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A multi-objective dynamic RTO for plant-wide control

Arvind Ravi * **Niket S. Kaisare** *

* *Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai 600036, Tamil Nadu (e-mail: arvindpravi@gmail.com)*

Abstract: This work addresses a dynamic multi-objective control problem that achieves the desired product quality while ensuring the best profitable operation. A two-layered architecture is presented: The upper layer dynamic real-time optimizer (D-RTO), designed to handle multiple objectives, determines the best Pareto optimal trajectories for the lower level MPC. The proposed optimizer computes different trade-off solutions between the objectives using lexicographic approach. Here, the quality objective is formulated as a set point tracking problem whereas the economic objective is a nonlinear cost function. The trade-off solutions, which correspond to the Pareto points in the function space, are obtained by varying the rate of convergence of the quality variable to the desired set point. The Pareto point closest to the utopian or the ideal solution of the objectives is chosen to calculate the best optimal trajectory. The applicability of the proposed control framework is demonstrated on a reactor-separator system. Performance of this dynamic controller scheme is investigated by comparing with different control methodologies that compute optimal trajectories over a fixed, predefined horizon.

Keywords: Dynamic real-time optimization, multiple-criterion optimization, nonlinear control systems, model-based control, extended Kalman filters

1. INTRODUCTION

Chemical industries have shifted their focus towards handling multiple objectives to sustain or improve their overall business in the current competitive environment. Performance and operational objectives, such as product quality and safety respectively, cannot be compromised at the expense of maximizing profits in any process unit (Tatjewski, 2008). Traditional method of augmenting the objectives with consistent weighing parameters is challenging due to the difficulties in assigning values for these weights a priori (Das and Dennis, 1997). Additionally, optimal planning and scheduling strategies drive more dynamism into plant operations and thus increasing the necessity for constant retuning of weights. Different optimization approaches are proposed (Gambier and Badreddin, 2007) to compute optimal solutions for a multiobjective problem irrespective of the varied domains of these objectives (For eg. Temperature, total cost, quality).

Traditionally, the single objective controller schemes focus on achieving optimal economic operation. These frameworks are conceptualized under two broad categories, a multi-layer hierarchical architecture (Scattolini, 2009) or an unified single-layer (Amrit et al., 2013) control design. A common two-layered control framework consists of upper level steady state real time optimizer (RTO) which optimizes the economic objective modelled as a stationary non linear function based on the steady state plant parameters (Engell, 2007). The RTO function includes complex plant characteristics and therefore the computational requirements are usually high for calculation of optimal solutions which then form the set points for the lower level controllers. Nevertheless, the RTO cannot handle high frequency disturbances and dynamic process and cost parameters. Secondly, model inconsistencies between the RTO and lower level MPC can affect the computation of feasible and optimal target values (De Souza et al., 2010). Single-layered approach, commonly known as Economic MPC (E-MPC) (Rawlings et al., 2012; Amrit et al., 2013) can address these issues as the controller scheme incorporates the economic cost function directly in the MPC framework. However, with increasing complexity of process plants, optimization of the cost function within the control instances may become computationally intractable (Würth et al., 2011). Hence, a two-layered dynamic-RTO strategy, which was introduced earlier by Kadam et al. (2003) and Tosukhowong et al. (2004), is adopted to handle multiple control objectives for complex systems. Unlike the prior works on hierarchical single objective control, a multi-objective control problem targeting the desired product quality and also maximize overall profit on plant scale is considered in this work.

Different variants of economic MPC with simultaneous set point tracking can be found in literature (Zambrano and Camacho, 2002; Gutiérrez-Limón et al., 2011). Recently, (Tian et al., 2019) demonstrated a single-layer multi-objective control where the trade-off between the economic and set point tracking objective was based on the convergence of controlled variable to the respective set point. The algorithm is derived based on the closed looped stability property of the conventional tracking MPC which assumes the availability of optimal solution within the next

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control instance. Secondly, the required trade-off is to be ascertained manually depending on the requirement. The current work addresses a similar multi-objective control problem in a hierarchical framework, incorporating the proposed lexicographic-based algorithm in its optimization layer, to handle delays in computation of optimal solutions. Additionally, the algorithm also includes the decision step to choose the best trade-off trajectory online.

The dynamic optimizer present in the upper layer operates at a slower rate compared to the lower level nonlinear MPC (NMPC). Computational time is considered for the multi-objective optimization and the optimal trajectory is transmitted to the lower layer after some delay, Δ. The quality objective is identified as a set point tracking problem with certain modifications. Conventional methodology to achieve the best tracking performance minimizes the sum of squared deviations between all predicted values and the desired set point over the entire prediction horizon. However, the proposed methodology is reformulated to minimize only the squared deviation of the final prediction value from the set point. Reducing the domain of optimization to the terminal point reduces the speed of convergence to the given set point. As the algorithm uses the lexicographic approach (Gambier and Badreddin, 2007), this relaxation of the quality objective negotiates improved solution for the profit function. At each optimization instance, different Pareto solutions are generated by varying the prediction horizons between specified limits. Subsequently, the optimal Pareto solution and the corresponding prediction horizon is chosen close to the ideal solution which represents the standalone or single objective optimal solution of the respective objective functions. The optimizer communicates the Pareto optimal trajectory, derived from the chosen solution, to the lower level controller. This lower-level nonlinear MPC applies a successive linearization approach to generate future predictions (Lee and Ricker, 1994) and computes the optimal control moves for the plant. This work restricts the performance analyses only to the scenarios with low frequency disturbances such as decisions from the scheduling layer affecting the controller. With the exception of sensor noise, other high frequency disturbances such as model-plant mismatch are not assumed in this work. Performance of the proposed controller is compared with various control schemes including the framework which incorporates the conventional tracking methodology in the lexicographic optimization module.

The next section illustrates the two-layered control architecture and the proposed algorithm. The third section demonstrates the applicability of the controller scheme for a reactor-separator case study. The penultimate section discusses the results obtained followed by the conclusion and future extensions to this work.

2. CONTROL ARCHITECTURE

Dynamics of the multi-unit chemical process is represented by a discrete time nonlinear function given by:

$$\begin{aligned} x_{k+1} &= f\left(x_k, u_k\right) \\ y_{k+1} &= g\left(x_k\right) + \nu_k \\ y^c_{k+1} &= h\left(x_k\right) \end{aligned} \tag{1}$$

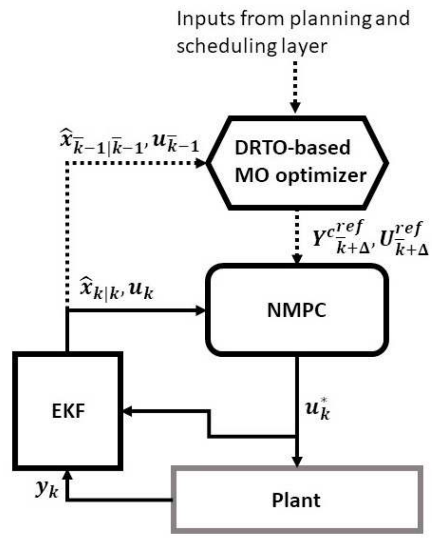

Fig. 1. Schematic of the proposed two-layered dynamic multi-objective controller framework

Here, $x \in \Re^n$, $u \in \Re^m$, are the variables representing states and inputs respectively. $y \in \Re^p$ and $y^c \in \Re^{p_c}$ denote the measured and controlled variables of the plant. The measurements are assumed to have an additive sensor noise ν_k with Gaussian white noise properties $\mathcal{N}(0, \sigma^2)$. The system states are estimated using the extended Kalman filter (EKF) and the complete set of state estimates are transmitted to the respective control layers.

2.1 Multi-objective D-RTO

The multi-objective controller is formulated as a hierarchical control framework, as shown in Figure 1. The dynamic-RTO (D-RTO) present in the upper layer implements the multi-objective control algorithm based on lexicographic approach. The proposed methodology identifies different plant trajectories corresponding to different Pareto solutions, and chooses the plant trajectory which provides the best optimal trade-off with respect to the least priority economic cost function. While the lower level MPC computes control action at all discrete time instances k, the dynamic optimizer operates at slower time scales and becomes online at infrequent time instances $\bar{k}$. Thus, the estimates computed by the nonlinear EKF are made available to these control layers depending on their respective frequency of operation. The delay in computing the best optimal trajectory is denoted by Δ, the value of which can be varied depending on the computational complexity. The priority objective of product quality, formulated as a terminal set point tracking objective is given by:

$$J^*_{Q,ter} = \min \left\|\hat{x}_{(k+N_{drto})|k} - x^{ref}\right\|^2 \tag{2}$$

$$\hat{x}_{k+i|k} - f\left(\hat{x}_{(k+i-1)|k}, u_k\right) = 0 \tag{3}$$

$$U^- \leq U \leq U^+ \tag{4}$$

$$\Delta U^- \leq \Delta U \leq \Delta U^+ \tag{5}$$

Let $U^*_{Q,ter}$ be its optimal solution. Only the squared error between the terminal prediction and set point (x^{ref}) is considered, unlike the conventional method (refer Eq. 9), to obtain improved trade-off for economic objective. The standalone economic objective for maximization of overall profit is given by:

$$J^*_{econ} = \max \sum_{i=0}^{N_{drto}} \Phi_{econ}\left(\hat{x}_{k+i|k}, u_{k+i}\right) \tag{6}$$

subject to constraints $(3) - (5)$

The notion of lexicographic method retains the optimal solution of the priority quality objective through an additional constraint (as in Eq. 8) while optimizing the economic objective. Thus the optimization formulation is given by:

$$J_{econ} = \max \sum_{i=0}^{N_{drto}-1} \Phi_{econ}\left(\hat{x}_{k+i|k}, u_{k+i}\right) \tag{7}$$

$$J_{Q,ter} \leq J^*_{Q,ter} \tag{8}$$

subject to constraints $(3) - (5)$

At each optimization instance, the algorithm performs the lexicographic optimization, as shown in Equation 7, for different horizon lengths, N_{drto}, thereby generating set of Pareto optimal points for the multi-objective problem. Accordingly, varying the horizon length affects the tracking performance of the quality objective as the algorithm considers only the terminal value for optimization. Thus, the lexicographic method applied for different horizon lengths generates different trade-off or the Pareto solutions for the economic objective. The best trade-off trajectory is computed from the Pareto point closest to the ideal or the standalone optimal solution of the respective objective functions.

The implementation of the algorithm begins with a vectorial representation of objectives in the function space (Gambier and Badreddin, 2007), thus the Pareto points in 2-D space are defined as

$$\tilde{\mathbf{J}}_\ell = \left(\tilde{J}^*_Q, \tilde{J}_{econ}\right)_\ell$$

where $\tilde{J}^*_Q$ and $\tilde{J}_{econ}$ denotes the normalized values. ℓ are index values between the maximum and the minimum N_{drto}. J^*_Q represents the optimal objective function value of the conventional set point tracking function calculated using $(U^*_{Q,ter})_\ell$ (computed in Eq. (2)) and given by:

$$J^*_Q = \sum_{i=1}^{N_{drto}} \left\|\hat{x}_{(k+i)|k} - x^{ref}\right\|^2 \tag{9}$$

The optimal horizon is chosen as value of N_{drto} corresponding to the point closest to the desired solution, which is minimum value of the conventional tracking function and maximum profit

$$\tilde{\mathbf{J}}_{ideal} = \left(\min(\tilde{J}^*_Q), \max(\tilde{J}_{econ})\right)$$

This can be calculated by the 2-norm minimization objective given by:

$$N^{opt}_{drto} = \underset{\ell}{\operatorname{argmin}} \left\|\tilde{\mathbf{J}}_\ell - \tilde{\mathbf{J}}_{ideal}\right\|^2 \tag{10}$$

The detailed steps of the proposed methodology are described below.

Step 1: Obtain $\hat{x}_{\bar{k}-1|\bar{k}-1}$ and $u_{\bar{k}-1}$ from the EKF.

Step 2: **for** $\ell = N^{min}_{drto}$ to N^{max}_{drto}

- **o** Solve Eq. 2, calculate $\{J^*_{Q,ter}\}_\ell$
- **o** Determine $(J^*_Q)_\ell$ using Eq. 9
- **o** Solve Eq. 7, calculate $\{J_{econ}\}_\ell$

end for

Step 4: Normalize the values of J^*_Q and J_{econ}. Construct the Pareto points in 2-D space.

Step 5: Determine $\tilde{\mathbf{J}}_{ideal}$.

Step 6: Solve Eq. 10 to calculate N^{opt}_{drto}.

Step 7: Obtain the reference trajectories Y^{ref} and U^{ref} corresponding to N^{opt}_{drto}

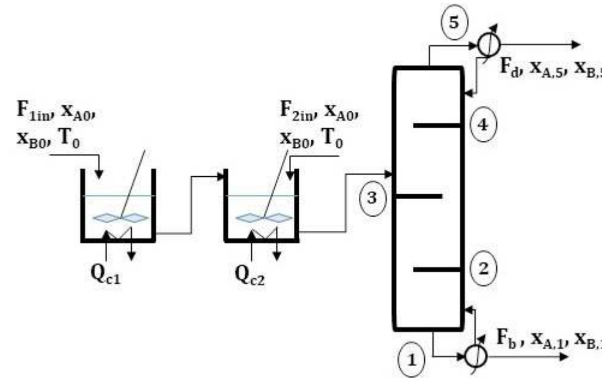

Fig. 2. Schematic of the reactor-separator system

Table 1. Steady state parameter values of reactor-separator system

Parameter	Value	Parameter	Value
F_{1in}	35 (kmol/h)	M_{c1}	10 (kmol)
F_{2in}	35 (kmol/h)	M_{c2}	50 (kmol)
Q_{c1}	75 (kmol/h)	T_0	360 (K)
Q_{c2}	75 (kmol/h)	T_w	300 (K)
k_{10}	8e10 (1/h)	k_{20}	2e9 (1/h)
F_b	60 (kmol/h)	P	1 atm
R	50 (kmol/h)	M_{r1}	10 (kmol)
$\frac{E1}{R}$	9300 (1/K)	M_{r2}	25 (kmol)
$\frac{E2}{R}$	9000 (1/K)	α_A	18
ΔH_1	-4e4 (kJ/kmol)	α_B	9
ΔH_2	-4e4 (kJ/kmol)	α_C	1
C_p	700 (kJ/kmol K)	x_{A0}	1
C_{pw}	76 (kJ/kmol K)	x_{B0}	0

The reference trajectories are communicated to the lower layer nonlinear MPC at $k = \bar{k} + \Delta$ which operates at all the sampling instances. Here, the nonlinear quadratic controller based on successive linearization (Lee and Ricker, 1994) is implemented to handle the model consistency issues generally prevalent in hierarchical control (Kadam et al., 2003).

3. CASE STUDY: REACTOR SEPARATOR SYSTEM

Performance of the proposed hierarchical multi-objective controller is analyzed for a multi-unit system consisting of two CSTRs followed by a separator column. Series reaction ($\mathcal{A} \xrightarrow{k_1} \mathcal{B} \xrightarrow{k_2} \mathcal{C}$) takes place in the two reactors and the desired product $\mathcal{B}$ is obtained from bottom stream F_b of the separator column. The priority objective is to maintain the composition of desired product $\mathcal{B}$ in the reboiler outlet flow (F_b) at a user-defined set point and simultaneously achieve the best possible overall profit. Total of 18 states describe the system which includes 4 states in each of the reactors and 10 states in the separator (tray compositions of $\mathcal{A}$ and $\mathcal{B}$). The schematic of the system is shown in Figure 2. The model equations are given in the Appendix A and corresponding the steady state parameter values are tabulated in Table 1. The measured variables are the reactor temperatures T_1, T_2 and feed tray temperature T_f which is calculated as follows.

$$T_f = \frac{3860}{12.8 - log\frac{\alpha_{\mathcal{A}}.P}{\kappa}} \quad \kappa = \sum_{m=\mathcal{A},\mathcal{B},\mathcal{C}} \alpha_m x_{m,f}$$

The manipulated and controlled variables are Q_{c1}, Q_{c2}, F_b and $T_1, T_2, x_{\mathcal{B},1}$ respectively. The set point objective $J_{Q,ter}$ and the economic objective for profit maximization J_{econ} are given by:

$$\begin{aligned} J_{Q,ter} &= \left\|(\hat{x}_{\mathcal{B},1})_{(k+N_{drto})|k} - (x_{\mathcal{B},1})^{ref}\right\|^2 \\ J_{econ} &= \sum_{i=0}^{N_{drto}-1} \beta_B (\hat{x}_{\mathcal{B},1})_{(k+i)|k}(F_b)_{k+i} \\ &\quad - \beta_W \left((Q_{c1})_{k+i} + (Q_{c2})_{k+i}\right) \end{aligned} \tag{11}$$

Here, $\beta_B = 3; \beta_W = 0.5$ are the cost parameters. Refer Table 2 for the control parameters assumed for this study.

Table 2. Values of control parameters

Parameter	Value	Unit
Sample time	3	min
min N_{drto}	3	sample time steps
max N_{drto}	20	sample time steps
M_{drto}	3	sample time steps
P_{nmpc}	15	sample time steps
M_{nmpc}	2	sample time steps

4. RESULTS AND DISCUSSION

The simulation study analyses the performance of the proposed algorithm in comparison with other controller schemes. It is desired to reach the required product quality in two steps with the first step change to 0.6 given at t = 1.5 h and the second step change to 0.7 given at t = 8.5 h. The external disturbances are neglected in this study. The delay in optimization, Δ, is assumed as 1 sampling instant in this work. The dynamic optimizer is taken online from t = 0.5 h.

Table 3 reports the values of average profit and RMSE for various controller scenarios which are calculated as

$$\text{Average profit} = \frac{\sum_{k=0}^{T_k-1} \beta_B (x_{\mathcal{B},1})_k (F_b)_k - \beta_W (Q_{c1})_k + (Q_{c2})_k}{T_k}$$

$$\text{RMSE} = \sqrt{\frac{\sum_{k=1}^{T_k}\left((x_{\mathcal{B},1})_k - (x_{\mathcal{B},1})_k^{ref}\right)^2}{T_k}} \tag{12}$$

These are the performance indicators of economic and the quality objective respectively. T_k denotes the total number of sample time steps considered for the simulation study.

Table 3. Performance of various controller schemes. A single layer control is considered for the case only with the quality objective, rest are two-layer D-RTO-based controllers.

Controller scheme	Average profit	RMSE
Quality objective only	-29.956	0.0207
Proposed method	**16.489**	**0.0223**
Conventional tracking	6.709	0.0238
$N_{drto} = 5$	16.306	0.0230
$N_{drto} = 10$	16.325	0.0244
$N_{drto} = 15$	16.424	0.0278
$N_{drto} = 20$	15.773	0.0236
Economic objective only	35.506	0.1544

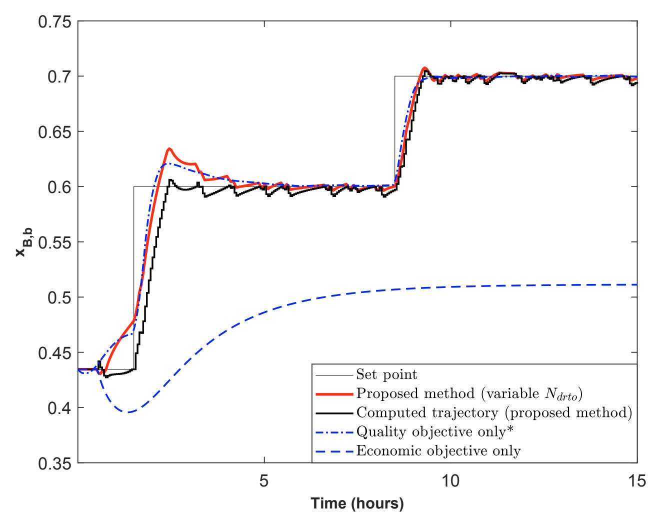

Fig. 3. Quality tracking performance of proposed algorithm compared to the single objective controller schemes. *single-layer control implemented for the case with only the quality objective.

The first case compares the performance of proposed controller with the extreme case scenarios comprising of either the quality or the profit targets. As indicated by the performance indices (Eq. 12) tabulated in Table 3, controller scenario satisfying only the quality objective indicate worst economic performance with the best set point tracking. Similarly, the economic objective is handled in the multi-layer D-RTO and report maximum profit and worst set point tracking performance among the controllers. Dashed-blue lines in Figure 3 reiterate the poor tracking performance of the controller. However, the control trajectory accomplished by the proposed method (solid-red) almost coincides with the single objective quality tracking controller (dashed-dotted blue) with substantial increase in the average profit (refer Table 3).

The performance analysis is further extended to two other major controller schemes: fixed prediction horizon where the value of N_{drto} remains constant for all dynamic optimization instance and the conventional method which applies the lexicographic approach for the quality objective which optimizes all the prediction values close to the

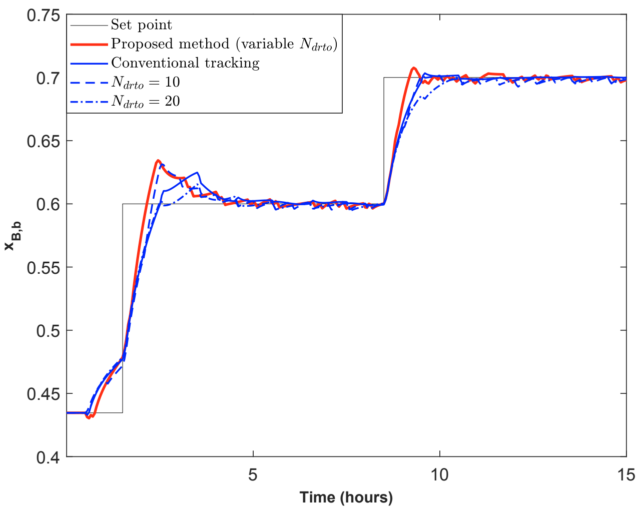

Fig. 4. Performance of proposed algorithm compared to the controllers with fixed prediction horizons.

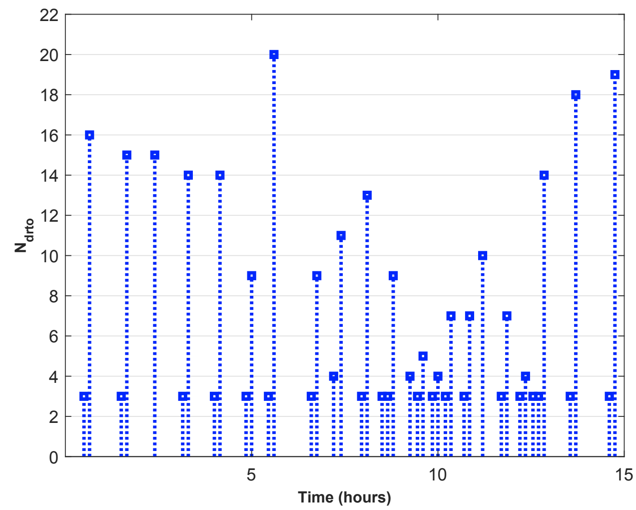

Fig. 5. Variation of N_{drto} values of the proposed controller with respect to time

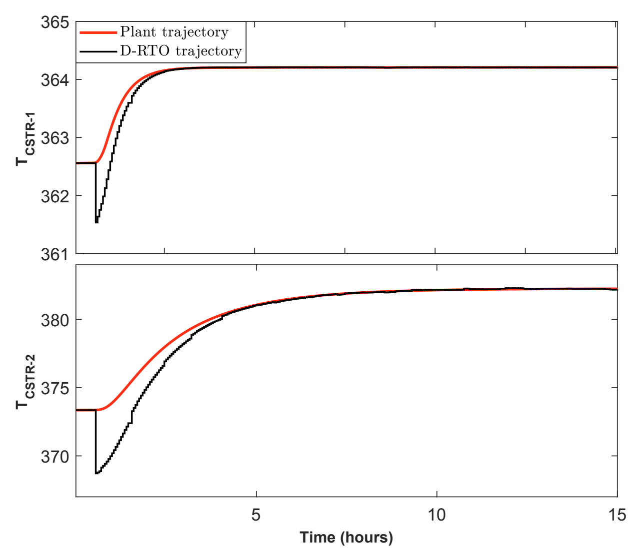

Fig. 6. Asymptotic controller tracking of reactor temperatures to a steady state value as cooling water flows reach the respective minimum flow constraints

set point (Eq. 9). The proposed algorithm dynamically determines the optimal trajectory along with the optimal length, N_{drto}^{opt} time steps, at every D-RTO instance. Examination of the performance indices tabulated in Table 3 demonstrates better performance of the proposed scheme with both the objectives performing better than the controllers with fixed horizons. The average computational time for the calculation of Y^{ref} and U^{ref} for the proposed method is approximately 7 min and for the fixed horizon case studies are 8 s ($N_{drto} = 5$) and 40 s ($N_{drto} = 20$). The increased computational effort is offset by the efficacy of the proposed method with time taken for the multi-objective optimization managed by the computational delay incorporated in the algorithm.

The corresponding plots in Figure 3 and 4 compares the tracking performance of various control schemes with the proposed algorithm. As mentioned earlier, the D-RTO is taken online at t = 0.5 h. Hence an initial increase in the mole fraction $x_{\mathcal{B},1}$ is observed before the proposed set point change at t = 1.5 h. The step plot in black (Fig. 4) represents the plant trajectory communicated to the NMPC layer.

Figure 5 presents the different horizon lengths of the optimal plant trajectory computed by the optimizer across the entire simulation time. The gaps between stem plots indicate that the D-RTO is off line in those instances and becomes online after the NMPC executes all the reference values computed in the previous D-RTO run. Figure 6 exhibits the NMPC tracking of reactor temperatures. Since reduction in the cooling water flow rates Q_{c1} and Q_{c2} have a positive effect on both the objectives (reduction in flow increases formation of $\mathcal{B}$ in the reactors and increase the profit as well), minimum values of the flow rates are reached and hence the reactor temperatures gradually settles at an higher value.

5. CONCLUSION

This work presents a new dynamic framework to handle multiple objectives of quality and profit. The hierarchical structure consists of control layers operating at different frequencies to handle the rigors of multi-objective optimization. The optimizer incorporates a lexicographic approach and calculates different Pareto solutions by varying the prediction horizons of the objective functions. The best solution among the computed Pareto set to chosen to calculate the best trade-off trajectory along with the optimal horizon length. This offers advantage as there is no requirement for pretuning the optimal length of the trajectory and its value computed dynamically at every D-RTO instance. The proposed algorithm is shown to demonstrate better performance for both the objectives for various control scenarios. A possible extension to this work would be to handle high frequency disturbances such as model-plant mismatch. Also, the multi-objective problem will be reformulated to include safety objectives in addition to the quality and economic objective prioritized in that order. Finally, a distributed control implementation could be attempted at the lower level as the decentralized control structure offers more reliability in handling faults in individual control loops.

REFERENCES

Amrit, R., Rawlings, J.B., and Biegler, L.T. (2013). Optimizing process economics online using model predictive control. *Computers & Chemical Engineering*, 58, 334–343.

Das, I. and Dennis, J.E. (1997). A closer look at drawbacks of minimizing weighted sums of objectives for pareto set generation in multicriteria optimization problems. *Structural optimization*, 14(1), 63–69.

De Souza, G., Odloak, D., and Zanin, A.C. (2010). Real time optimization (rto) with model predictive control (mpc). *Computers & Chemical Engineering*, 34(12), 1999–2006.

Engell, S. (2007). Feedback control for optimal process operation. *Journal of process control*, 17(3), 203–219.

Gambier, A. and Badreddin, E. (2007). Multi-objective optimal control: An overview. In *2007 IEEE International Conference on Control Applications*, 170–175. IEEE.

Gutiérrez-Limón, M.A., Flores-Tlacuahuac, A., and Grossmann, I.E. (2011). A multiobjective optimization approach for the simultaneous single line scheduling and control of cstrs. *Industrial & Engineering Chemistry Research*, 51(17), 5881–5890.

Kadam, J., Marquardt, W., Schlegel, M., Backx, T., Bosgra, O., Brouwer, P., Dünnebier, G., Van Hessem, D., Tiagounov, A., and De Wolf, S. (2003). Towards integrated dynamic real-time optimization and control of industrial processes. *Proceedings foundations of computer-aided process operations (FOCAPO2003)*, 593–596.

Lee, J.H. and Ricker, N.L. (1994). Extended kalman filter based nonlinear model predictive control. *Industrial & Engineering Chemistry Research*, 33(6), 1530–1541.

Rawlings, J.B., Angeli, D., and Bates, C.N. (2012). Fundamentals of economic model predictive control. In *2012 IEEE 51st IEEE conference on decision and control (CDC)*, 3851–3861. IEEE.

Scattolini, R. (2009). Architectures for distributed and hierarchical model predictive control–a review. *Journal of process control*, 19(5), 723–731.

Tatjewski, P. (2008). Advanced control and on-line process optimization in multilayer structures. *Annual Reviews in Control*, 32(1), 71–85.

Tian, H., Lu, Q., Gopaluni, R.B., Zavala, V.M., and Olson, J.A. (2019). An economic model predictive control framework for mechanical pulping processes. *Control Engineering Practice*, 85, 100–109.

Tosukhowong, T., Lee, J.M., Lee, J.H., and Lu, J. (2004). An introduction to a dynamic plant-wide optimization strategy for an integrated plant. *Computers & chemical engineering*, 29(1), 199–208.

Würth, L., Hannemann, R., and Marquardt, W. (2011). A two-layer architecture for economically optimal process control and operation. *Journal of Process Control*, 21(3), 311–321.

Zambrano, D. and Camacho, E.F. (2002). Application of mpc with multiple objective for a solar refrigeration plant. In *Proceedings of the International Conference on Control Applications*, volume 2, 1230–1235. IEEE.

Appendix A. MODEL EQUATIONS

CSTR-1

$$\frac{\mathrm{d}x_{\mathcal{A}1}}{\mathrm{d}t} = \frac{F_{1in}}{M_{r1}}(x_{\mathcal{A}0} - x_{\mathcal{A}1}) - k_{11}x_{\mathcal{A}1}$$

$$\frac{\mathrm{d}x_{\mathcal{B}1}}{\mathrm{d}t} = \frac{F_{1in}}{M_{r1}}(x_{\mathcal{B}0} - x_{\mathcal{B}1}) + k_{11}x_{\mathcal{A}1} - k_{21}x_{\mathcal{B}1}$$

$$\frac{\mathrm{d}T_1}{\mathrm{d}t} = \frac{F_{1in}}{M_{r1}}(T_0 - T_1) + \frac{UA_{r1}}{C_pM_{r1}}(T_{c1} - T_1) - \frac{(k_{11}x_{\mathcal{A}1}\delta H_1 + k_{21}x_{\mathcal{B}1}\delta H_2)}{C_p}$$

$$\frac{\mathrm{d}T_{c1}}{\mathrm{d}t} = \frac{Q_{c1}}{M_{c1}}(T_w - T_{c1}) + \frac{UA_{r1}}{C_{pw}M_{c1}}(T_1 - T_{c1})$$

CSTR-2

$$\frac{\mathrm{d}x_{\mathcal{A}2}}{\mathrm{d}t} = \frac{F_{1out}}{M_{r2}}x_{\mathcal{A}1} + \frac{F_{2in}}{M_{r2}}x_{\mathcal{A}0} - \frac{(F_{1out} + F_{2in})}{M_{r2}}x_{\mathcal{A}2} - k_{12}x_{\mathcal{A}2}$$

$$\frac{\mathrm{d}x_{\mathcal{B}2}}{\mathrm{d}t} = \frac{F_1}{M_{r2}}x_{\mathcal{B}1} + \frac{F_{2in}}{M_{r2}}x_{\mathcal{B}0} - \frac{(F_{1out} + F_{2in})}{M_{r2}}x_{\mathcal{B}2} + k_{12}x_{\mathcal{B}2} - k_{22}x_{\mathcal{B}2}$$

$$\frac{\mathrm{d}T_2}{\mathrm{d}t} = \frac{F_{1out}}{M_{r2}}T_1 + \frac{F_{2in}}{M_{r2}}T_0 - \frac{(F_{1out} + F_{2in})}{M_{r2}}T_2 + \frac{UA_{r2}}{C_pM_{r2}}(T_{c2} - T_2) - \frac{(k_{12}x_{\mathcal{A}1}\delta H_1 + k_{22}x_{\mathcal{B}2}\delta H_2)}{C_p}$$

$$\frac{\mathrm{d}T_{c2}}{\mathrm{d}t} = \frac{Q_{c2}}{M_{c2}}(T_w - T_{c2}) + \frac{UA_{r2}}{C_{pw}M_{c2}}(T_2 - T_{c2})$$

Separator

The column consists of 5 trays, numbered from the reboiler to the condenser. The feed from CSTR-2 outlet enters tray 3. A constant hold up system is assumed with $M_n = 10$ kmol.

$$\frac{\mathrm{d}x_{i,1}}{\mathrm{d}t} = \frac{(R + F_{2out})x_{i,2} - Vy_{i,1} - F_bx_{i,1}}{M_1}$$

$$\frac{\mathrm{d}x_{i,2}}{\mathrm{d}t} = \frac{(R + F_{2out})(x_{i,3} - x_{i,2}) + V(y_{i,1} - y_{i,2})}{M_2}$$

$$\frac{\mathrm{d}x_{i,3}}{\mathrm{d}t} = \frac{F_{2out}x_{i2} + Rx_{i,4} + V(y_{i,2} - y_{i,3})}{M_3} - \frac{(R + F_{2out})x_{i,3}}{M_3}$$

$$\frac{\mathrm{d}x_{i,4}}{\mathrm{d}t} = \frac{R(x_{i,5} - x_{i,4}) + V(y_{i,3} - y_{i,4})}{M_4}$$

$$\frac{\mathrm{d}x_{i,5}}{\mathrm{d}t} = \frac{Vy_{i,4} - Rx_{i,5} - F_px_{i,5}}{M_5}$$

$$i = \mathcal{A}/\mathcal{B}$$

$$k_{cd} = e^{\frac{-E_a}{RT}} \quad c = \text{reaction};\ d = \text{reactor}$$

$$F_p = F_{1in} + F_{2in} - F_b$$