Distributed optimal control of a Dimethyl Ether (DME) catalytic distillation column

Amir Alizadeh Moghadam, Ilyasse Aksikas, Stevan Dubljevic, J. Fraser Forbes

Abstract— This contribution addresses the development of a Linear Quadratic regulator (LQ) for controlling concentration profiles along a catalytic distillation column which is modelled by a set of coupled hyperbolic Partial Differential and Algebraic Equations (PDAEs). The methodology is based on an infinite-dimensional representation of the system and solving the related Operator Riccati Equation (ORE). The performance of the designed control policy is assessed through a numerical simulation.

I. INTRODUCTION

Reactive distillation (RD) has received much attention in the literature over recent years due to its advantages and inherent complexities. This process is a combination of chemical reaction and multi-component distillation in a counter-current column. When solid catalyst is used to accelerate the reaction, the process is called catalytic distillation (CD). The most important advantages in use of RD are; reduced downstream processing, using the heat of reaction for distillation, overcoming chemical equilibria by removing products from the reaction zone and etc.; however, the interaction between the simultaneous reaction and distillation introduces challenging problems in controlling the column such as steady-state multiplicity, strong interactions between process variables and process sign change [1].

Despite the complexities in control aspects of RD, a relatively small amount of research work has been reported in this area and most of the publications deal with modelling, simulation, process design and the analysis of steady-state multiplicity (e.g., [2], [3] and [4]). A significant portion of the literature on the area of control of RD concerns the effectiveness of different control structures including conventional proportional integral (PI) controllers (e.g., [5], [6] and [7]). Linear model predictive control (MPC) has also been investigated based on simplified dynamic models of RD (e.g., [8], [1] and [9]). In addition, a limited number of papers in the literature have dealt with the advanced nonlinear control of RD process (e.g., [10], [11] and [12]). The reactive distillation process can take place either in a trayed or a packed column [2]. In the case of packed column, the process is a distributed parameter system, meaning that the process variables are function of both time and spatial

coordinate. Such a system is modelled by a set of coupled PDAEs in which partial differential equations (PDEs) describe the mass and energy balances and algebraic equations represent the equilibrium condition. Lumping assumptions are often used [2] to convert the PDEs to sets of ordinary differential equations (ODEs), which allows the use of standard control methods applicable to ODEs systems; however, this approximation results in some mismatches in the dynamical properties of the original distributed parameter and the lumped parameter models, which affects the performance of the designed model-based controller. A more rigorous way to deal with distributed parameter processes is to exploit the infinite-dimensional characteristic of the system [13]. This approach has been ignored in the literature dealing with control of reactive distillation columns which the present work tries to address for the first time with the flavor of optimal control.

Classical methods in the optimal feedback controller synthesis is the well known Linear Quadratic regulator (LQ). The main objective of this control policy is to regulate a linear system by minimizing a quadratic performance index. An important advantage of LQ control is that it uses a state feedback law, in which the state feedback gain is calculated offline by using LTI system's dynamic and thereby the amount of on-line calculations is reduced, significantly. In solving an LQ problem for an infinite-dimensional (distributed) system, two common methods are available in the literature. The first approach is based on frequency domain description and is known as *spectral factorization*. In this method the control law is obtained via solving an *operator Diophantine equation* [14]. This technique is applied in [15] to control the temperature and the concentration in a plug flow reactor. The second methodology involves solving an operator Riccati equation (ORE) for a given state-space model [16]. This method was used in [17] for a particular class of hyperbolic PDEs. The methodology was then extended to a more general class of hyperbolic system by using an infinite-dimensional *Hilbert* state-space setting with distributed input and output [18]. When a state-space model is available, solving the optimal control problem with the ORE method requires less computational effort in comparison to the *spectral factorization* approach which is more convenient for transfer function models.

In this work, an ORE-based infinite-dimensional LQ control is used to control the mole fraction profiles in a DME packed catalytic distillation column through manipulating the liquid and the gas flowrates. Such a system is modelled by a set of hyperbolic PDAEs. In order to solve the LQ

control problem, the PDAEs system is converted to a system of pure PDEs by solving the algebraic equations and a linear system is calculated through linearizing the nonlinear PDEs around the desired steady-state profiles. In contrast to the previous work ([17] and [18]), the resulted linear model involves a velocity term which is not a diagonal matrix and in addition its elements are function of the states. First, a state transformation is used to make the velocity term diagonal. The related ORE is then formulated and its equivalent matrix Riccati equation is found when the velocity term is a space-varying and diagonal matrix. Finally, a numerical simulation is done to evaluate the performance of the designed controller.

II. PROCESS MODEL

The process under consideration is shown in Fig. 1. This catalytic distillation column is used for producing DME through liquid phase dehydration of methanol. The column has an effective packing height of 4 m including four sections of 1 m each. The rectifying zone at the top and the stripping zone at the bottom are filled with packing in which separation is taking place. The two middle sections are catalytically packed reactive zones in which the following reaction is taking place:

$$2Methanol \iff DME + Water \qquad (1)$$
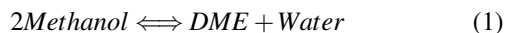
The kinetic of the above reaction is given by [19]:

$$r_D = \frac{k_s x_M^2}{(x_M + \frac{K_W}{K_M}(x_W))^2} \qquad (2)$$

where r_D is the rate of the reaction in $\frac{mol}{kgcat.sec}$; x_D, x_M and x_W are the mole fractions of DME, methanol and water in the liquid phase, respectively; and:

$$k_s = 6.12 \times 10^7 exp(\frac{-98(kJ/mol)}{RT})$$
$$\frac{K_W}{K_M} = exp(-6.46 + \frac{2964}{T})$$

where T is the temperature in K; and R is the gas universal constant.

Methanol feed, with flowrate F, enters the column at the top of the reaction zone and the liquid and gas with flowrates L and G, enter the column at the top and the bottom, respectively. Due to the difference between vapor pressures of methanol, DME and water, the gas and liquid leaving the column mainly contain DME and water, receptively. For the sake of simplicity, the condenser and reboiler are not considered here.

Various types of models, involving different levels of complexity, can be used to simulate the dynamics of reactive distillation column. In this work, we consider the simple and generic reactive distillation model studied by [20]. It should be noted that in [20] gas and liquid rates through stripping and rectifying zones are constant and these rates change in the reactive zone because the heat of reaction vaporizes some liquid. Since the heat of reaction (1) is negligible [19], we assume constant liquid and gas rates all through the column.
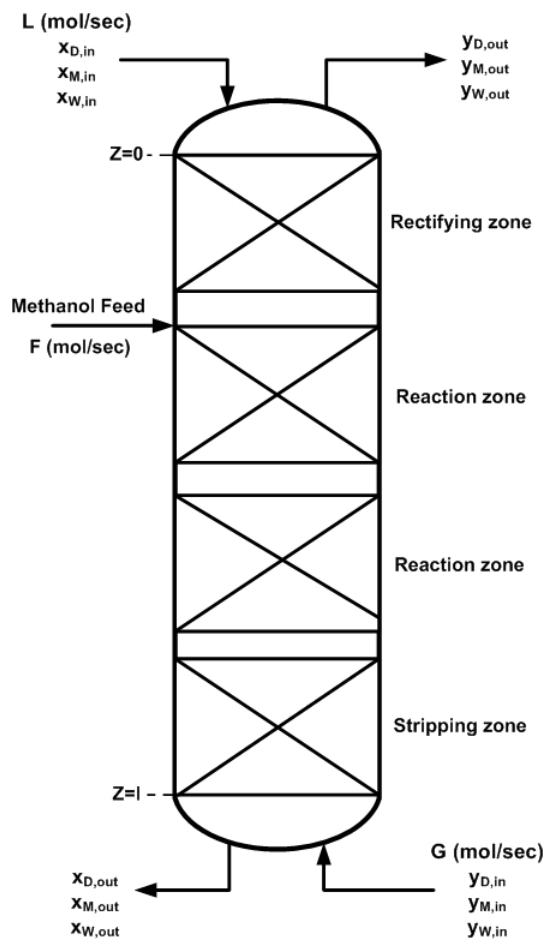

Fig. 1. Catalytic distillation column

Therefore, the model structure of the catalytic distillation column is developed based on the following assumptions:

- Negligible gas hold-up
- Constant liquid hold-up
- Constant gas and liquid rates
- Gas-liquid equilibrium
- No chemical reaction in the gas phase
- Perfect mixing in radial direction
- Fast energy dynamics
- Constant operating pressure
- Raoult's law for the gas-liquid equilibrium
- Constant relative volatilities

It should be noted that a more rigorous model will most likely give quantitatively different but qualitatively similar results. Regarding the above assumptions, the nonlinear process models describing the system under study are presented

as follows:

$$U_L \frac{\partial x_D}{\partial t} = -L\frac{\partial x_D}{\partial z} + G\frac{\partial y_D}{\partial z} + r_D\phi \qquad (3)$$

$$U_L \frac{\partial x_M}{\partial t} = -L\frac{\partial x_M}{\partial z} + G\frac{\partial y_M}{\partial z} - 2r_D\phi \qquad (4)$$

$$x_D + x_M + x_W = 1 \qquad (5)$$

$$y_D = \frac{\alpha_D x_D}{\alpha_D x_D + \alpha_M x_M + \alpha_W x_W} \qquad (6)$$

$$y_M = \frac{\alpha_M x_M}{\alpha_D x_D + \alpha_M x_M + \alpha_W x_W} \qquad (7)$$

$$y_D + y_M + y_W = 1 \qquad (8)$$

$$T = \frac{B_{vp,D}}{A_{vp,D} - \log_{10}\left(\frac{\alpha_D P}{\alpha_D x_D + \alpha_M x_M + \alpha_W x_W}\right)} - C_{vp,D} \qquad (9)$$

subject to the boundary and initial conditions:

$$x_D(0,t) = x_{D,in}, \quad x_M(0,t) = x_{M,in}, \quad x_W(0,t) = x_{W,in} \quad (10)$$

$$x_D(z,0) = x_{D,0}, \quad x_M(z,0) = x_{M,0}, \quad x_W(z,0) = x_{W,0} \quad (11)$$

where t is the time; z is the spatial coordinate; x_D, x_M and x_W are the mole fractions of DME, methanol and water in the liquid phase, respectively; y_D, y_M and y_W are the mole fractions of DME, methanol and water in the gas phase, respectively; U_L is the liquid hold-up; ϕ is the catalyst loading; P is the pressure; α_D, α_M and α_W are the relative volatilities of DME, methanol and water with respect to water (heaviest component), respectively; and $A_{vp,D}$, $B_{vp,D}$ and $C_{vp,D}$ are the Antoine equation parameters for DME.

It should be noted that the reaction terms in (3) and (4) for the rectifying and stripping zones are zero as there is no reaction is taking place in these sections.

The model parameters that are used in this work are give in Table I. In the table, subscripts "ss" denote the steady-state condition.

The model equations (3) to (10) are solved at steady-state condition in gPROMS® [21]. A finite difference method is used to solve the system of coupled differential and algebraic equations. The steady-state mole fraction profiles and also the temperature profile are shown in Fig. 2 to 4.

III. LQ CONTROL SYNTHESIS

In this section we are interested in an LQ control policy for regulating the mole fraction and temperature profiles along the catalytic distillation column according to the infinite dimensional model (3) to (11). Let us define $x_1 = x_D$, $x_2 = x_M$, $x = [x_1, x_2]$, $u_1 = L$, $u_2 = G$ and $u = [u_1, u_2]$. By taking the derivatives of y_D and y_M in (6) and (7) with respect to the spatial coordinate and substituting them into (3) and (4) we get:

$$\frac{\partial x_1}{\partial t} = f_{11}(x,u)\frac{\partial x_1}{\partial z} + f_{12}(x,u)\frac{\partial x_2}{\partial z} + \frac{r_D\phi}{U_L} \qquad (12)$$

$$\frac{\partial x_2}{\partial t} = f_{21}(x,u)\frac{\partial x_1}{\partial z} + f_{22}(x,u)\frac{\partial x_2}{\partial z} - \frac{2r_D\phi}{U_L} \qquad (13)$$

TABLE I

MODEL PARAMETERS

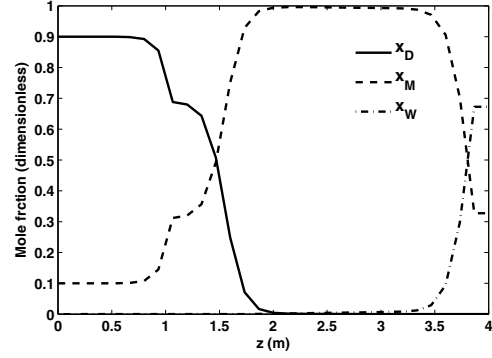| Parameter	Value
l	4 m
U_L	10 mol/m
P	8×10^5 Pa
ϕ	50 kg/m
F	0.017 mol/sec
L_{ss}	0.07 mol/sec
G_{ss}	0.0645 mol/sec
$x_{D,in}$	0.9
$x_{M,in}$	0.1
$x_{W,in}$	0.0
$y_{D,in}$	0.0
$y_{M,in}$	0.1
$y_{W,in}$	0.9
α_D	21.3
α_M	3.13
α_W	1
$A_{vp,D}$	4.441
$B_{vp,D}$	1025.560
$C_{vp,D}$	-17.1

Fig. 2.   Steady-state liquid phase mole fraction profiles

with the following boundary and initial conditions:

$$x_1(0,t) = x_{1,in}, \quad x_2(0,t) = x_{2,in} \qquad (14)$$

$$x_1(z,0) = x_{1,e}(z), \quad x_2(z,0) = x_{2,e}(z) \qquad (15)$$

where $f_{11}(x,u)$, $f_{12}(x,u)$, $f_{21}(x,u)$ and $f_{22}(x,u)$ are nonlinear functions of x and u and $x_{1,e}(z)$ and $x_{2,e}(z)$ are equilibrium profiles of x_1 and x_2 obtained from steady-state solution of (3) to (10). The matrix form of the above equations is:

$$\frac{\partial x}{\partial t} = f(x,u)\frac{\partial x}{\partial z} + R(x) \qquad (16)$$

$$x(0,t) = x_{in}, \quad x(z,0) = x_e(z)$$

where $\frac{\partial x}{\partial t} = [\frac{\partial x_1}{\partial t}, \frac{\partial x_2}{\partial t}]$, $\frac{\partial x}{\partial z} = [\frac{\partial x_1}{\partial z}, \frac{\partial x_2}{\partial z}]$, $R(x) = [\frac{r_D\phi}{U_L}, -\frac{2r_D\phi}{U_L}]$, $x_{in} = [x_{1,in}, x_{2,in}]$, $x_e(z) = [x_{1,e}(z), x_{2,e}(z)]$ and:

$$f(x,u) = \begin{bmatrix} f_{11}(x,u) & f_{12}(x,u) \\ f_{21}(x,u) & f_{22}(x,u) \end{bmatrix} \qquad (17)$$

In order to make the boundary conditions (14) homogenous, let us consider the following state transformation:

$$\tilde{x}_1 = \frac{x_1 - x_{1,in}}{x_{1,in}}, \quad \tilde{x}_2 = \frac{x_2 - x_{2,in}}{x_{2,in}} \qquad (18)$$
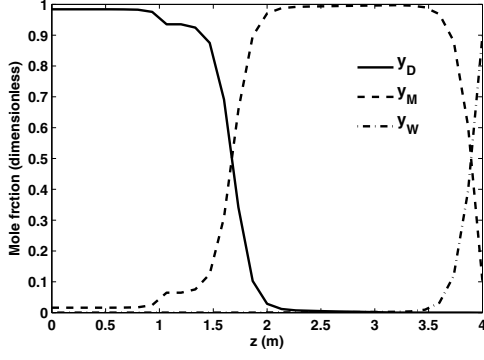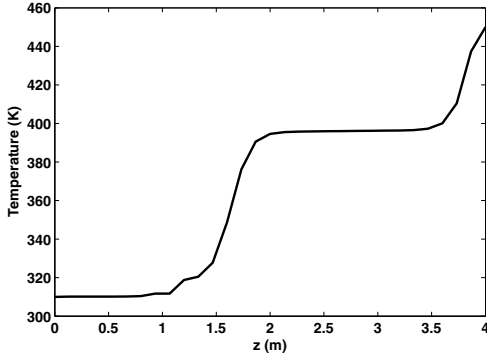
Fig. 3. Steady-state gas phase mole fraction profiles

Fig. 4. Steady-state temperature profile

Then we obtain the following equivalent representation of model (16):

$$\frac{\partial \tilde{x}}{\partial t} = \tilde{f}(\tilde{x},u)\frac{\partial \tilde{x}}{\partial z} + \tilde{R}(\tilde{x}) \qquad (19)$$
$$\tilde{x}(0,t) = 0$$

Linearizing model (19) about its equilibrium profile by using the Taylor series expansion leads to the following linear model on the Hilbert space $\mathscr{H} = L_2(0,l)^2$:

$$\frac{\partial \bar{x}}{\partial t} = V(z)\frac{\partial \bar{x}}{\partial z} + M(z)\bar{x} + B(z)\bar{u}$$
$$y = C(z)\bar{x} \qquad (20)$$
$$\bar{x}(0,t) = 0$$

where $\bar{x} \in \mathscr{H} = L_2(0,l)^2$ is deviation state variable, $\bar{u} \in \mathbb{R}^2$ is deviation input variable, $y \in \mathscr{Y} = L_2(0,l)^2$ denote the output variable, $V(z)$, $M(z)$ and $B(z)$ are continuous matrices whose entries are functions in $L_\infty(0,l)$.

Model (20) can be stated in an infinite-dimensional state-space in the *Hilbert* space $\mathscr{H} = L_2(0,l)^2$ [16]:

$$\dot{x}(t) = \mathscr{A}\bar{x}(t) + \mathscr{B}\bar{u}(t) \qquad (21)$$
$$y = \mathscr{C}\bar{x}(t)$$

Here $\mathscr{A}$ is a linear operator defined as:

$$\mathscr{A}h(z) = V(z)\frac{dh(z)}{dz} + M(z)h(z) \qquad (22)$$

with the following domain:

$$D(\mathscr{A}) = \{h(z) \in \mathscr{H} : h(z) \text{ and } \frac{dh(z)}{dz} \text{ are}$$
$$\text{a.c., and } \frac{dh(z)}{dz} \in \mathscr{H}\} \qquad (23)$$

where a.c. means absolutely continuous.

$\mathscr{B} \in (\mathbb{R}^2, \mathscr{H})$ is given by $\mathscr{B} = B(\cdot)I$; and $\mathscr{C} \in (\mathscr{H}, \mathscr{Y})$ is given by $\mathscr{C} = C(\cdot)I$ where I is the identity operator.

The LQ control design for system (20) is based on the minimization of an infinite-time horizon, quadratic objective function that requires the solution of an ORE (see [16] and [22]). The solution of the ORE can be achieved by converting it to an equivalent matrix Riccati equation. The optimal feedback operator can then be found by solving the resulting matrix Riccati equation. Let us consider the following infinite-time horizon quadratic objective function:

$$J(\bar{x}_0, \bar{u}) = \int_0^\infty (\langle \mathscr{C}x(t), \mathscr{P}\mathscr{C}\bar{x}(t)\rangle + \langle u(t), R\bar{u}(t)\rangle)dt \qquad (24)$$

where $\mathscr{P} = PI \in \mathscr{L}(\mathscr{Y})$ with $P \in \mathbb{R}^{2\times 2}$ is a positive semi-definite and symmetric matrix; and $R \in \mathbb{R}^{2\times 2}$ is a positive definite symmetric matrix. The minimization of the above objective function subject to system (20) results in solving the following ORE (see [16] and the references therein):

$$[\mathscr{A}^*\mathscr{Q} + \mathscr{Q}\mathscr{A} + \mathscr{C}^*\mathscr{P}\mathscr{C} - \mathscr{Q}\mathscr{B}R^{-1}\mathscr{B}^*\mathscr{Q}]\bar{x} = 0 \qquad (25)$$

According to Theorem 6.2.7 in [16], ORE (25) has a unique, non-negative, and self-adjoint solution $\mathscr{Q} \in \mathscr{L}(\mathscr{H})$, if system (20) is exponentially optimizable (stabilizable) and exponentially detectable. Under these conditions, the minimum cost function is given by $J(\bar{x}_0, \bar{u}_{opt}) = \langle \bar{x}_0, \mathscr{Q}\bar{x}_0\rangle$ and for any initial condition $\bar{x}_0 \in \mathscr{H}$ the unique optimal control variable $\bar{u}_{opt}$, which minimizes the objective function (24), is obtained on $t \geq 0$ as:

$$\bar{u}_{opt}(t) = K\bar{x}(t) \qquad (26)$$

where

$$K = -R^{-1}\mathscr{B}^*\mathscr{Q} \qquad (27)$$

In addition, $\mathscr{A} + \mathscr{B}K$ generates an exponentially stable $C_0-semigroup$ [16].

In [18] it is proven that if the matrix $V < 0$, then operator $\mathscr{A}$ given by (22) and (23) generates an exponentially stable C_0−semigroup. Therefore, ORE (25) has a unique, non-negative, and self-adjoint solution $\mathscr{Q} \in \mathscr{L}(\mathscr{H})$.

In order to solve the ORE it should be converted to an equivalent matrix Riccati equation. In [18] it is proven that when matrix V is a constant diagonal matrix, by choosing $\mathscr{Q} = diag(\phi_1(z), \phi_2(z))I$, ORE (24) can be converted to the following matrix Riccati equation:

$$V\frac{d\phi}{dz} = M^*\phi + \phi M + C^*PC - \phi BR^{-1}B^*\phi$$
$$\phi(l) = 0 \qquad (28)$$

However, matrix $V(z)$ in (20) is not diagonal and in addition its elements are space-varying. Therefore, in order to find the

equivalent matrix Riccati equation, first, we use the following state transformation to make $V(z)$ a diagonal matrix:

$$\bar{x} = T(z)\hat{x} \tag{29}$$

where matrix $T(z)$ is the transformation matrix whose columns are eigenvectors of $V(z)$. By applying this state transformation to (20) we have:

$$\frac{\partial \hat{x}}{\partial t} = \bar{V}(z)\frac{\partial \hat{x}}{\partial z} + \bar{M}(z)\hat{x} + \bar{B}(z)\bar{u}$$
$$y = \bar{C}(z)\hat{x} \tag{30}$$
$$\hat{x}(0,t) = 0$$

where:

$$\bar{V}(z) = T(z)^{-1}V(z)T(z)$$

is a diagonal matrix whose elements are the eigenvalues of $V(z)$; and $\bar{M}(z)$, $\bar{B}(z)$ and $\bar{C}(z)$ are given by:

$$\bar{M}(z) = T(z)^{-1}V(z)\frac{\partial T(z)}{\partial z} + T(z)^{-1}M(z)T(z)$$
$$\bar{B}(z) = T(z)^{-1}B(z)$$
$$\bar{C}(z) = C(z)T(z)$$

The infinite-dimensional state-space representation of (30) is:

$$\dot{\hat{x}}(t) = \bar{\mathscr{A}}\hat{x}(t) + \bar{\mathscr{B}}\bar{u}(t) \tag{31}$$
$$y = \bar{\mathscr{C}}\hat{x}(t)$$

where $\bar{\mathscr{A}}$ is a linear operator defined as:

$$\bar{\mathscr{A}}h(z) = \bar{V}(z)\frac{dh(z)}{dz} + \bar{M}(z)h(z) \tag{32}$$

with the same domain defined in (23); $\bar{\mathscr{B}} \in (\mathbb{R}^2, \mathscr{H})$ is given by $\bar{\mathscr{B}} = \bar{B}(\cdot)I$; and $\bar{\mathscr{C}} \in (\mathscr{H}, \mathscr{Y})$ is given by $\bar{\mathscr{C}} = \bar{C}(\cdot)I$. The ORE for system (30) is the same as (25) with new operators $\bar{\mathscr{A}}$, $\bar{\mathscr{B}}$, and $\bar{\mathscr{C}}$. By assuming $\mathscr{Q} = diag(\phi_1(z), \phi_2(z))I$, with the same argument used in the proof of Theorem 5 in [18], it can be proven that the equivalent matrix Riccati equation for (30) is:

$$\frac{d(\bar{V}\phi)}{dz} = \bar{M}^*\phi + \phi\bar{M} + \bar{C}^*P\bar{C} - \phi\bar{B}R^{-1}\bar{B}^*\phi$$
$$\phi(l) = 0 \tag{33}$$

The above matrix Riccati equation can be solve numerically and the feedback operator can be found from:

$$K = -R^{-1}\bar{\mathscr{B}}^*\mathscr{Q} \tag{34}$$

IV. SIMULATION RESULTS

In order to assess the performance of the controller, the designed feedback operator is used with the original nonlinear system (3) to (11). Since we are interested in controlling both state variables, matrix $C(z)$ is the identity matrix. The weighting matrices are chosen to be $P = diag(17 \times 10^{-6}, 17 \times 10^{-6})$ and $R = diag(28 \times 10^3, 20 \times 10^3)$. The set of coupled nonlinear PDAEs (3) to (11) along with the matrix Riccati equation (33) are solved numerically in gPROMS. We use an arbitrary initial condition $x_1(z,0) = 0.6$ and $x_2(z,0) = 0.4$ to measure the performance of the designed controller. The
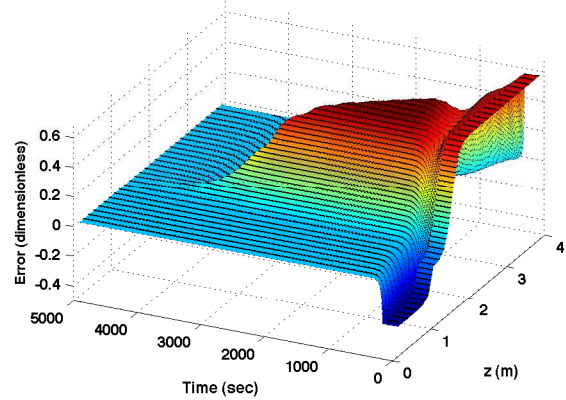

Fig. 5. Control error profile for x_1

control error profiles for DME and methanol liquid mole fractions $(x_1(z,t) - x_{1,e}(z)$ and $x_2(z,t) - x_{2,e}(z))$ are shown in Fig. 5 and Fig. 6. These figures show how the error between the states and their desired equilibrium profiles (Fig. 2) converges to zero when the system is initiated from the selected initial condition. To have a measure of how fast the designed controller is, the spatially averaged control error for the closed-loop and the open-loop systems are compared in Fig. 7. This figure shows that the closed-loop system is able to reject the effect of the initial condition in about 4×10^3 sec while for the open-loop system it takes near 8×10^4 sec to do so. It means that the closed-loop system is more than 1000 times faster than the open-loop system with respect to the residence time of the column which is 72.4 sec. Finally, the control input profiles are shown in Fig. 8. The control efforts are not particularly aggressive, and are physically realizable.

V. CONCLUSIONS

In this work an ORE-based infinite-dimensional LQ control policy is used to control mole fraction profiles along a packed catalytic distillation column. The column is modelled by a set of coupled hyperbolic partial differential and algebraic equations. The system of equations is converted to a set of pure PDEs and a linear system is calculated through linearizing the nonlinear PDEs around the desired steady-state profiles which is stated in the form of infinite-dimensional state-space. A state transformation is then applied to find a system with diagonal velocity term. The ORE equation for the new system is formulated and its equivalent matrix Riccati equation is obtained. Finally, in order to assess the performance of the designed controller it is implemented on the column which resulted in a high performance closed-loop system.

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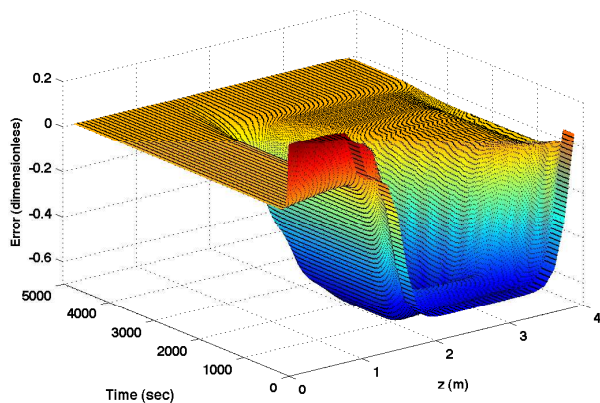[2] R. Taylor and R. Krishna. Modelling reactive distillation. *Chemical Engineering Science*, 55:5183–5229, 2000.
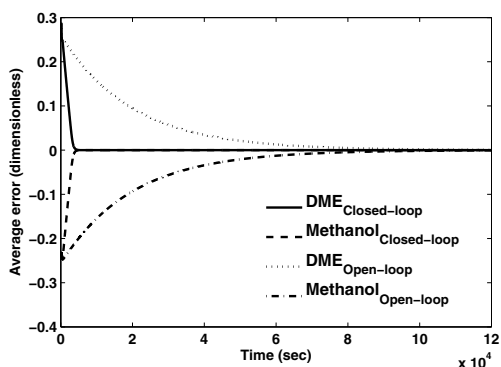
Fig. 6. Control error profile for x_2

Fig. 7. Spatially averaged error
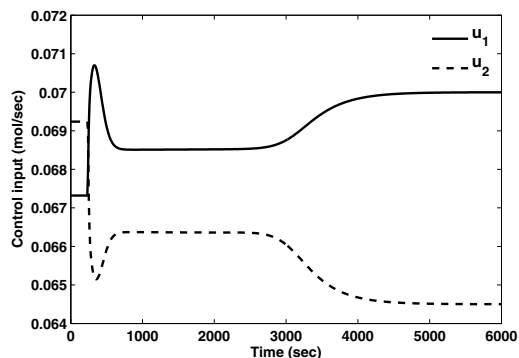

Fig. 8. Control input profies

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