Real-Time Regulatory Control Structure Selection Based on Economics

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Real-time optimization (RTO) is the lowest level in the decision-making process for operating chemical processes at which economics is directly taken into consideration. This work presents a systematic methodology for incorporating decisions pertinent to the structure and functionality of the regulatory control system (RCS) at the real-time optimization level. The proposed formulation consists of a set of linear constraints that determines the set of manipulated and controlled variables and the steady-state operating policy that minimizes the effects of disturbances on process economics. The methodology is applied to two case studies, including an evaporator process and a fluid catalytic cracking process. The results demonstrate that the methodology can be used to decrease the sensitivity of process economics to disturbances and to operate processes in a near optimal way with less frequent RTO executions.

1. Introduction

The decisions related to the operation of modern manufacturing facilities are currently made at three different levels.[1,2] At the lowest level, advanced process control (APC) achieves operating targets such as product quality, production level, and safety with an execution frequency of seconds or minutes. At the highest level, planning and scheduling provide coordination of activities over significant time periods (weeks or years). Real-time optimization (RTO) connects these two levels, and its role is crucial, since it is the lowest level in the decision-making process at which economics is taken into consideration explicitly.[1,3,4] APC and RTO advanced significantly through the last 50 years and, to a certain extent, did so independently, since they were conceived as having different functionalities. However, in the past decade, mainly due to the introduction of nonlinear model predictive control (MPC) and the advances in the optimization algorithms, the distinction between APC and RTO has become less clear.[3,5] Arguably, their main distinction is that RTO is mainly concerned with steady-state economics and uses nonlinear models while, at the APC level, the objective functions used are not directly related to economics and the models employed are linear.

Current RTO systems adopt a steady-state view of plant operations, and execution is triggered when disturbances with a significant effect on economics are taking place. The aim is to determine the corrective action needed to optimize the steady-state economics of the plant. Installation and maintenance of RTO systems can only be justified for the cases where disturbances with significant economic effect (major disturbances) are frequent and degrees of freedom are available for optimization purposes, i.e., not all of them have been effectively removed by the two other levels.[1,3] On the other hand, there is little discussion in the literature on how disturbances that are more frequent and have less significant implications for the process economics (minor disturbances) can be handled in an RTO system. Although the occurrence of a major disturbance normally triggers the execution of the RTO and corrective action is taken to alleviate the disturbance's effect on economics, minor disturbances are handled by the APC system in a way that is not always related to process economics.

Marlin and Hrymak,[1] when discussing the challenges involved in transmitting the results of the RTO system to the APC system, state that "RTO results should include not only the optimum operating point, but also the manner for responding to disturbances," and they also stress the importance of modeling, at the RTO level, the process control system implemented in the plant. They implicitly propose that all disturbances must be handled by the APC system in a way dictated by the results of the RTO. An important consequence of their proposition is that the structure of the regulatory control system (RCS) should be determined at the RTO level as well. This might be less important when the regulatory controller is of an MPC type but can be critical when other controller types, such as decentralized proportional−integral−derivative (PID) controllers, are used at the regulatory level.

The aim of this work is to address the last issue. It is proposed that the RCS, i.e., the selection of sets of controlled and manipulated variables and possibly the structure of their interconnection, should be determined at the RTO level, and a systematic methodology is proposed for achieving that. Since RTO is the lowest level at which economics, the key driving force, is explicitly taken into consideration, it is beneficial to make as many decisions as possible at this level and then transmit the results to the lower levels for implementation. One might argue that such an approach might significantly increase the computational load at the RTO level and the complexity of the APC system. However, the size of the optimization problems solved currently at the RTO level is already impressive. As computational power is becoming less expensive and numerical algorithms are becoming more robust, high fidelity models and complicated methodologies will inevitably find their way into the RTO systems and

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technology. In addition, as is discussed in the section that follows, the proposed methodology offers the opportunity of significantly reducing the frequency of RTO execution and, thus, increasing the time available for additional computations. An important advantage is that the RCS does not need to be fixed but can be variable, as determined by the execution of the RTO system. Since the occurrence of disturbances causes the process to operate at points with different characteristics, we cannot assume that the same RCS is the best structure at all possible operating points. A control strategy that is based on a variable (optimally adapted) RCS is clearly more appropriate in the long term, especially when the determination of this structure is based explicitly on economics. Increasing the complexity of the APC system is a drawback of the proposed methodology but can be justified if the economic potential is significant.

2. Proposed Methodology for RCS Selection at the RTO Level

As has been extensively discussed in the literature, the optimization problem solved at the RTO level is of the following general form[6,7]

$$\min_{\mathbf{x},\mathbf{u}} \mathrm{E}_{\theta\in\Theta}\,[J(\mathbf{x},\mathbf{u},\boldsymbol{\theta})] \tag{1}$$

s.t.

$$\mathbf{f}(\mathbf{x},\mathbf{u},\boldsymbol{\theta}) = 0$$

$$\mathbf{g}(\mathbf{x},\mathbf{u},\boldsymbol{\theta}) \le 0$$

where E denotes the expected value, $\mathbf{x} \in \mathrm{X} \subseteq \mathbb{R}^{n_x}$ is the n_x vector of differential and algebraic variables (dependent variables) of the process model, $\mathbf{u} \in \mathrm{U} \subseteq \mathbb{P}^{n_u}$ is the n_u vector of manipulated variables (independent variables), $\boldsymbol{\theta} \in \Theta \subseteq \mathbb{P}^{n_\theta}$ is the n_θ vector of disturbances, and $\mathbf{f}{:}R^{n_x+n_u+n_\theta} \rightarrow R^{n_x}$ and $\mathbf{g}{:}R^{n_x+n_u+n_\theta} \rightarrow R^{n_g}$ are the equality and inequality constraints, respectively, of the process model. By selecting discrete realizations for the varying process parameters $\theta^p \in \Theta$**,** where $p \in \mathrm{P}$ and P is the index set, the optimization problem (eq 1) can be written in the following multiperiod form

$$\min_{x^p,u^p} \sum_{p\in P} w^p\, J(x^p,u^p,\theta^p) \tag{2}$$

s.t.

$$\begin{bmatrix} \mathbf{f}(x^p,u^p,\theta^p) = 0 \\ \mathbf{g}(x^p,u^p,\theta^p) \le 0 \end{bmatrix} \forall p \in P$$

i.e., the expected value of the objective function is approximated, using, for instance, a quadrature scheme over Θ, to determine the optimum value of the available degrees of freedom $\mathbf{u}$. w^p are weights that reflect the frequency of occurrence of the disturbance realization θ^p, which can be calculated on-line based on historical data. An implicit assumption in the above formulation (eq 2) is that all disturbances are measurable since all manipulated variables are adapted perfectly to optimize plant performance at all periods. Furthermore, it is interesting to note that this optimal adaptation of the operating point to the changing disturbances is done in a complete open-loop, model-based fashion. However, this can only be the case if the frequency of the RTO execution matches that of the disturbances, all disturbances are measurable, and the available model perfect. As a result, the multiperiod optimization problem given by eq 2 can be extremely optimistic and a more realistic formulation is needed (see also discussion by Rooney and Biegler[8,9] and Pistikopoulos[10]). Such a formulation should at least contain some elements of the feedback and/or feedforward strategy adopted at the regulatory level to limit the arbitrary adaptation of the available degrees of freedom.

To this end, we first define the vector $\mathbf{y} \in \mathrm{Y} \subseteq \mathbb{R}^{n_y}$ of the available measured variables to be an arbitrary function of the independent and dependent variables

$$\mathbf{m}(\mathbf{x},\mathbf{u},\mathbf{y}) = 0 \tag{3}$$

Normally the measured variables have upper and lower bounds which must be enforced at all periods

$$y_j^{\mathrm{L}} \le y_j^p \le y_j^{\mathrm{U}},\ \forall j, p \tag{4}$$

where the superscript L (U) denotes the lower (upper) bound. We also define a binary variable δ_j for each measured variable as follows

$$\delta_j = \begin{bmatrix} 1, \text{ if the measured variable } y_j \text{ is selected} \\ \quad \text{as the controlled variable} \\ 0, \text{ otherwise} \end{bmatrix} \tag{5}$$

Furthermore, if a measured variable is selected at the regulatory level as a controlled variable then, at the RTO level, this variable will always be equal to its set point value since, as seen from the RTO level, the process is always at steady state, i.e.,

$$\delta_j = 1 \Rightarrow y_j^p = y_j^{\mathrm{sp}},\ \forall p \tag{6}$$

Combining eqs 4–6, we obtain the following equivalent set of linear constraints

$$\begin{bmatrix} y_j^{\mathrm{sp}} + (1-\delta_j)y_j^{\mathrm{L}} \le y_j^p \le y_j^{\mathrm{sp}} + (1-\delta_j)y_j^{\mathrm{U}} \\ \delta_j y_j^{\mathrm{L}} \le y_j^{\mathrm{sp}} \le \delta_j y_j^{\mathrm{U}} \end{bmatrix} \forall j,p \tag{7}$$

In this formulation, the value of the set points is constant for all periods and independent from the values of the measurable disturbances. However, significant benefits might be achieved by using a feedforward scheme in which the set points are time-varying and are related in a linear or nonlinear way to the value of the measurable disturbances. A way of expressing this mathematically is the following:

$$y_j^{\mathrm{sp},p} = \psi_j^0 + \sum_{k\in K_\mathrm{m}} \psi_{jk}^1\left(\frac{\theta_k^p - \theta_k^{\mathrm{N}}}{\Delta\theta_k}\right) + \psi_{jk}^2\left(\frac{\theta_k^p - \theta_k^{\mathrm{N}}}{\Delta\theta_k}\right)^2 + \cdots = \psi_j^0 + \sum_{k\in K_\mathrm{m}} \sum_{q=1}^{n_q} \psi_{jk}^q \left(\frac{\theta_k^p - \theta_k^{\mathrm{N}}}{\Delta\theta_k}\right)^q \tag{8}$$

i.e., each set point is determined as a sum of a constant term and a polynomial function (of the order n_q) of the measurable disturbances. It should be noted that index k belongs to the index set K_m of the measurable disturbances. When the index set K_m is empty, then all set points are constant. Superscript N in eq 8 denotes the nominal value, while $\Delta\theta$ is the maximum absolute deviation of θ from its nominal value (θ^N). Although other functional forms are also possible, an interesting feature of eq 8 is that the polynomial coefficients appear linearly in the optimization, preserving the linearity of the proposed formulation. Finally, combining eq 7 and eq 8 we obtain

$$\begin{bmatrix} y_j^{sp,p} + (1-\delta_j)y_j^L \le y_j^p \le y_j^{sp,p} + (1-\delta_j)y_j^U \\ \delta_j y_j^L \le y_j^{sp,p} \le \delta_j y_j^U \\ y_j^{sp,p} = \psi_j^0 + \sum_{k\in K_m}\sum_{q=1}^{n_q} \psi_{jk}^q \left(\frac{\theta_k^p - \theta_k^N}{\Delta\theta_k}\right)^q \\ \delta_j \Psi_j^L \le \psi_{jk}^q \le \delta_j \Psi_j^U,\ \forall q, k \in K_m \end{bmatrix} \forall j, p \quad (9)$$

Following similar arguments, we define the binary variable λ_i associated with the manipulated variables u_i as follows

$$\lambda_i = \begin{bmatrix} 1, \text{ if the manipulated variable } u_i \text{ is used} \\ \quad \text{at the regulatory controller} \\ 0, \text{ otherwise} \end{bmatrix} \quad (10)$$

to finally obtain

$$\begin{bmatrix} u_i^{opt,p} + \lambda_i u_i^L \le u_i^p \le u_i^{opt,p} + \lambda_i u_i^U \\ (1-\lambda_i)u_i^L \le u_i^{opt,p} \le (1-\lambda_i)u_i^U \\ u_i^{opt,p} = \upsilon_i^0 + \sum_{k\in K_m}\sum_{q=1}^{n_q} \upsilon_{ik}^q \left(\frac{\theta_k^p - \theta_k^N}{\Delta\theta_k}\right)^q \\ (1-\lambda_i)U_i^L \le \upsilon_{ik}^q \le (1-\lambda_i)U_i^U,\ \forall q, k \in K_m \end{bmatrix} \forall i, p \quad (11)$$

It should be noted that if $\lambda_i = 1$ (i.e., manipulated variable u_i is used at the regulatory controller) then it follows from the second constraint that $u_i^{opt,p} = 0$, from the fourth constraint that $\upsilon_{ik}^p = 0$, $\forall k, p$, and also from the first constraint

$$u_i^L \le u_i^p \le u_i^U,\ \forall p \quad (12)$$

i.e., when a manipulated variable is selected at the regulatory control structure, then it can obtain any feasible value. When $\lambda_i = 0$ (i.e. manipulated variable u_i is not used at the regulatory controller and, thus, it is available for steady-state optimization), then

$$u_i^p = u_i^{opt,p},\ \forall p \quad (13)$$

$$u_i^L \le u_i^{opt,p} \le u_i^U,\ \forall p \quad (14)$$

Again, the optimal steady-state values of the manipulated variables can be either constant or polynomial functions of the measured disturbances.

Finally, it is important to note that the available degrees of freedom for optimizing purposes are equal to the dimension of the vector **u**. Clearly, the number of additional specifications introduced by eqs 9 and 11 must be equal to this number, and this can be included in the mathematical formulation in the form of the following constraint

$$\sum_{j=1}^{n_y}\delta_j + \sum_{i=1}^{n_u}(1-\lambda_i) = n_u \quad (15)$$

The complete formulation is obtained by augmenting eq 2 with eqs 9, 11, and 15

$$\min_{\substack{\mathbf{x}^p \\ \upsilon_i^0, \upsilon_{ik}^q, \lambda_i \\ \psi_j^0, \psi_{jk}^q, \delta_j}} \sum_{p\in P} w^p J(x^p, u^p, \theta^p) \quad (16)$$

s.t.

$$\begin{bmatrix} \mathbf{f}(x^p, u^p, \theta^p) = 0 \\ \mathbf{g}(x^p, u^p, \theta^p) \le 0 \\ \mathbf{m}(x^p, u^p, y^p) = 0 \end{bmatrix} \forall p$$

$$\begin{bmatrix} y_j^{sp,p} + (1-\delta_j)y_j^L \le y_j^p \le y_j^{sp,p} + (1-\delta_j)y_j^U \\ \delta_j y_j^L \le y_j^{sp,p} \le \delta_j y_j^U \\ y_j^{sp,p} = \psi_j^0 + \sum_{k\in K_m}\sum_{q=1}^{n_q} \psi_{jk}^q \left(\frac{\theta_k^p - \theta_k^N}{\Delta\theta_k}\right)^q \\ \delta_j \Psi_j^L \le \psi_{jk}^q \le \delta_j \Psi_j^U,\ \forall q, k \in K_m \end{bmatrix} \forall j, p$$

$$\begin{bmatrix} u_i^{opt,p} + \lambda_i u_i^L \le u_i^p \le u_i^{opt,p} + \lambda_i u_i^U \\ (1-\lambda_i)u_i^L \le u_i^{opt,p} \le (1-\lambda_i)u_i^U \\ u_i^{opt,p} = \upsilon_i^0 + \sum_{k\in K_m}\sum_{q=1}^{n_q} \upsilon_{ik}^q \left(\frac{\theta_k^p - \theta_k^N}{\Delta\theta_k}\right)^q \\ (1-\lambda_i)U_i^L \le \upsilon_{ik}^q \le (1-\lambda_i)U_i^U,\ \forall q, k \in K_m \end{bmatrix} \forall i, p$$

$$\sum_{j=1}^{n_y}\delta_j + \sum_{i=1}^{n_u}(1-\lambda_i) = n_u$$

$$x \in X, \quad u \in U, \quad y \in Y$$

$$\delta_j \in \{0,1\}, \quad \lambda_i \in \{0,1\}$$

3. Discussion of the Proposed Formulation

The proposed methodology has a number of interesting characteristics that are worth discussing further. Formulation 16 (eq 16) can be used to determine not only the optimum operating point for a range of disturbances but also the optimal operating policy and regulatory control structure. An implicit assumption is that, for the range of disturbance variation considered, a feasible solution always exists, i.e., the flexibility problem has been solved at the design stage and enough overdesign has been implemented to guarantee that.

It is interesting to note that eqs 9, 11, and 15 for describing and optimizing the RCS structure are linear equations. If the initial problem solved at the RTO level (eq 2) is a linear problem, then the overall formulation will be a mixed integer linear programming problem (MILP). However, since the models employed at the RTO level are nonlinear, in most cases the overall formulation will correspond to mixed integer, nonlinear programming problem (MINLP). In both cases, since the additional equations are linear in nature, the robustness of optimizing the process model will not be affected. The size and complexity, however, will increase due to the presence of the binary variables.[11]

The proposed formulation can be seen as a mathematical generalization of ideas that have been presented independently in the past by many research groups from both industry and academia. If, for instance, we consider the economics to be dominated by the nominal steady state and only enforce feasibility for all other periods, then we obtain an extension of the previous work by Kookos and Perkins[12] on the "back-off" idea as applied to the simultaneous design and control problem. If we assign equal weights to all periods and restrict the set points to be constant for all periods considered, then we obtain the mathematical description of the "*concept of eigenstructure*" as was proposed by Luyben.[13,14] Luyben[14] states that the purpose of his paper was "to put forward the notion that each process has an intrinsically self-regulating control structure which makes the system as insensitive as possible to load disturbances and is self-optimizing". In most of the examples considered by Luyben (see ref 14 and the references therein), economics was the key performance indicator for comparing alternative constant set point strategies and control structures using rating programs. The reader is also encouraged to read the discussion in ref 14 about the connections between Luyben's conjecture of the existence of "*self-regulating*" or "*self-optimizing*" control and other relevant control methodologies. Recently, Skogestad[15] has defined control as "*self-optimizing*" when "an acceptable loss can be achieved using constant setpoints for the controlled variables", where "*loss*" is the difference between the value of the objective using a constant set point policy and the true optimal value. His methodology can also be obtained as a special case of formulation 16 (eq 16).

In developing the proposed methodology, we have assumed that the exact value of the set points is required by the regulatory level, which then achieves zero steady-state offset at all periods. This necessitates integral action at all regulatory loops, which might not be the case. Alternatively, eq 9 can be replaced by the following

$$\begin{bmatrix} y_j^{\mathrm{sp,L}} + (1-\delta_j)y_j^{\mathrm{L}} \le y_j^p \le y_j^{\mathrm{sp,U}} + (1-\delta_j)y_j^{\mathrm{U}} \\ \delta_j y_j^{\mathrm{L}} \le y_j^{\mathrm{sp,L}} \le y_j^{\mathrm{sp,U}} \le \delta_j y_j^{\mathrm{U}} \end{bmatrix} \forall j, p \tag{17}$$

where the new variables $y_j^{\mathrm{sp,L}}$ and $y_j^{\mathrm{sp,U}}$, that also appear linearly, are new tighter lower and upper bounds, respectively, on the steady-state value of the corresponding controlled variable. If $\delta_j = 0$, then eq 4 is obtained, while when $\delta_j = 1$, then it follows that

$$y_j^{\mathrm{L}} \le y_j^{\mathrm{sp,L}} \le y_j^p \le y_j^{\mathrm{sp,U}} \le y_j^{\mathrm{U}} \forall j, p \tag{18}$$

i.e., the controlled variable y_j is restricted to lie between the tighter lower and upper bounds.

The values of the integer variables at the solution of eq 16 unambiguously define the set of controlled variables and the set of manipulated variables. In addition, the (possibly time-varying) set points for the controlled variables and the unused manipulated variables are obtained from the same solution. This information can be used to design a centralized controller. However, if a fully decentralized (such as decentralized PID) controller is used at the regulatory level, the pairing problem needs to be solved. There is a vast amount of literature available on the issue, and the interested reader is referred to the book by Skogestad and Postlethwaite[16] for a review of the controllability tools available for solving the pairing problem. Automated methods that are based on mathematical programming techniques are also available and might be more appropriate from the implementation point of view (see ref 17 and the references therein).

Finally, as has already been mentioned, an implicit assumption of this work is that, for the range of disturbance variation considered, a feasible solution always exists. However, since the selection of the RCS in the proposed formulation does not take feasibility directly into account, a validation step is necessary to guarantee that the selected structure is feasible for the whole range of disturbances considered. To achieve that, we consider the initial description of the process augmented by the specifications imposed by the control system as obtained by the solution of the proposed formulation (such as eq 8, for instance). The augmented description can be written as

$$\begin{aligned} \mathbf{f}(\mathbf{x},\mathbf{u},\boldsymbol{\theta}) &= 0 \\ \mathbf{m}(\mathbf{x},\mathbf{u},\mathbf{y}) &= 0 \\ \mathbf{c}(\mathbf{x},\mathbf{u},\mathbf{y},\boldsymbol{\theta}) &= 0 \\ \mathbf{g}(\mathbf{x},\mathbf{u},\boldsymbol{\theta}) &\le 0 \end{aligned} \tag{19}$$

where $\mathbf{c}:R^{n_x+n_u+n_y+n_\theta} \rightarrow R^{n_u}$ is the steady-state specification imposed by the RCS. We then define the following

$$\mathbf{h}(\mathbf{x},\mathbf{u},\mathbf{y},\boldsymbol{\theta}) = \begin{bmatrix} \mathbf{f}(\mathbf{x},\mathbf{u},\boldsymbol{\theta}) \\ \mathbf{m}(\mathbf{x},\mathbf{u},\mathbf{y}) \\ \mathbf{c}(\mathbf{x},\mathbf{u},\mathbf{y},\boldsymbol{\theta}) \end{bmatrix} = 0 \tag{20}$$

where $\mathbf{h}:R^{n_x+n_u+n_y+n_\theta} \rightarrow R^{n_x+n_y+n_u}$, i.e., if the disturbances are specified (θ), then solving the set of equations given by $\mathbf{h}(\mathbf{x},\mathbf{u},\mathbf{y},\boldsymbol{\theta}) = 0$ completely determines all the remaining variables ($\mathbf{x}$, $\mathbf{u}$, and $\mathbf{y}$). To determine the maximum disturbance set for which feasibility is guaranteed, we can solve the following flexibility index determination problem[18]

$$\min_{\eta,\sigma,x,u,y,\theta} \eta \tag{21}$$

s.t.

$$\mathbf{h}(\mathbf{x},\mathbf{u},\mathbf{y},\boldsymbol{\theta}) = 0$$

$$\mathbf{g}_l(\mathbf{x},\mathbf{u},\boldsymbol{\theta}) + \sigma_1 = 0, \forall l$$

$$0 \le \sigma_l \le B_{\mathrm{M}}(1-\gamma_l), \forall l$$

$$\sum_l \gamma_l = 1$$

$$\theta^{\mathrm{N}} - \eta\Delta\theta \le \theta \le \theta^{\mathrm{N}} + \eta\Delta\theta$$

$$\gamma_l \in \{0,1\}, \forall l$$

where η is the scalar flexibility index which is used to scale (relative to $\Delta\theta$) the disturbance set considered in our analysis, B_{M} is a large positive number, and σ_λ are the positive variables. If $\eta = 1$, then feasibility can only be guaranteed for disturbances in $[\theta^{\mathrm{N}} + \Delta\theta, \theta^{\mathrm{N}} - \Delta\theta]$, while if $\eta < 1$, then there is at least one combination in

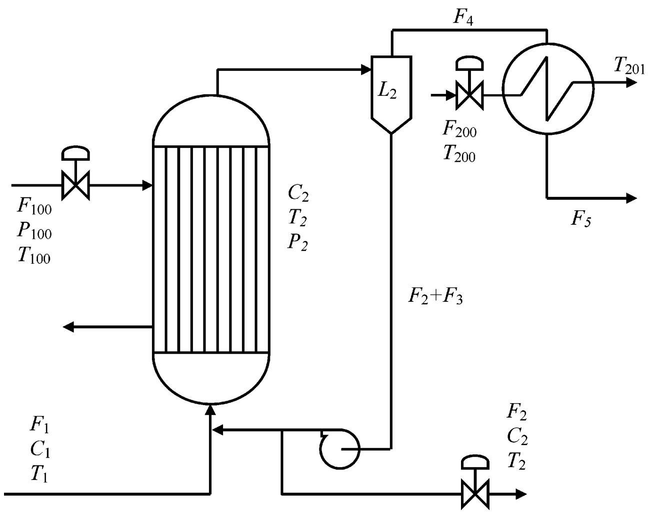

Figure 1. Evaporator system.

Table 1. Major Variables of the Evaporation Process Model and Their Values at Optimal Nominal Operating Point

notation	variable	value	units
F_1	feed flow rate	10.000	kg/min
F_2	product flow rate	1.429	kg/min
F_4	vapor flow rate	8.571	kg/min
F_5	condensate flow rate	8.571	kg/min
F_{100}	steam flow rate	9.884	kg/min
F_{200}	cooling water flow rate	213.952	kg/min
T_1	feed temperature	40.000	°C
T_2	product temperature	91.785	°C
T_4	vapor temperature	84.263	°C
T_{100}	steam temperature	129.466	°C
T_{200}	cooling water inlet temperature	25.000	°C
T_{201}	cooling water outlet temperature	47.034	°C
C_1	feed composition	5.000	%
C_2	product composition	35.000	%
P_2	operating pressure	57.717	kPa
P_{100}	steam pressure	256.606	kPa

$[\theta^N + \Delta\theta, \theta^N - \Delta\theta]$ that will result in infeasible operation. Clearly, in the latter case, the RCS selected should be rejected and the proposed methodology should be applied again by using an integer cut to exclude the previous structure from any further consideration.

4. Case Studies

In all case studies the NLP or MINLP problems were solved using the GAMS interface to the MINOS and DICOPT (MINOS/CPLEX) solvers.[19]

4.1. Evaporator Process. The evaporation process examined in this case study is shown in Figure 1.[12,20] This is a process that removes a volatile liquid from a nonvolatile solute, thus concentrating the solution, and it mainly consists of a heat exchange vessel with a recirculating pump. The vapor is condensed by the use of a process heat exchanger. The major variables of interest are summarized in Table 1, while the dynamic model of the evaporator is given by[12]

Equality Constraints

$$F_1C_1 - F_2C_2 = 0 \quad (22)$$

$$F_4 - F_5 = 0 \quad (23)$$

$$F_1 - F_4 - F_2 = 0 \quad (24)$$

$$F_1C_pT_1 - F_4(\lambda + C_pT_4) - F_2C_pT_2 + Q_{100} = 0 \quad (25)$$

$$0.5616P_2 + 0.3126C_2 + 48.43 - T_2 = 0 \quad (26)$$

$$0.5070P_2 + 55 - T_4 = 0 \quad (27)$$

$$0.1538P_{100} + 90 - T_{100} = 0 \quad (28)$$

$$Q_{100} - UA_1(T_{100} - T_2) = 0 \quad (29)$$

$$Q_{100} - F_{100}\lambda_S = 0 \quad (30)$$

$$Q_{200} - F_{200}C_p(T_{201} - T_{200}) = 0 \quad (31)$$

$$Q_{200} - UA_2(T_4 - (T_{201} + T_{200})/2) = 0 \quad (32)$$

$$F_5\lambda - Q_{200} = 0 \quad (33)$$

Inequality Constraints

$$35 - C_2 \le 0 \quad (34)$$

$$40 - P_2 \le 0 \quad (35)$$

$$P_2 - 80 \le 0 \quad (36)$$

$$P_{100} - 400 \le 0 \quad (37)$$

$$F_{200} - 400 \le 0 \quad (38)$$

$$T_{201} - T_4 + 5 \le 0 \quad (39)$$

Objective Function (Operating Cost in \$/yr)

$$J = 8000(F_{100} + 10^{-3}F_{200}) \quad (40)$$

where $C_p = 0.07$ kW/kg, $\lambda = 38.5$ kW/kg, $\lambda_S = 36.6$ kW/kg, $UA_1 = 9.6$ kW/°C and $UA_2 = 6.84$ kW/°C. We further define the following vectors

$$\mathbf{y} = \begin{bmatrix} C_2 \\ P_2 \\ T_2 \\ T_4 \\ T_{201} \end{bmatrix}, \quad \mathbf{u} = \begin{bmatrix} P_{100} \\ F_{200} \end{bmatrix}, \quad \boldsymbol{\theta} = \begin{bmatrix} F_1 \\ C_1 \end{bmatrix} \quad (41)$$

To find the optimum point of steady-state operation, the following nominal input conditions are selected: $F_1 = 10$ kg/min and $C_1 = 5\%$. Table 1 summarizes the results of the optimization for this nominal case, and the corresponding objective function is 80 780 \$/yr. The product purity constraint is the only constraint that is active at the optimal point. It is assumed that $F_1 \in [8,12]$ and $C_1 \in [4,6]$ and that their distribution is uniform (i.e., $w^p = 1/n_p$). Equation 2 was then solved using 441 periods uniformly distributed on $[8,12] \times [4,6]$ to obtain a slightly increased average operating cost of 80 890 \$/yr.

The proposed formulation was then applied to obtain the RCS and the (possibly time-varying) set points that will keep the process as close as possible to optimality. Of the two disturbances (F_1 and C_1), only F_1 is considered to be measurable. The five potential controlled variables and the two potential manipulated variables

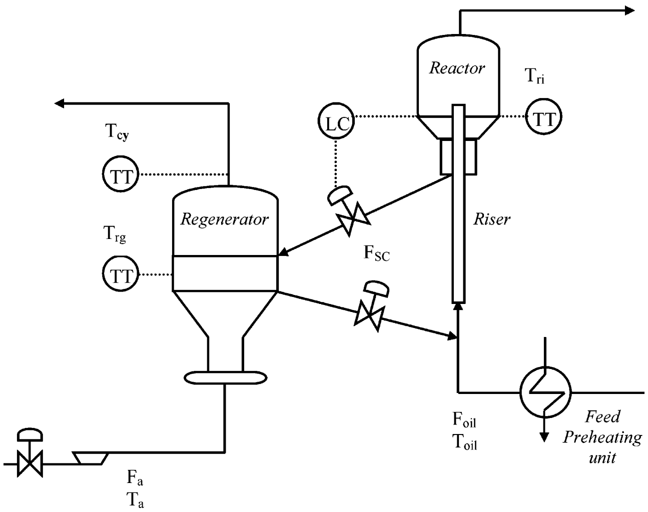

Figure 2. Fluid catalytic cracking process.

are given in eq 41. In the solution obtained, both manipulated variables are used in the regulatory level while the product composition (C_2) and operating pressure (P_2) are the selected controlled variables. The product composition has a constant set point = 35%, while the set point for the pressure is given by

$$P_2^{sp} = 58.35 + 18.35\left(\frac{F_1 - 10}{2}\right) \tag{42}$$

The corresponding objective function is 80 907 \$/yr. When the set points are restricted to be time-invariant, then we obtain the same set of manipulated and controlled variables, the same set point for C_2, but a different set point for pressure of P_2 = 73.24. The average operating cost, however, increases and becomes 81 460 \$/yr.

Formulation 21 (eq 21) was then solved to determine whether the optimal RCS ensures feasibility for all $F_1 \in [8,12]$ and $C_1 \in [4,6]$. The solution corresponds to $\eta = 1$, and thus, feasibility can be guaranteed for all disturbances considered. The worst case disturbance corresponds to $F_1 = 8$, and it is independent of the value of C_1. For this value of F_1, the pressure set point becomes 40 kPa and the pressure constraint becomes active. Any further decrease in F_1 results in infeasible operation. The constant set point strategy also corresponds to $\eta = 1$, but the worst case disturbance combination is different and corresponds to $F_1 = 12$ and $C_1 = 4$, which causes the cooling water flowrate to hit its upper bound of 400 kg/min.

At this point, it is interesting to compare the proposed control structure with variable set point with the control structure that keeps the set points of C_2 and P_2 constant and equal to the values at the nominal optimal operating point (see Table 1). By solving formulation 21 (eq 21) for the latter, it was found that the system under this control strategy is significantly less flexible, since $\eta = 0.4$ (the worst case disturbance combination corresponds to $F_1 = 10.8$ and $C_1 = 4.6$, which causes the cooling water flowrate to hit its upper bound of 400 kg/min). Thus, the structure obtained using the proposed formulation achieves not only near optimal operation but also ensures feasibility for the whole range of disturbances considered, while "classical" structures fail to achieve either.

4.2. Fluid Catalytic Cracking Process. In this section, a fluid catalytic cracking (FCC) process case study is considered (see Figure 2). The FCC process converts heavy oils into lighter and more valuable products. The dynamics of the FCC process are described by a low order but highly nonlinear set of differential algebraic equations (DAEs). The actual operation of the process is dominated by economics, which is sensitive to a number of disturbances. Furthermore, the most appropriate control structure for this process is a matter of some controversy, with the conventional structure being criticized in a number of recent publications.

Table 2. Parameters of the FCC Model

notation	variable	value	units
C_{p_a}	heat capacity of air	1.074	kJ/(kg K)
C_{p_d}	heat capacity of dispersing stream	1.9	kJ/(kg K)
$C_{p_{oil}}$	heat capacity of oil	3.133 5	kJ/(kg K)
C_{p_s}	heat capacity of catalyst	1.005	kJ/(kg K)
E_{cb}	activation energy for coke burning	158 600	kJ/kmol
E_{cf}	activation energy for coke formation	41 790	kJ/kmol
E_f	activation energy for gasoil cracking	101 500	kJ/kmol
h_1	parameter	521 150	kJ/kmol
h_2	parameter	245	kJ/(kmol K)
k_{com}	rate constant for coke burning	0.488 96	1/s
k_o	rate constant for gasoil cracking	962 000	1/s
m	empirical deactivation parameter	80	
n	hydrogen content in coke	2	
O_{in}	oxygen mole fraction in air	0.213 6	
T_a	air input temperature	320	K
W	catalyst holdup in regenerator	175 738	kg
W_a	air holdup in regenerator	20	kmol
W_{ri}	catalyst holdup in riser	2 724	kg
$y_f(0)$	weight fraction of gasoil in feed	1	
z_r	dimensionless position		
α	catalyst decay rate constant	0.12	1/s
ΔH_f	heat of reaction of gasoil cracking	506	kJ/kg
λ	weight fraction of steam in riser feed	0.035	

The model used in this study is based on a model first presented by Lee and Groves[21] as modified by Balchen et al.[22] and Loeblein and Perkins.[23] On the basis of a simplified, three-lump kinetic model, Lee and Groves[21] proposed that the following equations can be used to describe the riser (The nomenclature used can be found in Balchen et al.,[22] while the values of the parameters of the model are given in Table 2.)

$$\frac{1}{\tau_c}\frac{d}{dz}(y_f) = -K_1 y_f^2 \rho\phi \tag{43}$$

$$\frac{1}{\tau_c}\frac{d}{dz}(y_g) = (K_2 y_f^2 - K_3 y_g)\rho\phi \tag{44}$$

$$(F_{rc}C_{p_{rc}} + F_{oil}C_{p_{oil}} + \lambda F_{oil}C_{p_d})\frac{d}{dz}(T_{ri}(z) - T_{ri}(0)) = \Delta H_f F_{oil}\frac{d}{dz}(y_f) \tag{45}$$

where ρ is the catalyst-to-oil ratio (COR). Balchen et al.[22] presented a simplified solution of the above simultaneous differential equations

$$y_f(1) = \frac{a}{a + K_r\phi_0\,[1 - \exp(-a\tau_c\rho)]}y_f(0) \tag{46}$$

$$y_g(1) = 10[y_f^{0.9}(1) - y_f(1)] \tag{47}$$

$$T_{ri}(1) = \left\{1 - \frac{\gamma K_r \phi_0 [1 - \exp(-a\tau_c\rho)]}{a + K_r\phi_0[1 - \exp(-a\tau_c\rho)]} y_f(0)\right\} T_{ri}(0) \quad (48)$$

where

$$T_{ri}(0) = \frac{(C_{p_{oil}} F_{oil} + \lambda C_{p_d} F_{oil}) T_{oil} + C_{p_s} F_{rc} T_{rg}}{C_{p_{oil}} F_{oil} + \lambda C_{p_d} F_{oil} + C_{p_s} F_{rc}} \quad (49)$$

$$\gamma = \frac{\Delta H_f F_{oil}}{T_{ri}(0)\,(C_{p_{oil}} F_{oil} + \lambda C_{p_d} F_{oil} + C_{p_s} F_{rc})} \quad (50)$$

$$K_0 = k_0 \exp[-E_f/RT_{ri}(0)] \quad (51)$$

$$T_r = \left\{1 - \frac{\gamma K_0 \phi_0 [1 - \exp(-a\tau_c\rho z_r)]}{a + K_0\phi_0[1 - \exp(-a\tau_c\rho z_r)]}\right\} T_{ri}(0) \quad (52)$$

$$K_r = k_0 \exp[-E_f/RT_r] \quad (53)$$

$$\phi_0 = 1 - mC_{rc} \quad (54)$$

The model of the regenerator consists of the coke balance, the oxygen balance, and the enthalpy balance

$$F_{sc}(C_{sc} - C_{rc}) - kO_d C_{rc} W = 0 \quad (55)$$

$$R_a(O_{in} - O_d) - \frac{n + 2 + (n + 4)\sigma}{4M_c(1 + \sigma)} kO_d C_{rc} W = 0 \quad (56)$$

$$T_{ri}(1)\, F_{sc} C_{p_s} + F_a C_{p_a} T_a - T_{rg}(F_{sc} C_{p_s} + F_a C_{p_a}) - \Delta H \frac{kO_d C_{rc} W}{M_c} = 0 \quad (57)$$

The amount of coke produced and the amount of coke on the catalyst leaving the riser are determined by

$$C_{cat} = k_c^{\,1} \sqrt{\frac{\tau_c}{C_{rc}^{N}} \exp\left(-\frac{E_{cf}}{RT_{ri}(1)}\right)} \quad (58)$$

$$C_{sc} = C_{rc} + C_{cat} \quad (59)$$

The remaining variables are calculated as follows

$$k = k_{com} \exp\left[\left(\frac{1}{960} - \frac{1}{T_{rg}}\right)\frac{E_{cb}}{R}\right] \quad (60)$$

$$\Delta H = -h_1 - h_2(T_{rg} - 960) + 0.6(T_{rg} - 960)^2 \quad (61)$$

$$\sigma = 1.1 + \sigma_2(T_{rg} - 873) \quad (62)$$

$$T_{cy} = T_{rg} + c_t O_d \quad (63)$$

The economic objective function of the FCC process has the form[23]

$$J = 1440\{P_{gl} y_g(1)\, F_{oil} + P_{gs}\{[1 - y_f(1) - y_g(1)]F_{oil} - F_{sc}C_{cat}\} + P_{ugo}[y_f(1) - 1]F_{oil} - P_h F_{oil}(T_{oil} - 400)\} \quad (64)$$

where P_{gl} = 0.14 \$/kg, P_{gs} = 0.132 \$/kg, P_{ugo} = 0.088 \$/kg, P_h = 0.000 017 8 \$/(kg K) (J is the profit in \$/day). The following constraints define the feasible space of operation

$$g_1 = T_{ri}(0) - 1000 \le 0 \quad (65)$$

$$g_2 = T_{ri}(1) - 1000 \le 0 \quad (66)$$

$$g_3 = 760 - T_{ri}(0) \le 0 \quad (67)$$

$$g_4 = 760 - T_{ri}(1) \le 0 \quad (68)$$

$$g_5 = T_{cy} - 1000 \le 0 \quad (69)$$

$$g_6 = 895 - T_{rg} \le 0 \quad (70)$$

$$g_7 = 400 - T_{oil} \le 0 \quad (71)$$

$$g_8 = T_{oil} - 640 \le 0 \quad (72)$$

$$g_9 = F_a - 3600 \le 0 \quad (73)$$

$$g_{10} = F_{sc} - 24000 \le 0 \quad (74)$$

The vectors of state, disturbance, manipulated, and measured variables are defined as

$$\mathbf{y} = \begin{bmatrix} T_{ri}(1) \\ T_{rg} \\ T_{cy} \end{bmatrix}, \quad \mathbf{u} = \begin{bmatrix} F_{sc} \\ F_a \\ T_{oil} \end{bmatrix}, \quad \boldsymbol{\theta} = \begin{bmatrix} F_{oil} \\ k_c^1 \end{bmatrix} \quad (75)$$

The disturbance k_c^1 (the rate constant for coke formation) is selected to represent changes in the feed oil composition. This is, together with changes in the feed flowrate, probably the most significant disturbance to the FCC process. Only the feed flowrate is assumed to be a measured disturbance in this case study.

The nominal values of the disturbances are assumed to be F_{oil} = 2 438 kg/min and k_c^1 = 0.018 97. The optimum operating point is defined by the upper bounds on the cyclone and feed temperatures (the corresponding Lagrange multipliers are λ_5 = 368.6 \$/K and λ_8 = 55.3 \$/K). The value of the objective function is 73 623 \$/day.

Formulation 2 (eq 2) was then solved using 49 periods distributed uniformly in the space defined as $F_{oil} \in$ [2 194.2, 2 681.8] and $k_c^1 \in$ [0.017 073, 0.020 867]. The optimal solution has an objective function of 73 561 \$/day, and the upper bounds on the cyclone and feed temperatures are active constraints in all periods. Then the proposed formulation is solved and the regulatory control structure (F_{sc},F_a) − (T_{rg},T_{cy}) is obtained. The optimal value of the third manipulated variable is found to be equal to its upper bound value, while the set point of the cyclone temperature is also equal to its upper bound value. A time varying set point was found for T_{rg}

$$T_{rg}^{sp} = 898.68 - 1.012\left(\frac{F_{oil} - 2438}{243.8}\right) \quad (76)$$

The corresponding objective function is 73 528 \$/day. When a constant set point is considered, then the objective function is 73 479 \$/day, i.e., the benefit from using the time-varying set point is ~17 885 \$/yr. The feasibility formulation (eq 21) was then applied, and it was found that the flexibility index is 3.19 (i.e., the closed loop system will be steady-state feasible for a significantly larger parameter set than the one for which it was designed). The worst case disturbance corresponds to a significant decrease in feed flowrate that causes the lower bound constraint on the initial riser temperature to become active.

5. Conclusions

A systematic methodology for integrating decisions related to the structure and functionality of the regulatory control system into the RTO level has been presented. A set of linear constraints involving integer variables has been proposed to achieve the goal of this work, and possible connections with other methodologies have been discussed. In addition, a feasibility index test is proposed to evaluate the maximum range of disturbances for which feasibility is guaranteed for any selected control structure. The proposed methodology was applied in two realistic case studies, namely, an evaporator process and a fluid catalytic cracking process. In both cases, the proposed methodology was successful in identifying the structure and functionality of a steady-state regulatory control system that significantly reduces the effects of disturbances on the economics.

Nomenclature

$\mathbf{c}$ = vector function of constraints imposed by the regulatory controller
E = expected value
$\mathbf{f}$ = vector function of the process equality constraints
$\mathbf{g}$ = vector function of the inequality constraints that define the feasible operation
J = cost function
$\mathbf{m}$ = vector function defined in eq 3
p = index of periods
$\mathbf{u}$ = vector of control variables (variables that can change during operation)
$\mathbf{x}$ = vector of dependent variables
w = weights used in the multiperiod formulation
$\mathbf{y}$ = vector of potential measured variables

Greek Letters

γ = integer variables used in eq 21
Δ = deviation from the nominal value
δ = integer variables defined in eq 5
η = flexibility index
$\boldsymbol{\theta}$ = vector of disturbances
λ = integer variables defined in eq 10
σ = slack variables used in eq 21

Superscripts

L = lower bound
N = nominal case
opt = optimum value
sp = set point
U = upper bound

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