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Predictive Control of a Reactive Distillation Column using Multi-rate DAE EKF

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Abstract: Control of product purity is of paramount importance in effective control of tightly integrated process such as reactive distillation. In practice, however, measurements of product concentrations may be unavailable or may be available at slower sampling rates when compared with other measurements. A cost effective approach to improve control of such systems is to develop a state estimator that can accommodate measurements at multiple rates and use it in controller development. In this work, DAE EKF formulation developed by Mandela et al. (2010) is modified to accommodate measurements available at multiple sampling rates. A successive linearization based nonlinear MPC scheme is then developed for controlling a system modeled as DAEs. Observer error feedback approach developed by Hunag et al. (2012) has been extended to achieve offset reduction and to improve regulatory control of a multi-rate sampled data system. The efficacy of the proposed approach is demonstrated by conducting simulation studies on an ideal reactive distillation system. Analysis of the simulation results reveals that the feedback introduced using the multi-rate concentration measurements reduces the offset significantly in the face of unmeasured disturbances of moderate magnitude.

Keywords: Differential Algebraic Systems; Multi-rate Sampling; Extended Kalman Filter; Nonlinear Model Predictive Control; Reactive Distillation.

INTRODUCTION

Reactive distillation (RD) has recently become one of the most important hybrid unit operation in the processes industry. Control of quality variables, such as product purity in a RD column, is of paramount importance in effective control of such a tightly integrated process. In practice, however, measurements of product concentrations may be unavailable or may be available only at slow sampling rates when compared with other measurements such as temperatures and pressures. A cost effective approach to improve control of such systems is to develop a state estimator using a reliable mechanistic model of the plant and use the estimated quality variables for improving the control performance (Patwardhan et al. (2012)).

State estimation approaches that can accommodate measurements sampled at multiple rates are at the core of the control schemes for multi-rate sampled data systems. Over the last two decades, many versions extended Kalman filter (EKF) that can deal with the measurements sampled at multiple rates have been developed and employed for combined state and parameter estimation in variety of applications (Patwardhan et al. (2012)). However, majority of the available approaches are for systems modelled as a set of ODEs. An RD system, on the other hand, is typically modelled as a system of coupled differential algebraic equations (DAEs). The systems governed by DAEs have received much less attention in the state estimation literature. The extension of the Kalman Filter for nonlinear DAE systems has been explored previously by Beccera (2001). Their estimation scheme can accommodate measurements obtained only from the differential states, which can prove to be a serious limitation for systems such as RD columns. To overcome this limitation, Mandela et al (2010) have recently developed formulations for EKF and UKF (Unscented Kalman Filter), which accommodate measurements of differential as well as algebraic states. However, in both the approaches (Beccera (2001), Mandela et al (2010)), it was assumed that all the measurements are available at the single (fast) rate.

In this work, the DAE EKF formulation developed by Mandela et al (2010) is further modified to accommodate measurements available at multiple sampling rates. The RD system under consideration exhibits simultaneous input and output multiplicity behavior in the desired operating region. To achieve tight control of such a highly nonlinear system over a wide operating range, a successive linearization based nonlinear predictive control scheme is developed. To achieve off-set free close loop behavior, Huang et al. (2009) have proposed observer error feedback scheme that introduces integral action in the controller. This observer error feedback approach is extended in the present work for controlling a multi-rate sampled data system. The efficacy of the proposed approach is demonstrated by conducting simulation studies on a ideal reactive distillation system (Olanrewaju and Al-Arfaj (2006)), which exhibits input and output multiplicities simultane-

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ously at the desired operating point (point A in figure 1) .

This paper is organized as follows. In Section 1, EKF formulation for DAE systems is modified for the multi-rate measurement scenario. Section 2 presents development of multi-rate NMPC formulation based on successive linearization of DAE model. The results of the simulation case study using the ideal RD system are described in Section 3, and, the conclusions reached through analysis of the results are presented in Section 4.

1. MULTI-RATE EKF FOR DAE SYSTEMS

1.1 Modeling Assumptions

The nonlinear DAE model of RD column can be re-written in an abstract form as follows

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}\left[\mathbf{x}(t), \mathbf{z}(\mathbf{t}), \mathbf{m}(t)\right] \tag{1}$$

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

where, $\mathbf{x} \in R^{n_d}$ represents the differential state variables, $\mathbf{z} \in R^{n_a}$ represents the algebraic state variables, $\mathbf{u} \in R^m$ represents the manipulated input variables and $\mathbf{d} \in R^d$ represent the unmeasured disturbance variables. Let h represents the smallest sampling interval and interval at which manipulated input moves are made.

Assumption 1 It is assumed that total of $r(= r_F + r_S)$ measurements are available from the system, where, r_F is defined as measurements available at fast rate and r_S is defined as measurements available at slow rate. In a *regularly sampled multi-rate scenario*, a subset of the measurements, $\mathbf{y}_F \in R^{r_F}$, are available at faster rate, i.e. at *minor sampling instant* $\{kh : k = 0, 1, 2, ...\}$, while remaining measurements $\mathbf{y}_S(k_j) \in R^{r_S}$ are available only the at slower rate, i.e. at *major sampling instant* $\{k_j = j(nh) : j = 0, 1, 2, ...\}$. The measurement vector, $\mathbf{y}(k)$, at k'th sampling instant is given as follows

- **Minor sampling instant** $(k \neq k_j)$

$$\mathbf{y}(k) = \mathbf{y}_F(k) \tag{3}$$

$$\mathbf{y}_F(k) = \mathbf{C}_F \begin{bmatrix} \mathbf{x}(k) \\ \mathbf{z}(k) \end{bmatrix} + \mathbf{v}_F(k) \tag{4}$$

- **Major sampling instant** $(k = k_j)$

$$\mathbf{y}(k) = \begin{bmatrix} \mathbf{y}_F(k) \\ \mathbf{y}_S(k) \end{bmatrix} = \begin{bmatrix} \mathbf{C}_F \\ \mathbf{C}_S \end{bmatrix} \begin{bmatrix} \mathbf{x}(k) \\ \mathbf{z}(k) \end{bmatrix} + \mathbf{v}(k) \tag{5}$$

$$= \mathbf{C} \begin{bmatrix} \mathbf{x}(k) \\ \mathbf{z}(k) \end{bmatrix} + \mathbf{v}(k) \tag{6}$$

Thus, at major sampling instants, all the measurements are available simultaneously. Here, measurement noise, $\mathbf{v}(k)$ is modelled as a zero mean white noise processes with Gaussian distribution, i.e. $\mathbf{v}(k) \sim \mathcal{N}(\overline{\mathbf{0}}, \mathbf{R})$ and $\mathbf{v}_F(k) \sim \mathcal{N}(\overline{\mathbf{0}}, \mathbf{R}_F)$, represents subset of measurement noise vector corresponding to the fast rate measurements.

Assumption 2 The manipulated inputs are piecewise constant over interval i.e.

$$\mathbf{m}(t) = \mathbf{m}(k) \quad \text{for} \quad t_k \leq t < t_{k+1} = t_k + h$$

Further, the true value of the manipulated inputs ($\mathbf{m}$) is related to the known / computed value of the manipulated inputs ($\mathbf{u}$) as follows

$$\mathbf{m}(k) = \mathbf{u}(k) + \mathbf{w}_u(k) \tag{7}$$

where $\mathbf{w}_{u,k} \in \mathbb{R}^m$ denotes an unknown disturbance in manipulated inputs such that $\mathbf{w}_u(k) \sim \mathcal{N}(\overline{\mathbf{0}}, \mathbf{Q}_u)$.

Assumption 3 The choice of the sampling interval is small enough so that the variation of the unmeasured disturbances can be adequately approximated using the piecewise constant functions of the form

$$\mathbf{d}(k) = \overline{\mathbf{d}} + \mathbf{w}_d(k) \quad \text{for} \quad t_k \leq t < t_{k+1} = t_k + h$$

$\mathbf{w}_d(k) \in \mathbb{R}^{d_u}$ denotes a disturbance in the unmeasured disturbance such that $\mathbf{w}_d(k) \sim \mathcal{N}(\overline{\mathbf{0}}, \mathbf{Q}_d)$ and $\overline{\mathbf{d}}$ represents the mean or the steady state value of the unmeasured disturbance at some desired operating point.

Thus, the plant is simulated by solving the following set of DAEs

$$\mathbf{x}(k+1) = \mathbf{x}(k) + \int_{k\Delta}^{(k+1)h} \mathbf{f}\left[\mathbf{x}(\tau), \mathbf{m}(k), \mathbf{d}(k)\right] d\tau \tag{8}$$

$$\overline{0} = \mathbf{G}\left[\mathbf{x}(\tau), \mathbf{z}(\tau)\right] \tag{9}$$

using a suitable DAE solver. For the sake of convenience, the following notation is adopted to represent the DAE represented by (8-9) in discrete form

$$\mathbf{x}(k) = \mathbf{F}\left[\mathbf{x}(k-1), \mathbf{u}(k-1), \overline{\mathbf{d}}, \mathbf{w}(k-1)\right] \tag{10}$$

$$\overline{0} = \mathbf{G}\left[\mathbf{x}(k), \mathbf{z}(k)\right] \tag{11}$$

where $\mathbf{w}(k)$ represents augmented state noise vector, i.e.

$$\mathbf{w}(k) = \left[\, \mathbf{w}_u^T(k) \;\, \mathbf{w}_d^T(k) \,\right]^T$$

with covariance matrices $\mathbf{Q} = \mathbf{diag}\left[\, \mathbf{Q}_u \;\, \mathbf{Q}_d \,\right]$.

1.2 Multi-rate EKF for Semi-implicit DAE System

In the present work, the EKF algorithm proposed by Mandela et al (2010) is modified for *multi-rate* scenario for the state estimation of the semi-implicit DAE system given by (10-11) together with the measurement model (3-6). EKF is preferred over UKF as the later formulation was found to result in significantly large (about 20 times) average computation time. The steps involved in the state estimation based on EKF for *multi-rate* scenario are as follows:

- **Prediction Step:** At every minor and major sampling instant, given estimates $(\widehat{\mathbf{x}}(k-1|k-1), \widehat{\mathbf{z}}(k-1|k-1)$, the predicted mean is computed using a DAE solver

$$\widehat{\mathbf{x}}(k|k-1) = \mathbf{F}\left[\widehat{\mathbf{x}}(k-1|k-1), \mathbf{u}(k-1), \overline{\mathbf{d}}, \overline{\mathbf{0}}\right] \tag{12}$$

$$\overline{0} = \mathbf{G}\left[\widehat{\mathbf{x}}(k|k-1), \widehat{\mathbf{z}}(k|k-1)\right] \tag{13}$$

Defining an augmented state vector

$$\mathcal{X}(k) = \left[\, \mathbf{x}^T(k) \;\, \mathbf{z}^T(k) \,\right]^T$$

and Jacobian matrix

$$\mathcal{A}(k-1) = \begin{bmatrix} \underbrace{\left[\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right]_{(\bullet)}}_{a_{21}} & \underbrace{\left[\frac{\partial \mathbf{f}}{\partial \mathbf{z}}\right]_{(\bullet)}}_{a_{22}} \end{bmatrix}$$

$$\mathcal{B}_w(k-1) = \begin{bmatrix} \underbrace{\left[\frac{\partial \mathbf{f}}{\partial \mathbf{w}}\right]_{(\bullet)}}_{b_w} \end{bmatrix}$$

where,

$$a_{21} = -\left[\frac{\partial \mathbf{G}}{\partial \mathbf{z}}\right]^{-1}_{(\bullet)}\left[\frac{\partial \mathbf{G}}{\partial \mathbf{x}}\right]_{(\bullet)}\left[\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right]_{(\bullet)}$$

$$a_{22} = -\left[\frac{\partial \mathbf{G}}{\partial \mathbf{z}}\right]^{-1}_{(\bullet)}\left[\frac{\partial \mathbf{G}}{\partial \mathbf{x}}\right]_{(\bullet)}\left[\frac{\partial \mathbf{f}}{\partial \mathbf{z}}\right]_{(\bullet)}$$

$$b_{w} = -\left[\frac{\partial \mathbf{G}}{\partial \mathbf{z}}\right]^{-1}_{(\bullet)}\left[\frac{\partial \mathbf{G}}{\partial \mathbf{x}}\right]_{(\bullet)}\left[\frac{\partial \mathbf{f}}{\partial \mathbf{d}}\right]_{(\bullet)}$$

such that the derivatives are evaluated at

$$(\bullet) \equiv (\widehat{\mathbf{x}}(k|k-1), \widehat{\mathbf{z}}(k|k-1), \mathbf{u}(k-1), \overline{\mathbf{d}}) \tag{14}$$

The update of the predicted covariance matrix, $\mathbf{P}(k|k-1)$,of the augmented state estimates, $\widehat{\mathcal{X}}(k|k-1)$,is carried out as follows

$$\mathbf{P}(k|k-1) = \mathbf{\Phi}(k-1)\mathbf{P}(k-1|k-1)\mathbf{\Phi}(k-1)^T + \mathbf{\Gamma}_w^T(k-1)\mathbf{Q}\mathbf{\Gamma}_w(k-1) \tag{15}$$

$$\mathbf{\Phi}(k) = e^{\mathcal{A}(k)h} \quad ; \quad \mathbf{\Gamma}_w(k) = \int_0^h e^{\mathcal{A}(k)\tau}\mathcal{B}_w(k)d\tau$$

- **Update step:** Calculations for the update step are different at minor and major sampling instant.
  - **Minor sampling instant** ($k \neq k_j$)**:** The Kalman gain can be computed as follows

$$\mathbf{L}_F(k) = \mathbf{P}(k|k-1)\mathbf{C}_F^T\left[\mathbf{V}_F(k)\right]^{-1}$$

$$\mathbf{V}_F(k) = \mathbf{C}_F\mathbf{P}(k|k-1)\mathbf{C}_F^T + \mathbf{R}_F \tag{16}$$

$$\begin{bmatrix} \widehat{\mathbf{x}}(k|k) \\ \widetilde{\mathbf{z}}(k|k) \end{bmatrix} = \begin{bmatrix} \widehat{\mathbf{x}}(k|k-1) \\ \widehat{\mathbf{z}}(k|k-1) \end{bmatrix} + \mathbf{L}_F(k)\mathbf{e}_F(k)$$

$$\mathbf{e}_F(k) = \mathbf{y}_F(k) - \mathbf{C}_F\widehat{\mathcal{X}}(k|k-1) \tag{17}$$

$$\mathbf{P}(k|k) = \left[\mathbf{I} - \mathbf{L}_F(k)\mathbf{C}_F\right]\mathbf{P}(k|k-1)$$

  - **Major sampling instant** ($k = k_j$)**:** The Kalman gain can be computed as follows

$$\mathbf{L}(k) = \mathbf{P}(k|k-1)\mathbf{C}^T\left[\mathbf{C}\mathbf{P}(k|k-1)\mathbf{C}^T + \mathbf{R}\right]^{-1} \tag{18}$$

$$\begin{bmatrix} \widehat{\mathbf{x}}(k|k) \\ \widetilde{\mathbf{z}}(k|k) \end{bmatrix} = \begin{bmatrix} \widehat{\mathbf{x}}(k|k-1) \\ \widehat{\mathbf{z}}(k|k-1) \end{bmatrix} + \mathbf{L}(k)\mathbf{e}(k)$$

$$\mathbf{e}(k) = \mathbf{y}(k) - \mathbf{C}\widehat{\mathcal{X}}(k|k-1) \tag{19}$$

$$\mathbf{P}(k|k) = \left[\mathbf{I} - \mathbf{L}(k)\mathbf{C}\right]\mathbf{P}(k|k-1)$$

In each case, since the updated differential and algebraic states, $(\widehat{\mathbf{x}}(k|k), \widetilde{\mathbf{z}}(k|k))$ together may not satisfy the algebraic equations, the algebraic states, $\widehat{\mathbf{z}}(k|k)$, are recomputed using the differential states $\widehat{\mathbf{x}}(k|k)$ by solving for

$$\overline{0} = \mathbf{G}\left[\widehat{\mathbf{x}}(k|k), \widehat{\mathbf{z}}(k|k)\right] \tag{20}$$

2. NMPC SCHEMES BASED ON OBSERVER ERROR FEEDBACK

Let $\mathbf{y}_c$ represent set of controlled outputs

$$\mathbf{y}_c(k) \equiv \mathbf{y}_c(k) = \mathbf{C}_S\begin{bmatrix} \mathbf{x}(k) \\ \mathbf{z}(k) \end{bmatrix}$$

which, in the present case, corresponds to the slowly sampled measurements. Consider the problem of generating future predictions using continuous time model

$$\frac{d\widetilde{\mathbf{x}}}{dt} = \mathbf{f}\left[\widetilde{\mathbf{x}}(t), \widetilde{\mathbf{z}}(t), \mathbf{u}(t), \mathbf{d}(t)\right] \tag{21}$$

$$\overline{0} = \mathbf{G}\left[\widetilde{\mathbf{x}}(t), \widetilde{\mathbf{z}}(t)\right] \tag{22}$$

with initial condition $\widetilde{\mathbf{x}}(kh) = \widehat{\mathbf{x}}(k|k)$, $\mathbf{z}(kh) = \widehat{\mathbf{z}}(k|k)$ and using future input sequence

$$\mathbf{U}_f \equiv \{\mathbf{u}(k|k), \mathbf{u}(k+1|k)........\mathbf{u}(k+p-1|k)\} \tag{23}$$

To make the problem computationally tractable, it is proposed to linearize the DAE in the neighborhood of the current operating point

$$(\bullet) \equiv \left(\widehat{\mathbf{x}}(k|k), \widehat{\mathbf{z}}(k|k), \mathbf{u}(k-1), \overline{\mathbf{d}}\right) \tag{24}$$

and then the linear model is used for carrying out predictions.

2.1 Successive Linearization of DAE Model

RHS of equation (21) can be linearized in the neighborhood of point $(\bullet)$ as follows

$$\frac{d\widetilde{\mathbf{x}}}{dt} \approx \mathbf{f}(k) + \mathcal{A}_x(k)\delta\widetilde{\mathbf{x}}(t) + \mathcal{A}_z(k)\delta\widetilde{\mathbf{z}}(t) + \mathcal{B}_u(k)\delta\mathbf{u}(t) + \mathcal{B}_d(k)\delta\mathbf{d}(t)$$

$$\delta\widetilde{\mathbf{x}}(t) = \widetilde{\mathbf{x}}(t) - \widehat{\mathbf{x}}(k|k), \qquad \delta\widetilde{\mathbf{z}}(t) = \widetilde{\mathbf{z}}(t) - \widehat{\mathbf{z}}(k|k)$$

$$\delta\mathbf{u}(t) = \mathbf{u}(t) - \mathbf{u}(k-1), \qquad \delta\mathbf{d}(t) = \mathbf{d}(t) - \overline{\mathbf{d}}$$

$$\mathbf{f}(k) = \mathbf{f}\left[\widehat{\mathbf{x}}(k|k), \widehat{\mathbf{z}}(k|k), \mathbf{u}(k-1), \overline{\mathbf{d}}\right]$$

$$\mathcal{A}_x(k) = \left[\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right]_{(\bullet)} \quad ; \quad \mathcal{A}_z(k) = \left[\frac{\partial \mathbf{f}}{\partial \mathbf{z}}\right]_{(\bullet)}$$

$$\mathcal{B}_u(k) = \left[\frac{\partial \mathbf{f}}{\partial \mathbf{u}}\right]_{(\bullet)} \quad ; \quad \mathcal{B}_d(k) = \left[\frac{\partial \mathbf{f}}{\partial \mathbf{d}}\right]_{(\bullet)}$$

Also, equation (22) can be linearized in the neighborhood of point $(\bullet)$ as follows

$$\mathbf{G}\left[\widetilde{\mathbf{x}}(t), \widetilde{\mathbf{z}}(t)\right] \approx \mathbf{g}_k + \mathcal{G}_x(k)\delta\widetilde{\mathbf{x}}(t) + \mathcal{G}_z(k)\ \delta\widetilde{\mathbf{z}}(t) = \overline{\mathbf{0}}$$

$$\mathbf{g}(k) = \mathbf{G}\left[\widehat{\mathbf{x}}(k|k), \widehat{\mathbf{z}}(k|k)\right]$$

$$\mathcal{G}_x(k) = \left[\frac{\partial \mathbf{G}}{\partial \mathbf{x}}\right]_{(\bullet)} \quad ; \quad \mathcal{G}_z(k) = \left[\frac{\partial \mathbf{G}}{\partial \mathbf{z}}\right]_{(\bullet)}$$

$$\delta\widetilde{\mathbf{z}}(t) = -\left[\mathcal{G}_z(k)\right]^{-1}\left[\mathbf{g}(k) + \mathcal{G}_x(k)\delta\widetilde{\mathbf{x}}(t)\right]$$

Thus, equation (21) can be locally approximated as follows

$$\frac{d\widetilde{\mathbf{x}}}{dt} = \mathbf{f}(k) - \mathcal{A}_z(k)\left[\mathcal{G}_z(k)\right]^{-1}\mathbf{g}(k) + \mathcal{A}(k)\delta\widetilde{\mathbf{x}}(t) + \mathcal{B}_u(k)\delta\mathbf{u}(t) + \mathcal{B}_d(k)\delta\mathbf{d}(t) \tag{25}$$

$$\mathcal{A}(k) = \left[\mathcal{A}_x(k) - \mathcal{A}_z(k)\left[\mathcal{G}_z(k)\right]^{-1}\mathcal{G}_x(k)\right] \tag{26}$$

$$\widetilde{\mathbf{x}}(t = kh) = \widehat{\mathbf{x}}(k|k) \tag{27}$$

The equations (25) can be integrated over interval $t \in [kh, (k+1)h]$ as follows

$$\mathbf{x}(k+1) = \Psi(k)\mathcal{F}(k) + \mathbf{\Phi}(k)\mathbf{x}(k) + \mathbf{\Gamma}_u(k)\delta\mathbf{u}(k) + \mathbf{\Gamma}_d(k)\mathbf{w}(k) \tag{28}$$

$$\delta\mathbf{z}(k+1) = -\left[\mathcal{G}_z(k)\right]^{-1}\left[\mathbf{g}(k) + \mathcal{G}_x(k)\delta\mathbf{x}(k+1)\right] \tag{29}$$

where

$$\mathcal{F}(k) = \mathbf{f}(k) - \mathcal{A}_z(k)\left[\mathcal{G}_z(k)\right]^{-1}\mathbf{g}(k) \\ -\mathcal{A}(k)\widehat{\mathbf{x}}(k|k)$$

$$\Psi(k) = \int_0^h \exp\left(\mathbf{A}(k)\tau\right)d\tau \ ; \quad \mathbf{\Phi}(k) = \exp\left[\mathbf{A}(k)h\right] \quad (30)$$

$$\mathbf{\Gamma}_u(k) = \int_0^h \exp\left(\mathbf{A}(k)\tau\right)\mathcal{B}_u(k)d\tau \quad (31)$$

$$\mathbf{\Gamma}_d(k) = \int_0^h \exp\left(\mathbf{A}(k)\tau\right)\mathcal{B}_d(k)d\tau \quad (32)$$

The resulting discrete DAE is then used for carrying out predictions.

2.2 Model Predictions

Given the set of future manipulated inputs, the model predictions are carried out using the local linear model as follows:

- It is proposed to use the innovation sequence $\{\mathbf{e}(k_j)\}$ generated at major sampling instants as a proxy for model plant mismatch (MPM) and unmeasured disturbances affecting the plant. Additional degrees of freedom are introduced by making use of filtered innovations while carrying out model predictions. Thus, during two major sampling instant, $k_j \le k < k_{j+1}$, innovation sequence filtered through a unity gain filter is evaluated at the fast rate as follows
$$\boldsymbol{\varepsilon}(k+1) = \mathbf{\Phi}_\varepsilon \boldsymbol{\varepsilon}(k) + \left[\mathbf{I} - \mathbf{\Phi}_\varepsilon\right]\mathbf{e}(k_j)$$
$$\mathbf{\Phi}_\varepsilon = \mathbf{diag}\left[\,\alpha_1 \ \alpha_2 \ ... \ \alpha_m\,\right]$$
Here, α_i with $0 \le \alpha_i < 1$ are treated as tuning parameters, which can be used for shaping the regulatory response.
- To carry out state predictions at minor as well as the major sampling instant, observer gain $\mathbf{L}(k_j)$, evaluated at the previous major sampling instant, is used as follows
$$\widetilde{\mathbf{x}}(k+l+1|k) = \Psi(k)\mathcal{F}(k) + \mathbf{\Phi}(k)\widehat{\mathbf{x}}(k+l|k) + \quad (33) \\ \mathbf{\Gamma}_m(k)\delta\mathbf{u}(k+l|k) + \mathbf{L}(k_j)\boldsymbol{\varepsilon}(k)$$
$$\widetilde{\mathbf{z}}(k+l+1|k) = \widehat{\mathbf{z}}(k|k) - \left[\mathcal{G}_z(k)\right]^{-1}[\circ] \quad (34)$$
$$[\circ] = \left[\mathbf{g}(k) + \mathcal{G}_x(k)\left(\widetilde{\mathbf{x}}(k+l+1|k) - \widehat{\mathbf{x}}(k|k)\right)\right]$$
$$\delta\mathbf{u}(k+l|k) = \mathbf{u}(k+l|k) - \mathbf{u}(k-1) \quad (35)$$
$$l = 0, 1, 2, ..., p-1 \quad (36)$$
- At *major sampling instants*, $\mathbf{y}_c(k)$ is a subset of $\mathbf{y}_m(k)$, and we estimate
$$\mathbf{e}_c(k_j) = \mathbf{y}_c(k_j) - \mathbf{C}_s\begin{bmatrix}\widehat{\mathbf{x}}(k_j|k_j) \\ \widehat{\mathbf{z}}(k_j|k_j)\end{bmatrix}$$
and use it during two major sampling instant, $k_j \le k < k_{j+1}$ to compute filtered output mismatch signal
$$\boldsymbol{\eta}(k) = \mathbf{\Phi}_\eta \boldsymbol{\eta}(k-1) + \left[\mathbf{I} - \mathbf{\Phi}_\eta\right]\mathbf{e}_c(k_j)$$
$$\mathbf{\Phi}_\eta = \mathbf{diag}\left[\,\beta_1 \ \beta_2 \ ... \ \beta_m\,\right]$$
Here, β_i with $0 \le \beta_i < 1$ are treated as tuning parameters. This filtered signal is then used then for correcting the output predictions at minor as well as major sampling instants as follows
$$\widetilde{\mathbf{y}}_S(k+l|k) = \mathbf{C}_s\begin{bmatrix}\widetilde{\mathbf{x}}(k+l|k) \\ \widetilde{\mathbf{z}}(k+l|k)\end{bmatrix} + \boldsymbol{\eta}(k) \quad (37)$$

for $l = 1, 2, ..., p$.

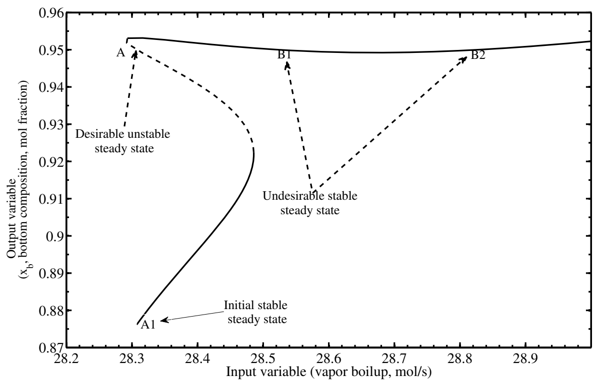

Fig. 1. Bifurcation diagram for Reactive Distillation Column

2.3 NMPC Formulation

Given the model predictions, at instant k, NMPC is formulated as a constrained optimization problem as follows

$$\min_{\mathbf{U}_f} \sum_{j=1}^{p} \left\|\mathbf{E}(k+j|k)\right\|^2_{2,\mathbf{W}_E} + \sum_{i=0}^{q-1}\left\|\Delta\mathbf{u}^T(k+i|k)\right\|^2_{2,\mathbf{W}_{\Delta\mathbf{u}}} \quad (38)$$

$$\mathbf{E}(k+j|k) = \widetilde{\mathbf{y}}_S(k+j|k) - \mathbf{y}_r \quad (39)$$

$$\Delta\mathbf{u}(k+j|k) = \mathbf{u}(k+j|k) - \mathbf{u}(k+j-1|k) \quad (40)$$

subject to

$$\mathbf{u}_L \le \mathbf{u}(k+j|k) \le \mathbf{u}_H \text{ for } j = 0, 1, .., q-1 \quad (41)$$

$$\mathbf{u}(k+j|k) = \mathbf{u}(k+q-1|k) \text{ for } j = q, q+1, .., p-1 \quad (42)$$

where $\mathbf{y}_r$ is the set point for the output, $\mathbf{W}_E$ and $\mathbf{W}_{\Delta\mathbf{u}}$ are positive semi-definite weighting matrices, p represents the prediction horizon and q represents the control horizon. The controller is implemented in moving horizon, i.e., the first optimal move $\mathbf{u}(k|k)$ is implemented the linearization and the optimization steps are repeated over the horizon $[k+1, k+p+1]$.

3. CONTROL OF IDEAL REACTIVE DISTILLATION COLUMN

An ideal reactive distillation column presented in Olanrewaju and Al-Arfaj (2006) is of interest in this work.

3.1 Ideal Reactive Distillation System

A benchmark reactive distillation system (Olanrewaju and Al-Arfaj (2006)), in which a quaternary hypothetical reaction of the form $a + b \leftrightarrow c + d$ is carried out, has been used in the present work to investigate the close loop performance of DAE observer based SLNMPC in multirate scenario. The reactive distillation system has $\mathbf{N}$ stages in the column and is numbered from bottom to the top. 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. Detailed model equations for this system are given Olanrewaju and Al-Arfaj (2006). For the RD system under consideration, the liquid compositions of all the components on all stages including reboiler stage and condenser stage and molar holdup of reboiler and condenser are considered as the differential state variables and while the temperatures on all the stages except total condenser are considered as the algebraic states. The algebraic constraints arise from the vapor liquid equilibrium on each stage of the distillation column. Kinetic and physical properties of the ideal RD system and VLE parameters are taken from Olanrewaju and Al-Arfaj (2006). Thus, the mathematical model consists of 90 differential states and 21 algebraic states. Process simulation was carried out using implicit Euler method with integration interval of 1 sec.

The following regularly sampled multi-rate scenario is considered

- **Fast rate measurements:** It is assumed that temperatures on alternate 11 stages starting from reboiler stage are being measured at the fast rate *with a interval of 30 sec.* Molar holdups in reboiler and condenser are also assumed as measured variables at the fast rate. Each temperature measurement is assumed to be corrupted with a zero mean, normally distributed white noise sequence with standard deviation 0.1 K. The measurements of the holdups are assumed to be corrupted with a zero mean white noise with a standard deviation of 2 mols.
- **Slow rate measurements:** The slow rate measurements are *feed stage composition of reactant a* (x_a), *composition of heavy product d in the bottom* (x_b) *and composition of light product c in the distillate* (x_d), which are assumed to be *available at every 2 minute interval or every 1 minute interval.* Each concentration measurement is assumed to be corrupted with zero mean, normally distributed white noise sequence with standard deviation of 0.001 mol fraction.

It is further assumed that the true manipulated inputs $(\mathbf{m})$ are corrupted with zero mean white noise $(\mathbf{w}_u)$ as given by equation (7) where the covariance matrix of $\mathbf{w}_u$ is given as

$$\mathbf{Q}_{\mathbf{w_u}} = diag\left[\, 0.1415^2 \; 0.165^2 \; 0.063^2 \,\right] \qquad (43)$$

3.2 Steady state multiplicity analyses

Before proceeding to closed loop studies, a bifurcation study is presented for the RD column. The vapor boilup is chosen as the continuation parameter in the bifurcation study while keeping the reflux flow constant. Figure 1 shows the steady state multiplicity behavior of the RD system for different values of vapor flow-rate at constant reflux flow rate. There are three steady state states (output multiplicity) for the system at vapor boilup rate (Vs) 28.3 mol/s. From the viewpoint of operation, the unstable steady state point A (x_b = 0.95), is the most desirable operating point as the desired purity can be achieved at lower vapor boilup and, in turn, with lower energy cost.

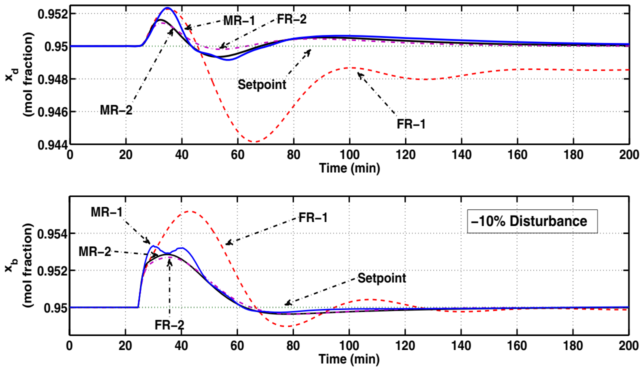

Fig. 2. Regulatory response for -10% disturbance in feed rate of reactant b: Compositions of top product c (x_d) and bottom product d (x_b)

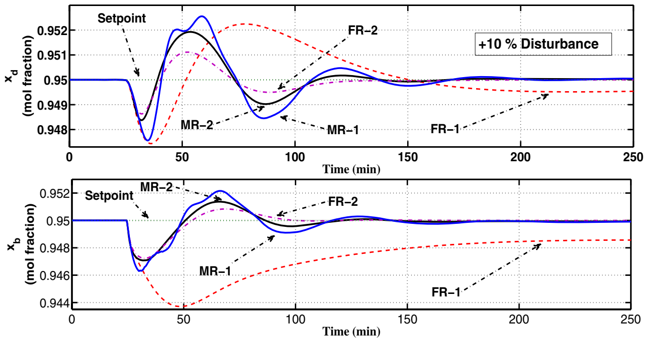

Fig. 3. Regulatory response for +10% disturbance in feed rate of reactant b: Compositions of top product c (x_d) and bottom product d (x_b)

However, the steady state A is locally unstable while the remaining two are locally stable steady states. Moreover, the desired purity (x_b = 0.95) can also be achieved at higher vapor boilup rates corresponding to points B1 (Vs = 28.5 mol/s) or B2 (Vs = 28.8 mol/s) (Fig. 1), which indicate the existence of input multiplicity. While the steady states corresponding to B1 and B2 are stable, operating at either of these points implies higher energy cost. Thus, the control problem is to operate the system at the unstable operating point A.

3.3 Regulatory Control Problem

In the close loop operation, reflux flow rate (F_R) and vapor boil-up rate (V_S) are treated as manipulated inputs. In addition, feed rate of reactant a (i.e. ,F_a) is also manipulated to maintain stoichiometric balance in reactive section. The NMPC scheme has three controlled outputs ,$\mathbf{y}_S$, i.e. x_a, x_b and x_d.

In the present work, the regulatory performance of SLN-MPC scheme is evaluated at desired unstable operating point (point A in Fig. 1). In particular, the regulatory behavior of the RD system in the presence of $\pm$ 10% step changes in the feed rate of reactant 'b' is considered in the simulation studies. The following four different measurement scenarios have been investigated.

- **Fast Rate Scenario 1 (FR-1):** Fast rate measurements of only temperature and liquid holdups (i.e.

Table 1. NMPC tunning parameters

Prediction horizon, p	20
Control horizon, q	2
Sampling time, T_s	30 sec
Weighting matrix, W_E	$[1.4912, 8.7460, 1] \times 10^6$

only $\mathbf{y}_F$) are available. This amounts to *inferential control* of $\mathbf{y}_S$.

- **Multi Rate Scenario 1 (MR-1):** In addition to $\mathbf{y}_F$, slow rate measurements of $\mathbf{y}_S$ are available at every 2 minute interval.
- **Multi Rate Scenario 2 (MR-2):** In addition to $\mathbf{y}_F$, slow rate measurements of $\mathbf{y}_S$ are available at every 1 minute interval
- **Fast Rate Scenario 2 (FR-2):** Measurements of $\mathbf{y}_F$ as well as $\mathbf{y}_S$ are available at the fast rate

The NMPC tuning parameters are shown in Table 1.

The model plant mismatch filter tuning matrices $\mathbf{\Phi}_\varepsilon$ and $\mathbf{\Phi}_\eta$ are chosen as follows

$$\mathbf{\Phi}_\varepsilon = 0.9\mathbf{I}_{n\times n} \text{ and } \mathbf{\Phi}_\eta = 0.9\mathbf{I}_{r\times r}$$

It may be noted that $\mathbf{W}_{\Delta\mathbf{u}}$ is chosen as null matrix. The state and the measurement noise model parameters have been used to develop multi-rate DAE EKFs. To highlight the offset reduction ability of the proposed scheme, the simulation results presented, however, are for scenarios where stochastic disturbances and measurement noise are absent. NMPC problem is solved using *fmincon* function from the *MATLAB*$^{(R)}$ Optimization Toolbox. Comparison of regulatory performances for different measurement scenarios are shown in Figures 2-5. The controlled variables are x_d, x_a *and* x_b. The unmeasured disturbances ($\pm 10\%$) in feed rate of reactant b are introduced after initial 25 minutes of operation with no model plant mismatch. In the absence of MPM, even the inferential control scheme (FR-1) is able to maintain the RD system at the desired concentration set points. However, the occurrences of step changes in the unmeasured disturbance leads to biased state estimation due to MPM, and, as a consequence, the inferential control scheme (FR-1) leads to large offsets. The offsets reduces significantly in the multi-rate scenarios MR-1 and MR-2 due to the feedback introduced through slowly sampled concentration measurements. Moreover, with the increase in the frequency of sampling of the concentration measurements, the offset reduces more and the regulatory performance improves. The offset disappears when concentration measurements are available at the fast rate (FR-2). The profiles of manipulated inputs are shown in Figure 5 for different measurement scenarios. The average computational times for all the different measurement scenarios considered is less than 5 sec on Intel CORE^{TM} i5 CPU 2.67 GHz with 4 GB RAM processor.

4. CONCLUSION

In this work, a DAE EKF based nonlinear MPC scheme is proposed, which can accommodate measurements of quality variables available at slower sampling rates. To achieve off-set reduction, the observer error feedback approach developed by Huang et al. (2009) is extended to accommodate multi-rate measurements. The efficacy of the proposed approach is demonstrated by conducting simulation studies on a ideal reactive distillation system

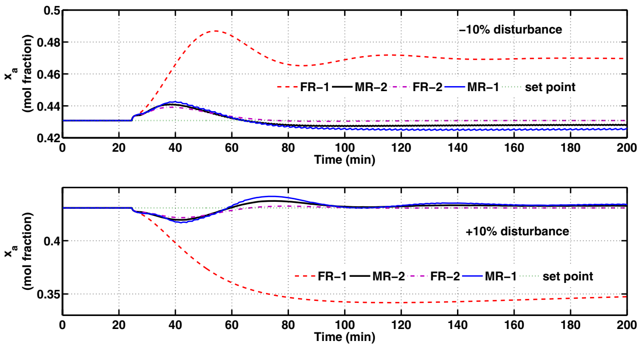

Fig. 4. Regulatory response for -/+ 10% disturbance: Feed Tray Composition

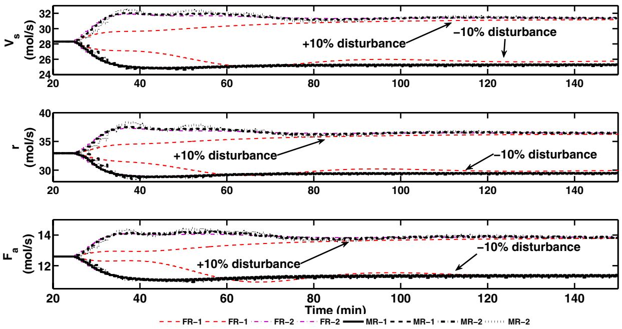

Fig. 5. Regulatory response for -/+10% disturbance: Manipulated Inputs

(Olanrewaju and Al-Arfaj (2006)). Analysis of the simulation results reveals that the offset reduces significantly and the regulatory performance improves with the increase in frequency of sampling of the quality variables. Possibility of employing target states for elimination of offset in the multi-rate scenarios is currently being investigated.

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