2(k) \\ M_3(k) \end{bmatrix} = \begin{bmatrix} \dfrac{1}{k}\displaystyle\sum_{j=1}^{k}\Big(j b_2 M_1(j) M_2(k-j)\Big) \\ \dfrac{1}{k}\displaystyle\sum_{j=1}^{k}\Big(j b_4 M_1(j) M_3(k-j)\Big) \end{bmatrix} \tag{21}$$

with $M_2(0) = \exp(b_2)M_1(0)$ and $M_3(0) = \exp(b_4)M_1(0)$

- Power nonlinearity, $m_4 = y_1^{n_1}$

$$M_4(k) = \frac{1}{kY_1(0)} \sum_{j=1}^{k} [(n_1+1)j - k] Y_1(j) M_4(k-j) \tag{22}$$

with $M_4(0) = Y_1(0)^{n_1}$

- Product nonlinearity, $r_1 = b_1 m_2 m_4$ and $r_2 = b_3 m_3 y_2$

$$\begin{bmatrix} R_1(k) \\ R_2(k) \end{bmatrix} = \begin{bmatrix} \displaystyle\sum_{j=0}^{k}\Big(b_1 M_2(j) M_4(k-j)\Big) \\ \displaystyle\sum_{j=0}^{k}\Big(b_3 M_3(j) Y_2(k-j)\Big) \end{bmatrix} \tag{23}$$

with $R_1(0) = b_1 M_2(0) Y_1(0)$ and $R_2(0) = b_3 M_3(0) Y_2(0)$

From the k-domain expressions, k spectrum of desirable order can be calculated recursively. This k spectrum can be used to obtain solution in original domain using inverse transform through Taylor or Pade approximation.

Application of DT can be similarly performed on the modified equation for the other characteristic line. Fig. 3 shows the dynamic response of adiabatic fixed bed reactor for a step down change of 20% in the inlet velocity. For DT based approximations shown in Fig. 3, the number of sub-domain (n) is taken to be 1 and the number of series terms (N) is taken to be 9. It is seen that the resulting response matches with the solution given by MOC with numerical integration using `ODE15s` in MATLAB. Table 2 gives the computational load involved in using DT and numerical integration for the solution of resulting differential equations. From the table it is clear that use of DT based MOC reduces the computational load significantly.

Table 2. Computational load for different type of approximation in MOC

Method	Nodes	Computational load, s
MOC - NL	11	5.9
MOC - DT with n= 1, N= 9	11	1.3

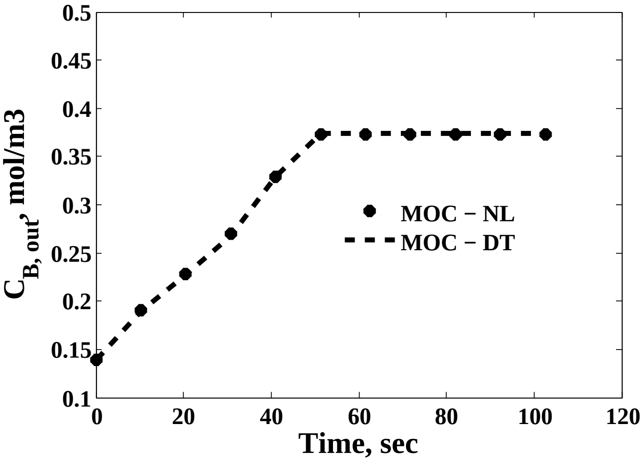

Fig. 3. Dynamic response of adiabatic FBR for 20% step down in inlet velocity using nonlinear integration method and DT method.

In another simulation, the model is tested with 70% step down in inlet velocity. As the velocity is reduced, slope of the characteristic line increases and hence, we need to use a larger number of terms (N) in the series solution and split the domain into sub-domains. Further we have used Pade based expansion of spectral terms for convergence. Thus in this case we have used 4 sub-domains and in each sub-domain Pade approximation is used with 3

Table 3. Computational load for different type of approximation in MOC

Method	Nodes	Computational load, s
MOC - NL	11	3.11
MOC - DT with n= 4, Nu= 3, Dn= 2	11	1.62

terms for the numerator and 2 terms for the denominator. The computational demand using DT based MOC and nonlinear integration (`ODE15s`) based MOC is shown in Table 3. This shows that use of DT-Pade approximation to the resulting ODE in MOC implementation can greatly help in reducing the computational load without degrading the resulting solution.

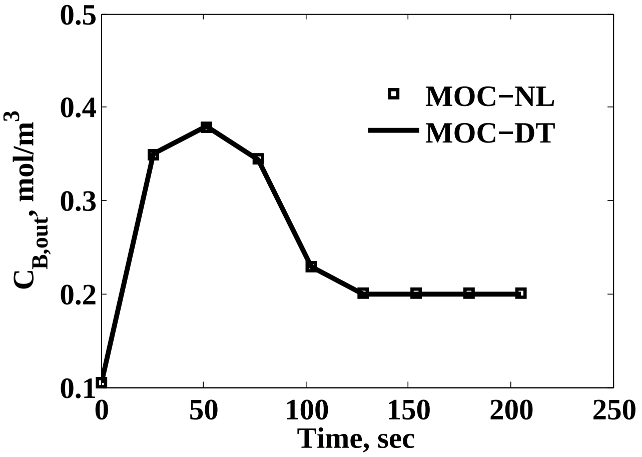

Fig. 4. Dynamic response of adiabatic FBR for 70% step down in inlet velocity using nonlinear integration method and DT method. Nu - number of terms in numerator, Dn - number of terms in denominator and n - number of sub-domains

4.2 Application of DT based MOC to non-adiabatic PFR with counter current heating - Dynamic simulation

The mathematical model for plug flow reactor with counter current heating is given below. It has characteristic lines with double slopes with, $\psi_1 = v_r > 0$ and $\psi_2 = -v_c < 0$ (Sudhakar et al. (2013b)).

$$\frac{\partial C_A}{\partial t} = -v_r \frac{\partial C_A}{\partial z} - r_A \tag{24}$$

$$\frac{\partial C_B}{\partial t} = -v_r \frac{\partial C_B}{\partial z} - \left(r_B - r_A\right) \tag{25}$$

$$\frac{\partial T_r}{\partial t} = -v_r \frac{\partial T_r}{\partial z} + \left(\frac{\Delta H_{r_A}}{\rho_r C p_r} r_A + \frac{\Delta H_{r_B}}{\rho_r C p_r} r_B\right) + \frac{U}{\rho_r C p_r V_r}(T_c - T_r) \tag{26}$$

$$\frac{\partial T_c}{\partial t} = v_c \frac{\partial T_c}{\partial z} - \frac{U}{\rho_c C p_c V_c}(T_c - T_r) \tag{27}$$

The above model is solved using MOC based on two approximations as mentioned previously, i.e, MOC-1 and MOC-2. Though the approximation involving boundary value problem show more accurate response compared to the one involving only initial value problem, the computational load involved in the former is higher compared to latter. As shown for adiabatic FBR, we use DT based approximation in MOC to reduce the computational load. This approximation results in algebraic equation as before and the boundary value problem now turn to be a solution of nonlinear algebraic equation which is solved using `fsolve` in MATLAB.

Table 4. Nodal and computational requirement for various approximations used in solving unsteady countercurrent PFR

Method	Nodes	Computational load, s
MOC-1	11	14.8
MOC-1 with DT	11	3.4
MOC-2	11	26.27
MOC-2 with DT	11	4.87

There are three types of nonlinearity for this model equation, inverse nonlinearity, product nonlinearity and exponential nonlinearity. As before, k-domain expression for each of this nonlinearity is based on recurrence relation as derived in Finkel (2012). As the problem is convection dominated and the velocity is not varied, the time interval over which equation for the solution variables solved is small. Thus we use $N = 2$ and number of sub-domain is fixed to one without any Pade approximation. The combination of MOC-DT as discussed above is applied to the countercurrent PFR. From Table 4 and Fig. 5, it is clear that the use of DT results in reduced computational load without compromising the accuracy of the resulting response.

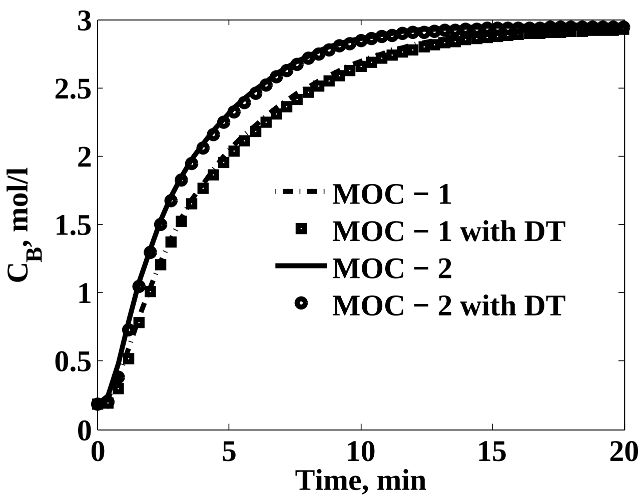

Fig. 5. Dynamic response of countercurrent PFR for 20% step up in inlet temperature of countercurrent heating fluid. DT is used with $k = 0, 1, 2$

5. CONCLUSION

In this contribution, DT based approximation is introduced in MOC model to reduce the computational load. Although DT is being used for solving differential equations in the literature, the radius of convergence is generally small as it is based on Taylor series approximation. Pade approximation is used to increase the radius of convergence of this method.

The DT based MOC model is obtained for two case studies involving fixed bed reactor and plug flow reactor. In both the case studies we have shown the use of DT resulted in reduced computational load through dynamic simulation. In the first case study, we have shown as the velocity decreases, the interval over which differential equations needs to be solved increases and the use of DT with Pade approximation is found to be useful. In the second case study, the DT based approximation results in nonlinear algebraic equations for the boundary value problem and found to be effective in reducing the computational load.

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