Adaptive Optimizing Control of an Ideal Reactive Distillation Column

Jayaram Valluru, Jalesh L. Purohit, Sachin C. Patwardhan*, Sanjay M. Mahajani

Department of Chemical Engineering, Indian Institute of Technology Bombay, Mumbai, India 400076

Abstract: Control of reactive distillation (RD) systems is a challenging problem due to nonlinear dynamic and steady state behavior arising from complex interactions between reaction kinetics and vapor liquid equilibria. The focus of work reported in the literature on control of RD systems is on solving servo and regulatory control problems. However, when the unmeasured disturbances / system parameters drift from their nominal values, the operating performance of a RD system can potentially be improved if real time optimization (RTO) techniques are employed for deciding the optimum operating point on-line. In this work, an integrated RTO and adaptive nonlinear model predictive control (NMPC) approach has been proposed for operating an RD system in a economically optimal manner. At the core of the integrated scheme is a nonlinear Bayesian state and parameter estimator, which is used as a common link between the RTO and the NMPC components. Estimates of the drifting unmeasured disturbances / parameters generated by the state estimator are used to update the steady state model used for RTO and the dynamic model used for predictions. This facilitates relatively frequent application of RTO without having to wait for the system to reach steady state and makes the NMPC formulation adaptive. Efficacy of the proposed integrated optimizing control scheme is demonstrated by conducting simulation studies on an ideal RD column. The control problem under investigation is optimal inferential control of product concentrations in the face of drifting reactant flow disturbance. Analysis of the simulation results reveals that the proposed integrated approach is able to satisfactorily identify and track economically beneficial optimum operating point of the system.

Keywords: Real Time Optimization, Nonlinear Predictive Control, State and Parameter Estimation, Reactive Distillation

1. INTRODUCTION

Reactive distillation systems exhibit highly nonlinear dynamic and steady state behavior due to complex interactions between reaction kinetics and vapor liquid equilibria (Purohit et al. (2013a)). As a consequence, optimal control of these systems poses a challenging problem. With reference to control of RD systems, most of the work in the literature has been carried out either on servo and regulatory control problems. (Purohit et al. (2013b), Olanrewaju and Al-Arfaj (2006)). However, disturbances in a plant, such as fluctuations in feed flow rates, feed compositions, variation in kinetic parameters, heat transfer coefficients and external disturbances, such as change in market conditions, shift the optimal point at which the economic benefits are maximized (Engell (2007)). Real time optimization (RTO) techniques, which create link between the advanced control layer and optimization of the economic performance of the process under consideration, have been extensively used in the literature for operating a plant optimally in the face of drifting disturbances and / or parameters (Marlin and Hrymak (1997)). Thus, when unmeasured disturbances / system parameters drift from their nominal values, the operating performance of a RD system can potentially be improved if the RTO techniques are employed for deciding the optimum operating point on-line. However, real time optimizing control of RD systems has received relatively less attention in the process control literature.

A typical RTO scheme consists of a steady state optimizer and a nonlinear controller, which is capable of shifting the plant operation from one optimum setpoint to other. RTO has been implemented by variety of approaches in the literature (Marlin and Hrymak (1997)). The conventional approach invokes the steady state optimization only when the system reaches its new steady state after occurrence of a disturbance / parameter change. The drawback of this approach that it is feasible only when the disturbances / parameters are slowly varying or changing abruptly but rarely (Tatjewski (2008)). When disturbances in a plant change frequently, the plant rarely operates at a steady state. The conventional RTO is not a good choice for optimally controlling such a system. To deal with slow as well as frequent external disturbances simultaneously, Würth et al. (2011) has proposed a two layer architecture where in the upper layer a dynamic RTO is used for rejecting the slowly varying disturbances and a model predictive controller is employed in the lower layer, which

⋆ * Corresponding author (e-mail: sachinp@iitb.ac.in)

tracks the optimal trajectory obtained from the upper layer and suppresses the high frequency disturbances. Another variant of RTO is the real time evolution (RTE) approach by Sequeira et al. (2002) where there is no wait for the plant to reach steady state to implement RTO. By this approach the optimal manipulated input changes computed by RTO are implemented directly without using an intermediate controller (Engell (2007)). However, this approach requires solving a constrained NLP at every time instant, which can prove to be computationally demanding task for a moderately large dimensional system such as reactive distillation.

For implementing the above mentioned approaches in an effective manner, the system states and the disturbances affecting the system need to be known with a reasonable accuracy. While developing RTO schemes, it is often assumed that the disturbances are measured and perfect information of the system states is available. However, such an ideal scenario is rarely found in practice. A way to alleviate this difficulty is to use a nonlinear state and parameter estimator as a common link between the control layer and the optimization layer (Deshpande et al. (2009)) . Estimates of the parameters generated by the nonlinear observer can be used in relatively frequent RTO implementation to arrive at revised optimum in real time. The state and parameter estimator can also be used to develop an adaptive controller that optimally tracks the setpoint trajectories generated by the RTO.

In this work, it is proposed to develop an integrated RTO and adaptive NMPC approach, in which a version of EKF for differential algebraic system (DAE) (Mandela et al. (2010)) is used as a common link between the RTO and the NMPC components, for operating an RD system in a economically optimal manner. Efficacy of the proposed integrated optimizing control scheme is demonstrated by conducting simulation studies on an ideal RD column (Purohit et al. (2013b)). The control problem under investigation is optimal inferential control of product concentrations in the face of drifting reactant flow disturbance.

This paper is organized in four sections. Details of the proposed integrated on-line optimizing control scheme are presented in the next section. Section 3 presents the simulation case study and the conclusions reached through analysis of the simulation results are summarized in Section 4.

2. ONLINE OPTIMIZING CONTROL SCHEME

2.1 Integrated RTO and Adaptive MPC Scheme

A schematic representation of the proposed integrated RTO and Predictive Control scheme is shown in Figure 1. At the core of the proposed integrated scheme is a nonlinear Bayesian state and parameter estimator (such as EKF), which is used to estimate drifting unmeasured disturbances / model parameters. The estimated model parameters are used to update the dynamic prediction model employed by NMPC scheme and the steady state model used by the RTO. When changes in estimated unmeasured disturbances cross a predefined threshold, the RTO is executed and the optimum setpoints are sent to the NMPC scheme, which moves the plant along the desired optimum trajectory. Distinguishing features of the proposed integrated scheme are as follows:

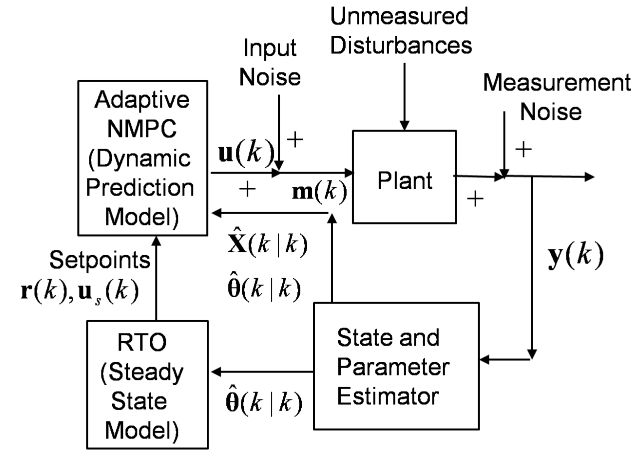

Fig. 1. Schematic Representation of the proposed integrated RTO and Adaptive NMPC Formulation

- A single model is used to perform RTO and multivariable control tasks
- Online update of parameters / unmeasured disturbances in the dynamic model used for prediction amounts to adaptive NMPC formulation
- Economic optimum tracking is carried out without waiting for the system to attain a steady state thereby eliminating the delays involved in tracking the optimum

The proposed integrated scheme has three components: (a) Nonlinear state estimator (b) Real Time Optimizer and (c) adaptive NMPC scheme, which are briefly described in the sub-sections that follow.

2.2 Model for RTO and Predictive Control

Consider a process represented by a set of semi-explicit differential algebraic equations (DAEs)

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}(t), \mathbf{z}(t), \mathbf{m}(t), \boldsymbol{\theta}(t)) \tag{1}$$

$$\overline{0} = \mathbf{G}[\mathbf{x}(t), \mathbf{z}\,(t)] \tag{2}$$

$$\mathbf{y}_T(t) = [\mathbf{C}_x \;\; \mathbf{C}_z] \begin{bmatrix} \mathbf{x}(t) \\ \mathbf{z}\,(t) \end{bmatrix} \tag{3}$$

where, $\mathbf{x} \in \mathbb{R}^n$ represents differential state variables, $\mathbf{z} \in \mathbb{R}^a$ represents algebraic state variables, $\mathbf{m} \in \mathbb{R}^u$ represents manipulated inputs, $\boldsymbol{\theta} \in \mathbb{R}^d$ represents slowly varying model parameters / unmeasured disturbances and $\mathbf{y}_T \in \mathbb{R}^r$ represents true measured variables. To develop the proposed integrated scheme, the following modelling assumptions have been made (Purohit et al. (2013b)) :

- **Assumption 1:** Measurements ($\mathbf{y}$) from plant simulation are available at a regular sampling interval h. *i.e.*

$$\mathbf{y}(k) = [\mathbf{C}_x \;\; \mathbf{C}_z] \begin{bmatrix} \mathbf{x}(k) \\ \mathbf{z}\,(k) \end{bmatrix} + \mathbf{v}(k) \tag{4}$$

  where, $\mathbf{v}(k) \in \mathbb{R}^r$ represents the measurement noise, which is modelled as a zero mean Gaussian white noise processes with covariance matrix $\mathbf{R}$.

- **Assumption 2:** Manipulated inputs ($\mathbf{m}$) are held as piece wise constant over a sampling interval (h) and the true values of the computed manipulated inputs ($\mathbf{u}$) are related to the true values of the manipulated inputs ($\mathbf{m}$) by
$$\mathbf{m}(k) = \mathbf{u}(k) + \mathbf{w}_u(k)$$
where, $\mathbf{w}_u(k) \,\epsilon\, \mathbb{R}^u$, is an unknown disturbance in manipulated inputs such that $\mathbf{w}_u(k) \sim \mathcal{N}(\overline{\mathbf{0}}, \mathbf{Q}_u)$.
- **Assumption 3:** Variation of the model parameters / unmeasured disturbance signal $\boldsymbol{\theta}(t)$ can be approximated as a piecewise constant function defined using the sampling interval h. Moreover, it is assumed that random walk model is sufficient to capture the drifting behavior of model parameters / unmeasured disturbance.
- **Assumption 4:** The control variables of interest, denoted by $\mathbf{y}_c$, (which, in general, need not correspond to the measured outputs) are assumed to be related to the states as follows
$$\mathbf{y}_c(k) = [\mathbf{H}_x \;\; \mathbf{H}_z] \begin{bmatrix} \mathbf{x}(k) \\ \mathbf{z}(k) \end{bmatrix} \tag{5}$$
where $[\mathbf{H}_x \;\; \mathbf{H}_z]$ represents appropriate coupling matrices.

Under the above assumptions, nonlinear plant is simulated by solving the set of DAEs given by equations (1)-(2)
$$\mathbf{x}(k+1) = \mathbf{x}(k) + \int_{kh}^{(k+1)h} \mathbf{f}(\mathbf{x}(\tau), \mathbf{z}(\tau), \mathbf{m}(k), \boldsymbol{\theta}(k)) d\tau \tag{6}$$
$$\overline{\mathbf{0}} = \mathbf{G}(\mathbf{x}(\boldsymbol{\tau}), \mathbf{z}(\boldsymbol{\tau})) \tag{7}$$
using a suitable DAE solver. To simplify the notation, the integration step is represented in a discrete form as follows
$$\mathbf{x}(k+1) = \mathbf{F}[\mathbf{x}(k), \mathbf{z}(k), \mathbf{m}(k), \boldsymbol{\theta}(k)] \tag{8}$$
$$\overline{\mathbf{0}} = \mathbf{G}[\mathbf{x}(k+1), \mathbf{z}\,(k+1)] \tag{9}$$
This discrete dynamic model is used for simulating the plant behavior and for developing the state estimator. On the other hand, to carry out steady state real time optimization, steady state model of the form
$$\mathbf{f}(\mathbf{x}_s,\ \mathbf{u_s},\ \mathbf{z}_s,\ \boldsymbol{\theta}) = \overline{\mathbf{0}} \tag{10}$$
$$\mathbf{G}(\mathbf{x}_s,\ \mathbf{z}_s) = \overline{\mathbf{0}} \tag{11}$$
derived from the dynamic model (1) and (2) is employed. The subscript s here denotes the steady state quantities.

2.3 State and Disturbance Estimation using DAE-EKF

The state and parameter estimator is central to the proposed integrated scheme. The dynamics associated with the drifting parameters / unmeasured disturbances is, in general, unknown. Thus, these drifting parameters / disturbances are modelled as an integrated white noise process, i.e.
$$\boldsymbol{\theta}(k+1) = \boldsymbol{\theta}(k) + \mathbf{w}_d(k), \tag{12}$$
where $\mathbf{w}_d(k)$ is assumed to be a zero mean Gaussian process with covariance, $\mathbf{Q}_d$. While developing the state estimator, the covariance is assumed to be diagonal matrix and the individual parameter variances are treated as tuning parameters. The unmeasured parameter / disturbance model is augmented with process dynamics to arrive at the following model
$$\mathbf{X}(k+1) = \mathcal{F}[\mathbf{X}(k), \mathbf{z}(k), \mathbf{u}(k) + \mathbf{w}_u(k)] \tag{13}$$
$$\overline{\mathbf{0}} = \mathbf{G}[\mathbf{X}(k+1), \mathbf{z}\,(k+1)] \tag{14}$$
where $\mathbf{X}(k) = [\mathbf{x}(k)^T \;\boldsymbol{\theta}\,(k)^T]^T$ and
$$\mathcal{F}[.] = \begin{bmatrix} \mathbf{F}[\mathbf{X}(k), \mathbf{z}(k), \mathbf{u}(k) + \mathbf{w}_u(k)] \\ \boldsymbol{\theta}(k) \end{bmatrix}$$
This augmented model together with the measurement model
$$\mathbf{y}(k) = [\mathbf{C}_x \;\; [\mathbf{0}] \;\; \mathbf{C}_z] \begin{bmatrix} \mathbf{X}(k) \\ \mathbf{z}\,(k) \end{bmatrix} + \mathbf{v}(k) \tag{15}$$
is used for developing the state and parameter estimation scheme. It maybe noted that, since, in practice, only the computed value of the manipulated input is known, true value of the manipulated input, $\mathbf{m}(k)$, appearing in equation (8) has been replaced by $\mathbf{u}(k)+\mathbf{w}_u(k)$ in equation (13). In the present work, it is proposed to use the DAE-EKF algorithm proposed by Mandela et al. (2010) for estimating the states of the augmented DAE system (13)-(14). Details of implementation of DAE-EKF on the ideal RD system under consideration can be found in Purohit et al. (2013b). An important feature of their approach is that it can accommodate measurements of differential as well as algebraic state variables. At each instant k, the estimated states $\hat{\mathbf{x}}(k|k)$, $\hat{\mathbf{z}}\,(k|k)$ the estimated disturbances $\widehat{\boldsymbol{\theta}}\,(k|k)$ are updated in the dynamic model used in the NMPC formulation. Update of the steady state model parameters using $\widehat{\boldsymbol{\theta}}\,(k|k)$ is discussed in the next sub-section.

2.4 Steady State Economic Optimization:

This component of the proposed integrated scheme solves a steady state economic optimization problem, where a suitable economic cost function $J(\mathbf{u_s})$ is considered, subject to the steady state nonlinear plant model (10)-(11) and bounds on the decision variables $\mathbf{u_s}$. While, in principle, the steady state optimization can be carried out at each sampling instant, solving the resulting constrained NLP in real time together with NMPC can be computationally demanding task. Thus, it is proposed to invoke the optimization step only when there is an appreciable change in the unmeasured disturbance / parameter values. Let k_l represent the last sampling instant when the steady state optimization was invoked. The steady state optimization is invoked at a subsequent instant $k = k_n$ where any one of the following criteria is satisfied
$$\left|\widehat{\boldsymbol{\theta}}_i(k|k) - \widehat{\boldsymbol{\theta}}_i(k_l|k_l)\right| \geq \Delta_i \tag{16}$$
Here, $\Delta_i : i = 1, 2, ...d$ represent pre-specified thresholds.

The optimization problem is formulated as follows:
$$\mathbf{u_s}(k_n) = \max_{\mathbf{u_s}} J(\mathbf{u_s}) \tag{17}$$
subject to
$$\mathbf{f}(\mathbf{x}_s,\ \mathbf{u_s},\ \mathbf{z}_s,\ \widehat{\boldsymbol{\theta}}(k_n|k_n)) = \overline{\mathbf{0}} \tag{18}$$
$$\mathbf{G}(\mathbf{x}_s,\ \mathbf{z}_s) = \overline{\mathbf{0}} \tag{19}$$
$$\mathbf{u}_{\mathbf{s}\,\min} \leq \mathbf{u_s} \leq \mathbf{u}_{\mathbf{s}\,\max} \tag{20}$$
The optimum solution to this problem yields the optimum setpoint
$$\mathbf{r}(k_n) = [\mathbf{H}_x \;\; \mathbf{H}_z] \begin{bmatrix} \mathbf{x}_s(k_n) \\ \mathbf{z}_s\,(k_n) \end{bmatrix}$$

After completion of the optimization step, we set $k_l = k_n$, and for $k \geq k_l$,

$$\mathbf{r}(k) = \mathbf{r}(k_l) \text{ and } \mathbf{u_s}(k) = \mathbf{u_s}(k_l)$$

are communicated to the NMPC for tracking till the RTO is invoked again.

2.5 Adaptive Nonlinear Model Predictive Control

Tracking of steady state optimal updated set-points $\mathbf{y}_r(k)$ is achieved by employing the observer error feedback and successive linearization based NMPC scheme developed by Purohit et al. (2013b) with the following modifications:

- *Model Predictions:* Model predictions are carried out as follows

$$\widetilde{\mathbf{x}}(j+1|k) = \mathbf{F}[\widetilde{\mathbf{x}}(j|k), \widetilde{\mathbf{z}}(j|k), \widehat{\boldsymbol{\theta}}(k|k)] + \mathbf{L}_d(k)\mathbf{e}(k) \quad (21)$$

$$\overline{\mathbf{0}} = \mathbf{G}[\widetilde{\mathbf{x}}(j+1|k), \widetilde{\mathbf{z}}\,(j+1|k)] \quad (22)$$

where $j = k, k+1, ...k+p$, p represents the prediction horizon, $\mathbf{L}_d(k)$ represents the observer gain matrix corresponding to the continuous states computed by DAE-EKF. Here, the initial conditions are

$$\tilde{\mathbf{x}}(0|k) = \hat{\mathbf{x}}(k|k) \text{ and } \tilde{\mathbf{z}}(0|k) = \hat{\mathbf{z}}(k|k)$$

It may be noted that this implicitly assumes

$$\widetilde{\boldsymbol{\theta}}(j+1) = \widetilde{\boldsymbol{\theta}}(j)$$

for $j \geq k$ i.e. over the prediction horizon with $\widetilde{\boldsymbol{\theta}}(0|k) = \widehat{\boldsymbol{\theta}}(k|k)$. The use of updated $\widehat{\boldsymbol{\theta}}(k|k)$ in predictions makes the NMPC formulation adaptive. The controlled outputs, $\tilde{\mathbf{y}}_c$, are predicted as follows

$$\tilde{\mathbf{y}}_c(j|k) = [\mathbf{H}_x \ \mathbf{H}_z] \begin{bmatrix} \tilde{\mathbf{x}}(j|k) \\ \tilde{\mathbf{z}}(j|k) \end{bmatrix}$$

- *Objective Function:* To strengthen the link between the RTO and NMPC, in addition to penalizing deviations from $\mathbf{y}_r(k)$, i.e.

$$\mathbf{E}(j|k) = \tilde{\mathbf{y}}_c(j|k) - \mathbf{y}_r(k) \quad \text{for } j = k, ..., k+p$$

and the change in the future input moves, the NMPC objective function is modified by including the following term

$$\sum_{i=0}^{q-1} \Delta\mathbf{u}_{\mathbf{s}}^T(k+i|k)\mathbf{W}_{\Delta u_s}\Delta\mathbf{u}_{\mathbf{s}}(k+i|k) \quad (23)$$

where

$$\Delta\mathbf{u}_{\mathbf{s}}(k+i|k) = \mathbf{u}(k+i|k) - \mathbf{u}_{\mathbf{s}}(k)$$

Here, p represents the prediction horizon, q represents the control horizon, $\mathbf{u}(k+i|k) : i = 0, 1, ..., q-1$ represents the future manipulated input moves and $\mathbf{W}_{\Delta u_s}$ is a positive definite weighting matrix.

3. REAL TIME OPTIMIZING CONTROL OF IDEAL REACTIVE DISTILLATION COLUMN

To demonstrate the effectiveness of the proposed integrated optimizing control scheme, a case study of real time optimizing control of an ideal reactive distillation (RD) (Olanrewaju and Al-Arfaj (2006); Purohit et al. (2013b)) system is presented in this section. A hypothetical reaction, $A + B \leftrightarrow C + D$ is carried out in the system. The reactive distillation column has total $\mathbf{N}(= N_s + N_{RX} + N_R)$ stages (excluding a reboiler and total condenser). The reactive section contains N_{RX} trays, the rectifying section contains N_R trays, and the stripping section below the reactive section contains N_S trays. Reaction occurs only in reactive section in which solid catalyst is present on trays. Pure reactant A enters the column on the first tray of the reactive section (i.e. tray no. $N_S + 1$) and pure reactant B enters the column on the last reactive stage (i.e. tray no. $N_S + N_{RX}$). In the present work, an RD column with $N_S = 7$, $N_{RX} = 6$, and $N_R = 7$ has been considered. In addition, the RD system consists of a reboiler and a total condenser. The differential state variables corresponds to compositions on all the trays, and molar hold ups in reboiler and condenser. The algebraic variables corresponds to temperatures in all the trays including the reboiler. These variables are obtained by using vapor liquid equilibrium on each tray and in the reboiler. The mathematical model of ideal RD system considered here consists of 88 differential equations, and 21 algebraic equations which result in semi-explicit DAEs of index 1. Details of the model parameters and operating conditions can be found in Olanrewaju and Al-Arfaj (2006); Purohit et al. (2013b). To solve DAEs for plant simulation and state estimation, an implicit Euler algorithm is employed with integration interval of 1 sec. A sampling time of $h = 30$ sec has been used for state estimation and control.

For this system, the measured outputs are temperatures on alternate trays, reboiler temperature, condenser and reboiler holdups. The controlled variables are (x_c, x_a, x_d) where x_c represents mole fraction of component C in the distillate, x_a represents concentration of A on the feed stage and x_d represents the mole fraction of component D on the bottom stage. It may be noted that the controlled outputs are different from the measured outputs. Manipulated inputs are feed flow rate of composition A (F_a), reflux flow rate (R), and vapor boilup (V_s). Inlet feed flow rate of composition B (F_b) is treated as an unmeasured disturbance variable / slowly varying model parameter. Details of the standard deviations of the measurement noise and noise in the manipulated inputs can be found in Purohit et al. (2013b). The standard deviation of noise in the random walk model for F_b is chosen as $Q_d = 1 \times 10^{-8}$. The prediction (p) and control horizon (q) in the NMPC formulation are chosen as 40 and 4, respectively. Other NMPC tuning parameters such as, bounds on the manipulated inputs and error weighting matrix can be found in Purohit et al. (2013b). In addition, matrix $\mathbf{W}_{\Delta u_s} = 10\mathbf{I}$ is used in the NMPC formulation. For invoking RTO, a dynamic threshold is selected as follows

$$\Delta_{F_b} = 0.005 \times \widehat{F}_b(k_l|k_l)$$

To avoid infeasibilities in iterations carried out by the optimizer while implementing RTO step, the decision variables are bounded between ±10% of their respective nominal values. Instead of checking this condition at each sampling instant, it is checked after regular intervals (every 230 samples). The constrained optimization problems in RTO and NMPC formulations are solved using MATLAB function *fmincon.*

It may be noted that, Purohit et al. (2013b) has developed observer error feed back based NMPC scheme for achieving offset free control of RD systems, by assuming that the controlled variables (x_c, x_d, x_a) are measured along with

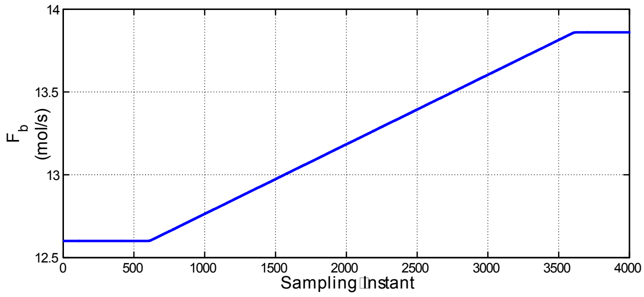

Fig. 2. Case A: Ramp disturbance in feed flow of reactant B

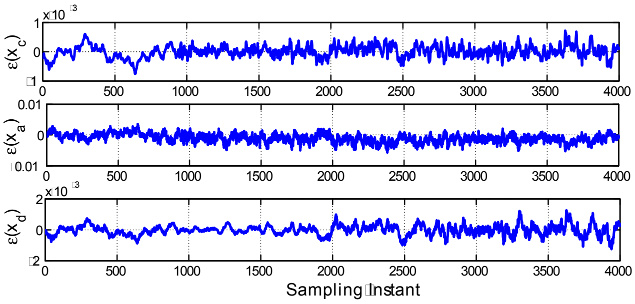

Fig. 3. Case A: Profile of state estimation errors in controlled variables

the temperatures. In practice, however, the composition measurements are rarely available. In the present work, observer error feed back based NMPC scheme developed by Purohit et al. (2013b) for DAE systems is used by considering only the temperature measurements. The key to achieve offset free control without the concentration measurements is estimation of the unmeasured disturbance.

The objective function for RTO is chosen as maximization of steady state top and bottom compositions (x_c, x_d) with respect to steady state reflux flow rate (R), and vapor boilup (V_s). The performance of the integrated optimizing control scheme is investigated under the following two scenarios:

- **Case A:** Perfect measurements of the feed flowrate (F_b) of reactant B are assumed to be available and are directly used for estimation, control and optimization.
- **Case B:** The feed flowrate (F_b) of reactant B is treated as unmeasured disturbance and estimated using DAE-EKF as discussed in the previous section. Estimated values of F_b are used for estimation, control and optimization.

Case A essentially provides a reference to evaluate Case B. The initial operating point is selected as unstable steady state point, $x_c = 0.95$, $x_d = 0.95$, $x_a = 0.4308$, with initial manipulated inputs maintained at $V_s = 28.3$ mol/s, $R = 32.9$ mol/s, $Fa = 12.6$ mol/s (Purohit et al. (2013b)). In the nominal conditions the disturbance variable F_b is maintained at 12.6 mol/s. A positive ramp disturbance is introduced in the F_b at 600^{th} sampling instant till F_b increases by 10% of its nominal value (see Figure 2).

Results of closed loop simulation for Case A are presented in Figures (4)-(5). Since perfect measurement of F_b is assumed to be available in this case, the estimation error

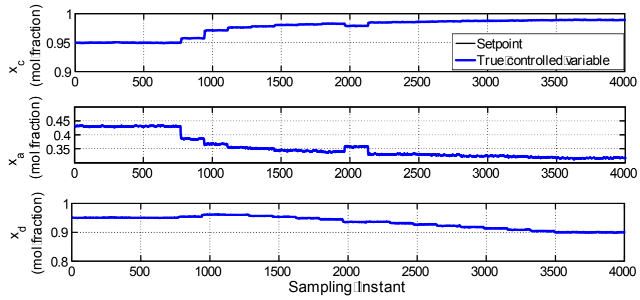

Fig. 4. Case A: Profiles of controlled variables

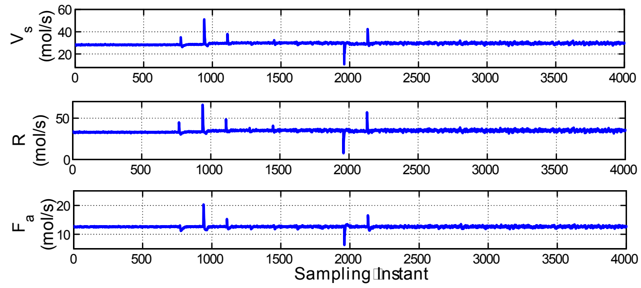

Fig. 5. Case A: Profile of manipulated inputs

for the controlled variables is practically zero as seen from Figure (3) i.e., estimated states quickly converge to the true states. When feed flowrate of B is increased, there is complete conversion of A, and, since A is the most volatile component, steady state x_c (i.e. x_c setpoint decided by RTO) increases from 0.95 to 0.9891 mole fraction (see Figure 4). On the other hand, since B is a heavy component, excess B goes out of the system through bottom product and, as a consequence x_d decreases from 0.95 to 0.899 mole fraction (see Figure 4). Figure (4) also shows that the optimal setpoints sent by the RTO are quickly tracked by the NMPC when the disturbance is perfectly known.

Results for Case B are presented in Figures (6) - (9). In this case, the flowrate F_b is unmeasured and is estimated along with the states using the DAE-EKF algorithm (see Figure 6). The behavior of the estimation errors for the controlled variables is presented in Figure (7). While the estimates of F_b differ significantly from the true value during the transient, estimated F_b eventually converges to the final true steady state value of F_b. As a consequence, the RTO moves the system close to the final optimum found in Case A (with approximately 1% difference from Case A). As can be expected, the performance of the NMPC deteriorates with reference to Case A. However, the performance shown in Figure (8) is certainly satisfactory from the viewpoint of achieving optimal operation in the face of drifting unmeasured disturbances. Moreover, offset free inferential control of product concentrations is achieved without requiring use of concentration measurements as suggested by Purohit et al. (2013b).

4. CONCLUSION

In this work, an integrated RTO and adaptive NMPC approach has been proposed for operating a reactive distillation system in a economically optimal manner. At the

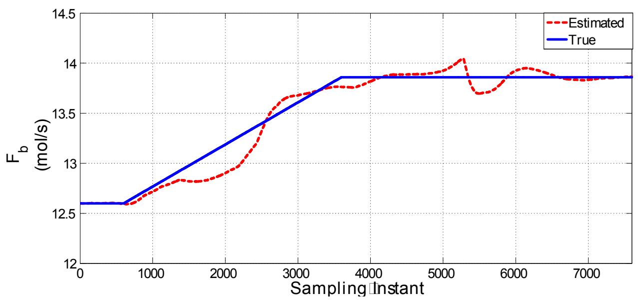

Fig. 6. Case B: Comparison of true and estimated disturbance variable

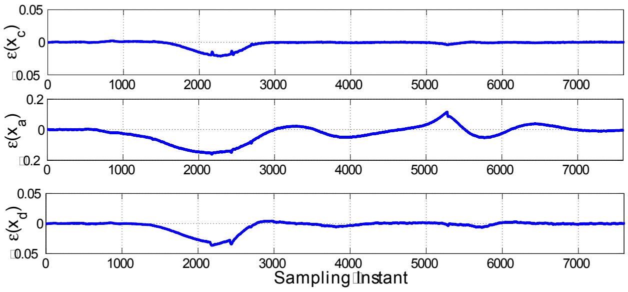

Fig. 7. Case B: Profiles of estimation errors

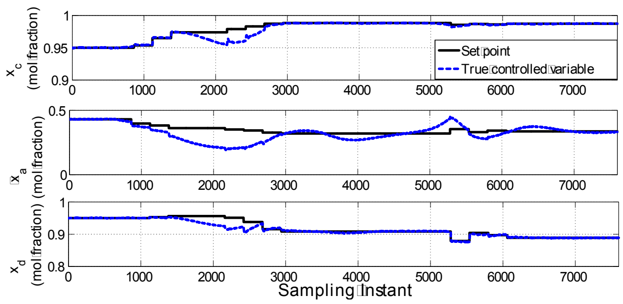

Fig. 8. Case B: Profiles of controlled variables

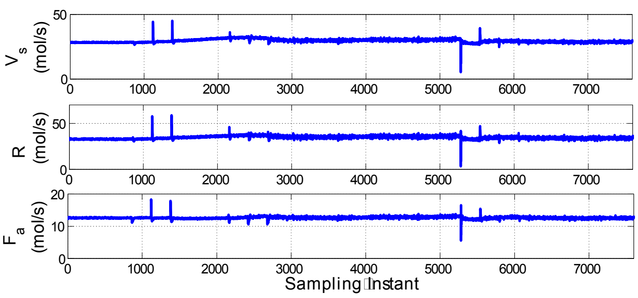

Fig. 9. Case B: Profiles of manipulated inputs

core of the integrated scheme is a state and parameter estimator (DAE-EKF), which connects the RTO and the NMPC components. Estimates of the drifting unmeasured disturbances / parameters generated by the state estimator are used to update the steady state model used for RTO and the dynamic model used for predictions. Efficacy of the proposed integrated optimizing control scheme is demonstrated by conducting simulation studies on an ideal RD column. The control problem under investigation is optimal inferential control of product concentrations in the face of drifting reactant flow disturbance. Analysis of the simulation results reveals that the proposed integrated approach is able to satisfactorily identify and track economically beneficial optimum operating point of the system. In response to the disturbance drift, the RTO increases the top product quality and decreases the bottom product quality from the nominal values, with minimal change in all the manipulated variables. Moreover, offset free control of product mole fractions is achieved without requiring to include concentration measurements.

While these initial studies have shown promising results, number of implementation issues remain to be sorted out. There is significant error in the estimation of the unmeasured disturbance during transient, which can possibly be reduced by employing alternate state estimation approaches such as DAE-UKF. Also, average computation time for implementation of RTO step was found to be about 20 min on a 3.4 GHz Pentium with i7 processor and using *fmincon*. Efforts are being made to reduce the time required for optimization by employing a more efficient NLP solver.

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