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Method of characteristics based model reduction for control of a counter-current reactor using approximate dynamic programming

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Abstract— **The aim of this paper is to use the method of characteristics (MOC) as a technique to obtain reduced order model for control of a counter-current reactor. The reactor is described by a system of quasi-linear hyperbolic partial differential equations (PDEs). Due to the counter-current operation, the system exhibits characteristic lines with double slopes; the slope of the characteristics have opposing signs. A reduced order model is obtained by using only a limited number of characteristic lines in the time-space plane. An approximation technique is proposed to obtain state variables at each sampling instance. This reduced-order MOC model is used for control in the approximate dynamic programming (ADP) framework for set-point tracking.**

I. Introduction

Counter-current operations are common in chemical engineering systems. The counter-current operation typically involves direct or indirect contact between two fluids moving in opposite directions. It allows for more effective heat and mass transfer between the two fluids than other modes of contact in majority of cases [1]. The objective of this work is to develop a method of characteristics (MOC) based reduced-order model for control of a counter-current process using the approximate dynamic programming (ADP) framework.

For typical processes of interest to the process industry, advective transport dominates over diffusive transport. Such processes can be reliably approximated as hyperbolic partial differential equations (PDEs). The state variables vary with time as well as along the length of the device. Since the two fluid media are convected in opposite directions, the model will have the following standard form:

$$\frac{\partial \Phi_1}{\partial t} = -\psi_1 \frac{\partial \Phi_1}{\partial z} + f_1(\Phi_1, \Phi_2) \quad (1)$$

$$\frac{\partial \Phi_2}{\partial t} = \psi_2 \frac{\partial \Phi_2}{\partial z} + f_2(\Phi_1, \Phi_2) \quad (2)$$

In the above equations, the vector Φ_1 consists of all the variables corresponding to the first fluid that get convected with a flow rate of ψ_1; Φ_2 consists of all the variables corresponding to the second fluid that get convected in the opposite direction with a flow rate of ψ_2. Therefore, the velocity or flow rate ψ_2 has an opposite sign in a counter-current system.

In our previous work [2], we presented an application of approximate dynamic programming (ADP) for control of water gas shift (WGS) reaction in a counter-current reactor–heat exchanger assembly. Finite difference method is a popular method to obtain finite dimensional model for control ([3], [4], [5]). The counter-current WGS reactor was discretized in space to convert the hyperbolic PDE into a system of ODEs, which is then represented in the standard state-space form. Although the control performance was excellent, the computation load was prohibitive due to the large state dimension of the discretized state-space model.

Model reduction techniques, such as proper orthogonal decomposition (POD), are often used to reduce the state dimension ([6], [7], [8], [9]). POD and similar methods that rely on modal decomposition generate a reduced-order model by discarding modes with low energy. These model reduction methods are not suitable for hyperbolic PDEs as these systems exhibit modes with nearly equal energy. Hence, reduction of first order hyperbolic systems needs special attention. Though there are several studies involve use of MOC for hyperbolic equations ([10], [11], [12], [13], [14], [15], [16], [17]), order reduction using MOC has not been well studied in literature.

In our previous work [18], MOC was used as a model reduction technique for a system involving characteristic lines with single and double slopes having positive values. The primary focus of this paper is to extend our previous work to hyperbolic PDEs with characteristics lines having positive and negative slope using MOC and use the obtained reduced order model in closed loop control using ADP. A generic non-adiabatic plug flow reactor with counter-current heating is used as an example. We propose a methodology to obtain reduced order model for such systems and demonstrate its use in ADP-based closed loop control.

II. Method of Characteristics

MOC is a technique used for the solution of first order hyperbolic PDEs, which aims to find characteristic curve(s) of the hyperbolic PDEs along which the solution of the original PDEs propagates. Specifically, MOC finds a relation between the two independent variables (time and space) in the hyperbolic PDE and this relation is given by the equation of the characteristic curve in the time-space plane. The original PDE becomes an ODE along this curve and hence the solution of PDEs finally turns out to be solution of only ODEs. One can also view this method as a Lagrangian technique of solving the PDE where one follows the dependent variables along certain paths in the time-space plane.

Hyperbolic PDE models with characteristic curves having double slopes are common in chemical engineering. The characteristic curve for Eq. (1), given by $dz/dt = \psi_1$

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is a line* in the t-z plane with slope ψ_1. The original PDE becomes an ODE along this characteristic line. It is straightforward to see that a similar transformation on Eq. (2) will lead to another characteristic, with slope $-\psi_2$. The slope of the characteristic lines depend on the magnitude and the direction of velocity of the corresponding variables. The model for counter-current systems will have characteristic lines with positive and negative slopes in the time-space plane.

In our previous work, we examined systems having characteristic lines with single and double positive slopes. Similar to the adiabatic fixed-bed reactor discussed therein (or any co-current system), the resultant ODEs will be solved along each of the characteristic lines and the solution is found at the intersection points. However, unlike the previous work, the solution for the counter-current system using MOC involves solving initial and boundary value problems. Consider the PDE model given by (3) and (4)

$$\frac{\partial \Phi_1}{\partial t} = -\psi_1 \frac{\partial \Phi_1}{\partial z} + f_1(\Phi_1, \Phi_2) \tag{3}$$
$$\frac{\partial \Phi_2}{\partial t} = \psi_2 \frac{\partial \Phi_2}{\partial z} + f_2(\Phi_1, \Phi_2) \tag{4}$$

with the following boundary and initial conditions:

$$\begin{bmatrix} \Phi_1(0,t) \\ \Phi_2(L,t) \\ \Phi_1(z,0) \\ \Phi_2(z,0) \end{bmatrix} = \begin{bmatrix} \Phi_{1in}(t) \\ \Phi_{2in}(t) \\ \Phi_{10}(z) \\ \Phi_{20}(z) \end{bmatrix} \tag{5}$$

In Eq. 3 and Eq. 4, Φ_1, Φ_2 can represent scalars or vectors. In this model the equations for the characteristic lines with two different slopes ($z_a(t)$ and $z_b(t)$) are given by,

$$\begin{bmatrix} \dfrac{dz_a}{dt}(t; z^0, t^0) \\ \dfrac{dz_b}{dt}(t; z^0, t^0) \end{bmatrix} = \begin{bmatrix} \psi_1 \\ -\psi_2 \end{bmatrix} \tag{6}$$

here (z^0, t^0) represent the starting point for the characteristic lines and is depicted as '•'in the Fig. 1 and the equation for the dependent variables along these characteristic lines are given by,

$$\begin{bmatrix} \dfrac{d\Phi_1}{dt}(t, z_a(t; z^0, t^0)) \\ \dfrac{d\Phi_2}{dt}(t, z_b(t; z^0, t^0)) \end{bmatrix} = \begin{bmatrix} f_1(\Phi_1, \Phi_2) \\ f_2(\Phi_1, \Phi_2) \end{bmatrix} \tag{7}$$

The space interval Δz at which the characteristic lines are placed depends on the number of nodal points (or order reduction) used and the time interval Δt is determined by the intersection of the two characteristic lines which again depends on the slope of the characteristic lines. The Eq. 7 has to be solved along these characteristic lines and the solutions are obtained at the intersection points.

The equation for characteristic lines, Eq. 6 has to be solved to find the intersection points and also to find the period of repetition of location of intersection points with the original nodal points as in for the adiabatic fixed bed reactor [12]. The period of repetition of the nodal points depends on the ratio of the two distinct slopes. The following Fig. 1 shows the intersection of characteristic lines ($z_a(t)$ and $z_b(t)$) in the time-space plane. Also it is seen that the intersection points repeats itself in the same location as in the distribution of original nodal points every 3Δt time, which is termed as period of repetition.

*Note that the characteristic is a curve if ψ_1 is time-varying.

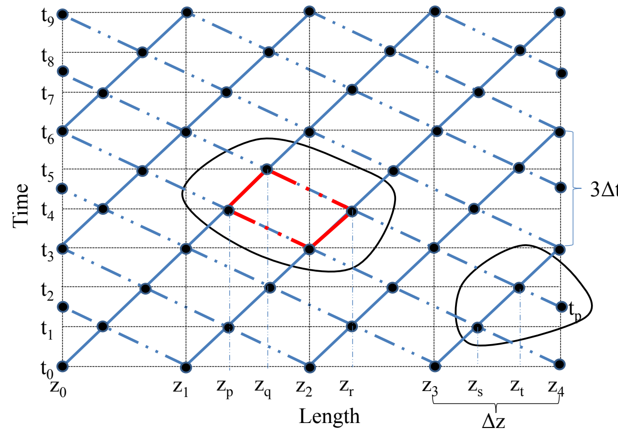

Fig. 1. Schematic figure showing intersection of two opposing characteristic line in the time-space plane

The accuracy of the resulting solution using MOC depends on the number of such characteristic lines in the time-space plane along which dependent variables needs to be solved. The reduction in the accuracy of resulting solution with the reduction in number of characteristic lines is much lower compared to conventional finite difference method. These characteristic lines correspond to nodal points along spatial direction and hence reduction in number density of characteristic lines will reduce the order of the original system while producing approximate solution. This property has been exploited in our previous work to get reduced order model for systems with characteristic lines having single and double positive slopes. In this work we extend this technique to the systems with characteristics having opposing slopes which involves the solution of initial and boundary value problems as against solution of only initial value problems in our previous studies.

Proposed methodology to obtain the reduced order model

The equation for the dependent variables (Eq. 7) needs to be solved simultaneously along each characteristic lines to obtain the solution at the intersection points. The simultaneous solution of Eq. 7 is difficult as each dependent variable vary along different characteristic lines and some kind of approximation is needed for the value of the other variable which does not vary along the particular characteristic line. Consider the region encircled in the Fig. 1 containing the points (z_p, t_4), (z_q, t_5), (z_2, t_3) and (z_r, t_4) and this region is enlarged in the Fig. 2. The Eq. 7 when solved starting from the point (z_p, t_4), Φ_1 varies along $z_a(t; z_p, t_4)$, whereas Φ_2 varies along $z_b(t; z_p, t_4)$. In order to simultaneously solve the

Eq. 7 along $z_a(t; z_p, t_4)$, one need the simultaneous variation of the other variable Φ_2 along this line. This is done through certain approximations and is explained in the following paragraphs.

Let the Eq. 6 is solved for different time interval dt_a and dt_b, keeping the same space interval ($dz_a = dz_b = dz$), then we have,

$$dt_a = -\frac{\Psi_2}{\Psi_1} dt_b \tag{8}$$

From the above relation, Eq. 7 is modified by multiplying the factor $-\frac{\Psi_1}{\Psi_2}$ as follows,

$$\begin{bmatrix} \frac{d\Phi_1}{dt_a}(t, z_a(t; z_p, t_4)) \\ \frac{d\Phi_2}{dt_a}(t, z_a(t; z_p, t_4)) \end{bmatrix} \approx \begin{bmatrix} f_1(\Phi_1, \Phi_2) \\ (-\frac{\Psi_1}{\Psi_2}) f_2(\Phi_1, \Phi_2) \end{bmatrix} \tag{9}$$

The above equation is solved with the initial condition at the point (z_p, t_4) along the characteristic line $z_a(t; z_p, t_4)$. The value of Φ_2 along this line is approximated from the other characteristic line $z_b(t; z_p, t_4)$. The factor $(-\frac{\Psi_1}{\Psi_2})$ in the Eq. 9 makes Φ_2 to be available simultaneously along $z_a(t; z_p, t_4)$. The value of the Φ_1 obtained at the point (z_q, t_5) is stored while the value of Φ_2 is discarded as it corresponds to other point. Similarly, one could solve for Φ_2 at the point (z_q, t_5), starting from the point (z_r, t_4), by solving the following modified equation,

$$\begin{bmatrix} \frac{d\Phi_1}{dt_b}(t, z_b(t; z_r, t_4)) \\ \frac{d\Phi_2}{dt_b}(t, z_b(t; z_r, t_4)) \end{bmatrix} \approx \begin{bmatrix} (-\frac{\Psi_2}{\Psi_1}) f_1(\Phi_1, \Phi_2) \\ f_2(\Phi_1, \Phi_2) \end{bmatrix} \tag{10}$$

The above equation is solved with the initial condition from the values at the point (z_r, t_4) and storing the value of Φ_2 obtained at the point (z_q, t_5) and discarding Φ_1. The above proposed methodology is represented in the Fig. 2 given below,

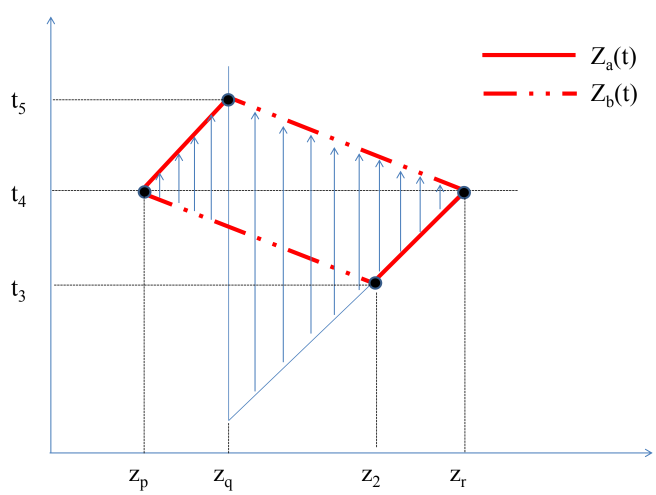

Fig. 2. Schematic figure showing approximation involved in solving for the dependent variables along the characteristic lines.

The arrow lines in Fig. 2 shows the direction of approximation. The above method of solving for the dependent variable is possible as long as we have the values for the initial conditions (like at the point (z_p, t_4) and (z_r, t_4) as discussed above). Now consider the encircled region in Fig. 1 containing the points (z_s, t_1), (z_t, t_2) and (z_4, t_p). In this case, the initial condition (the value of Φ_1) for solving the Eq. 10 along $z_b(t; z_4, t_p)$ is not available. This problem is addressed by first solving for Φ_1 from the known initial condition at (z_s, t_1) and then from the known values of Φ_1 at the point (z_t, t_2) and Φ_2 at the point (z_4, t_p), Eq. 10 can be solved as a boundary value problem along the line $z_b(t; z_4, t_p)$.

As an alternate to the above procedure, one can solve the boundary value problem for all the points in the time-space plane. Consider again the encircled region containing (z_p, t_4), (z_q, t_5), (z_2, t_3) and (z_r, t_4). The Eq. 9 can be solved along the line $z_a(t; z_p, t_4)$ as usual based on the information at the point (z_p, t_4) and a boundary value problem can be solved along the line $z_b(t; z_r, t_4)$ based on the information at the point (z_q, t_5) and at the point (z_r, t_4). This way the approximation involved by solving the Eq. 10 based on the information available only at the point (z_r, t_4) is avoided considerably. This can be seen in the improvement of the resulting response compared to the previous procedure. Though this way of solving reduces the approximation involved, the computational load involved gets increased. In this paper, the resulting initial value problems and boundary value problems are solved using `ode15s` and `bvp4c` in MATLAB respectively.

The computational load involved in solving the boundary value problem can be reduced by using approximation such as linearization of the resulting differential equations for every Δt. As we are dealing with convection dominated system, the dependent variables will be propagated relatively fast and hence the resulting characteristic lines will have lower slope. This would result in small Δt over which the differential equations for the dependent variables to be solved repeatedly and hence the linearized differential equations would well approximate the resulting solution.

In this paper, as mentioned in the previous paragraphs, we adopt three different approximations in the implementation of MOC,

- Approximation involving initial value problem for all the interior points and boundary value problems for the points near the boundary. This we refer to as MOC-1 in this paper.
- Approximation involving boundary value problem for all the points in the time-space plane. This we refer to as MOC-2 in this paper.
- Approximation involving linearized differential equations for each Δt, to reduce the computational load involved. This we refer to as MOC-3 in this paper.

III. Case Study - Plug Flow Reactor

We consider an example of a non-adiabatic plug flow reactor with counter-current heating to illustrate the use of MOC in obtaining reduced order model and its subsequent use in ADP based control. In the reactor, series reaction of the type, A $\rightarrow$ B $\rightarrow$ C, takes place with counter-current heating by

TABLE I

PARAMETERS FOR NON-ADIABATIC PLUG FLOW REACTOR

Parameter	Value
Length of the reactor (L, m)	1
Density of reactant (ρ_r, kg/l)	0.09
Density of jacket fluid (ρ_c, kg/l)	0.1
Specific heat of reactant (C_{pr}, kcal/kg/K)	0.231
Specific heat of jacket fluid (C_{pc}, kcal/kg/K)	0.8
Velocity of reactants (v_r, m/min)	0.5
Velocity of jacket fluid (v_c, m/min)	0.25
Heat Transfer coefficient (U_w, kcal/min/K)	1
Volume of the reactor(V_r, l)	10
Volume of the jacket fluid (V_c, l)	8
Inlet concentration of A ($C_{\rm Ain}$, mol/l)	4
Inlet concentration of B ($C_{\rm Bin}$, mol/l)	0
Inlet temperature of reactant($T_{\rm r,in}$, K)	400
Inlet temperature of jacket fluid ($T_{\rm c,in}$, K)	375
Arrhenius Constant (k_A, 1/min)	5×10^{12}
Activation Energy (E_A, kcal/kmol)	2.5×10^4
Heat of reaction (ΔH_{r_A}, kcal/mol)	0.5480
Arrhenius Constant (k_B, 1/min)	5×10^2
Activation Energy (E_B, kcal/kmol)	2×10^4
Heat of reaction (ΔH_{r_B}, kcal/mol)	0.9860

hot fluid. The following describes the mathematical model of the reactor (similar to the one used by [11])

$$\frac{\partial C_A}{\partial t} = -v_r \frac{\partial C_A}{\partial z} - r_A \tag{11}$$

$$\frac{\partial C_B}{\partial t} = -v_r \frac{\partial C_B}{\partial z} - \left(r_A - r_B\right) \tag{12}$$

$$\frac{\partial T_r}{\partial t} = -v_r \frac{\partial T_r}{\partial z} + \frac{\sum_j (-\Delta H_{r_j}) r_j}{\rho_r C_{pr}} + \frac{U(T_c - T_r)}{\rho_r C_{pr} V_r} \tag{13}$$

$$\frac{\partial T_c}{\partial t} = v_c \frac{\partial T_c}{\partial z} + \frac{U(T_r - T_c)}{\rho_c C_{pc} V_c} \tag{14}$$

The reaction kinetics is given by

$$r_A = k_A e^{\frac{-E_A}{RT}} C_A \tag{15}$$

$$r_B = k_B e^{\frac{-E_B}{RT}} C_B \tag{16}$$

The various parameters and operating conditions are given in Table I. The initial and boundary conditions are given by

$$\begin{bmatrix} C_A(0,t) \\ C_B(0,t) \\ T_r(0,t) \\ T_c(L,t) \end{bmatrix} = \begin{bmatrix} C_{A,in}(t) \\ C_{B,in}(t) \\ T_{r,in}(t) \\ T_{c,in}(t) \end{bmatrix} \quad \begin{bmatrix} C_A(z,0) \\ C_B(z,0) \\ T_r(z,0) \\ T_c(z,0) \end{bmatrix} = \begin{bmatrix} C_{A0}(z) \\ C_{B0}(z) \\ T_{r0}(z) \\ T_{c0}(z) \end{bmatrix} \tag{17}$$

Grid independence study using method of lines indicates the requirement of 251 nodal points to accurately describe the dynamics of the reactor. The dynamics from this model using MOL is considered as the reference solution (i.e., "plant") in further simulations.

A. Reduced Order Model from MOC

The hyperbolic PDE model of this PFR exhibits two characteristics determined by the velocity of the reactant (v_r) and the velocity of the heating fluid (v_c). The dependent variables in the Eq. 3 are given by $\Phi_1 \triangleq \begin{bmatrix} C_A & C_B & T_r \end{bmatrix}^T$ and $\Phi_2 \triangleq T_c$. The slopes of the characteristic lines ($z_a(t)$ and $z_b(t)$) are governed by $\psi_1 = v_r$ and $\psi_2 = v_c$. The equation for the dependent variables along the two characteristics are then given by

$$\frac{d}{dt}\begin{bmatrix} C_A(t, z_a(t; z^0, t^0)) \\ C_B(t, z_a(t; z^0, t^0)) \\ T_r(t, z_a(t; z^0, t^0)) \\ T_c(t, z_b(t; z^0, t^0)) \end{bmatrix} = \begin{bmatrix} -r_A \\ -(r_A - r_B) \\ \frac{\sum_j (-\Delta H_{r_j}) r_j}{\rho_r C_{pr}} + \frac{U(T_c - T_r)}{\rho_r C_{pr} V_r} \\ \frac{U(T_r - T_c)}{\rho_c C_{pc} V_c} \end{bmatrix} \tag{18}$$

The above equation is solved along the characteristic lines as described in the section II. The resulting differential equations are solved using `ode15s` routine in MATLAB. The Fig. 3 shows the open loop response of non-adiabatic PFR for a step-up input of 30% in the inlet hot fluid temperature. The comparison of response between grid independent solution (MOL) and MOC with 11 nodes shows that reduced order model from MOC gives reasonably accurate prediction. The MOC is implemented using three different approximations as mentioned in the section II. Fig. 3 shows that second and third approximations produces solution close to the one given by grid-independent MOL method. Also from the Table II, it is clear that implementation of MOC using linearized model shows similar behaviour with nonlinear model but with lower computational load.

TABLE II

COMPARISON OF DYNAMIC RESPONSE BETWEEN REDUCED ORDER AND HIGHER ORDER MODEL

Model	Nodes	Computational load, s
MOC-1	11	14.8
MOC-2	11	26.27
MOC-3	11	15

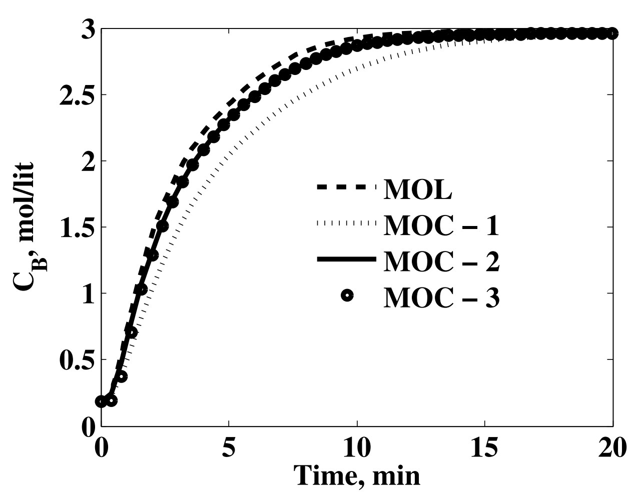

Fig. 3. Open loop response of the non-adiabatic PFR with lower order MOC with 11 nodes is compared with the reference model (MOL) to show the model order reduction capability of MOC.

B. Off-line learning of cost-to-go for ADP

ADP is one of the model based control techniques which requires reduced order model for its efficient performance.† The reduced order model obtained using MOC is used in ADP based control for set-point tracking problem. Reduced order model using two different approximations, i.e., MOC-2 and MOC-3 is used for prediction and optimization and grid independent MOL model with 251 nodes is considered as 'plant'. A set-point tracking problem is considered with the set-point for the outlet concentration of B as 3 mol/l. The temperature of the hot fluid is the manipulated variable which has significant effect on the reaction rate.

The small working region in the state space for the implementation of ADP is found from the closed loop data of sub-optimal controllers like PID and linear MPC. Total of 6 closed loop simulation were performed from 2 PID controllers and 4 linear MPC controllers of which 2 is linearized around initial steady state and 2 is linearized around final steady state and closed loop data were collected. The points which are repeated were removed and only distinct points are retained which forms the working region in the state space. Total of 338 points in 11 dimensional state space forms the working region and ADP finds an optimal path to reach the set-point within this region. Initial cost-to-go values are obtained from the sub-optimal controllers.

Local approximator like KNN with K=4 is used to find the mapping between cost-to-go values and the points in the working region. Quadratic penalty function is designed with $\sigma = 60$ which restrict the optimizer to search for the optimal path in the region of high data density. Value iteration is performed for all the point in the working region through Bellman equation to improve the initial cost-to-go values. The maximum absolute difference in the cost-to-go values of subsequent iteration is monitored for convergence. Total of 25 iterations were done and the final error converged to a value of 0.1, after which there is no significant decrease in the error. The values of cost-to-go obtained at 25^{th} iteration is approximated as optimal cost-to-go function using KNN approximator and used for online control.

C. Online ADP implementation

The converged cost-to-go values obtained from the Bellman iterations are then used for online control. The control objective is to track the given set-point of 3 mol/l of B at the outlet of the reactor from the steady state value of 0.18 mol/l using inlet temperature of jacket fluid as the manipulated variable. The profiles of controlled output and manipulated input for the six controllers are shown in Fig. 4 and Fig. 5.

The performance of ADP based controller using reduced order model from MOC is compared with PID and linear MPC controllers. The ADP based controller shows better performance compared to other sub-optimal controllers as seen from the Fig. 4. The closed loop response from ADP-MOC controller shows no oscillation and it reaches the set-point with small response time and hence has lower total cost-to-go values compared to all other controllers. Although ADP-MOC implementation gives better closed loop performance, it involves the solution of boundary value problem when using the model, MOC-2, which is computationally demanding. The computational load for the closed loop performance shown in the Fig. 4 using the model MOC-2 is about 2.5×10^3 s. As stated in the section III-A, we have also used linearized MOC model for online ADP implementation with the same converged cost-to-go values. The results indicate that this model, MOC-3 is able to give similar closed loop performance as given by the nonlinear model MOC-2, but with lesser computational demand. The computational load using this linearized model is about 1.39 $\times 10^3$ s. This indicates that as long as velocity is high, which makes the slope small, the linearization approximation produces closed loop performance similar to nonlinear model with the benefit of reduced computational load.

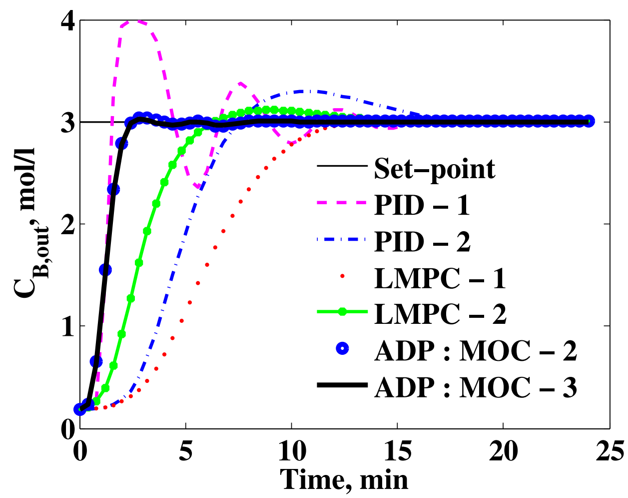

Fig. 4. Closed loop response from Linear MPC, PID and ADP with reduced order model from MOC for non-adiabatic PFR.

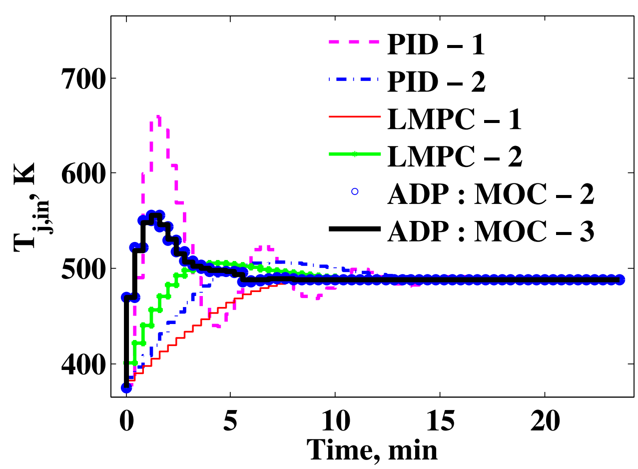

Fig. 5. Input moves for the different controllers for non-adiabatic PFR.

†For details on ADP, please refer to [18], [19], [20]

IV. Conclusion

Method of characteristics is found to be suitable in reducing the order of systems described by first order hyperbolic PDEs. Application of MOC for counter-current systems involve the solution of boundary value problem in addition to solving initial value problem. The computational load involved can be reduced by resorting to various approximations like the use of linearized model in this paper. Use of this reduced order model in ADP based control shows significant improvement in performance and computational requirement.

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