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Plantwide Control for Economic Optimum Operation of a Recycle Process with Side Reaction†

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ABSTRACT: Plantwide control system design for the economically optimum operation of a recycle process with side reaction, consisting of a continuous stirred tank reactor (CSTR) followed by two distillation columns, is studied. The steady-state operating profit is maximized over a large throughput range for an existing design. As the throughput is increased, constraints progressively become active until maximum throughput is reached where all the steady-state degrees of freedom are exhausted. A strategy of moving the throughput manipulator to the next constraint to become active as the throughput is increased is used to improve the control of the active constraint. This minimizes the variability and hence the back-off in the active constraint variables for economically optimal operation. The plantwide control system (CS1) so obtained is quantitatively compared with three other more conventional control systems (CS2−CS4) in terms of the required back-off to avoid hard constraint violation for disturbances. Results show that the most economical operation is achieved using CS1 and the traditional practice of fixing throughput at the feed (CS4) gives the highest (up to ∼7%) economic loss. A simple switching scheme to transition from low to maximum throughput is also demonstrated.

1. INTRODUCTION

The plantwide control system for chemical processes (Figure 1) typically consists of a regulatory layer that ensures safe and stable operation and a coordinating control layer on top for ensuring feasibility and economically optimal operation. The coordinating economic layer has two main tasks. First, there is a supervisory (logic) part that switches the controlled variables according to changes in active constraints at the economic optimum. Second, it controls the key active constraint variables ("economic variables") to drive them as close as possible to their limiting values. Model predictive control (MPC) is often used for the control function in the coordinating layer. In addition to these two layers, a real-time optimization layer may be further added to adjust key unconstrained set points for optimizing an economic criterion such as operating profit or energy consumption or feed processing rate (throughput). The overall plantwide control system is usually simplified in practice by selecting economically sound ("self-optimizing") controlled variables that obviate the need for the optimization layer.

The design of the regulatory plantwide control system has been extensively studied in the literature. The combinatorial complexity of the plantwide control structure design problem results in several reasonable structures that provide safe and stable process operation. To systematize the choice of the loop pairings in the regulatory layer, Luyben et al.[1] proposed a nine-step bottom-up heuristic design procedure for "smooth" process operation. An inherent disadvantage of this bottom-up approach is that economic issues are explicitly considered only at the end (step 9), although they are considered indirectly in the formulation of the control objectives such as product quality and product quality (step 1).

For chemical processes, the economic optimum steady-state operating point typically lies at the intersection of process constraints (i.e., multiple active constraints). The implemented regulatory control system affects the transients in these "active" constraint variables, and hence a "back-off" is necessary to avoid transient hard constraint violation. Structures minimizing the transients in the active constraints would require smaller back-offs with consequently better economic performance while ensuring safe and stable ("smooth") operation. On the basis of this concept, Skogestad[2,3] proposed a "top-down bottom-up" design procedure that uses a priori knowledge of active constraints at the economic optimum to synthesize the regulatory control system. The "top-down" part of the procedure is systematic, while some heuristics are employed in the subsequent "bottom-up" part.

Skogestad[4] has also formalized "self-optimizing" controlled variables, originally conceptualized by Morari et al.[5] These are chosen or designed such that holding them constant (at the set point) causes acceptable economic loss for different disturbance scenarios. A self-optimizing control structure thus does not require an explicit economic optimization layer. Self-optimizing control of complex chemical processes has been demonstrated in the literature.[6−8]

Notwithstanding the simplicity of self-optimizing structures, what constitutes "acceptable" economic loss is quite subjective. Further, mitigation of the back-off in active constraints through

Received: December 4, 2010
Accepted: June 10, 2011
Revised: May 22, 2011
Published: June 10, 2011

dx.doi.org/10.1021/ie1024358 | Ind. Eng. Chem. Res. 2011, 50, 8571–8584

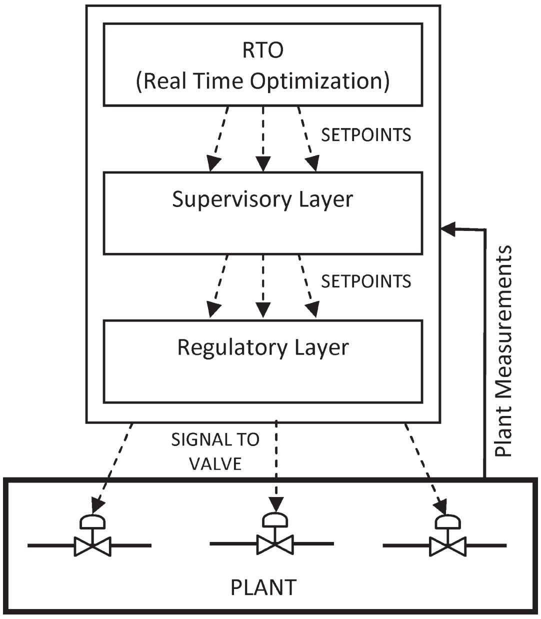

Figure 1. Plantwide control system.

appropriate supervisory and regulatory layer design may significantly impact operating profit. Even a small relative increase in production (say 1%) can translate into millions of dollars of additional revenue for the volume-driven continuous process industry. A quantitative evaluation of the economic performance of different regulatory control configurations with a supervisory economic optimizing control system on top is thus highly desirable.

In a recent article, Kanodia and Kaistha[9] show that both the choice of the regulatory control structure and the supervisory optimizing control can significantly affect the back-off in an active constraint and hence loss in profit for a hypothetical recycle process. The process considered in their work was, however, unrealistic with no side reaction(s). Also, consideration was given to a single active constraint when multiple constraints are usually active at the economic optimum. Further, plantwide control system design only for process operation at maximum throughput and not over a large throughput range was considered.

In this work, plantwide control system design for economically optimum operation over a large throughput range (including maximum throughput) of a more realistic recycle process with side reaction is considered. The case study illustrates the close coupling between plant economics and process control and shows how control structures can be derived in a systematic manner by considering the plant economics. The use of the location of the throughput manipulator (TPM) in order to improve economic performance is also demonstrated. The basis of the work is the systematic plantwide control procedure of Skogestad,[3] but because there are many factors to consider, including the objectives of "simplicity" and "robustness", which are difficult to capture mathematically, the procedure also relies on engineering insights and heuristics.

In the following, a brief description of the process is provided followed by optimized operating conditions for given fresh feed processing rates, maximum operating profit, and maximum throughput. It is shown that, as the throughput is increased, constraints progressively become active until, at maximum throughput, all steady-state degrees of freedom are exhausted. To minimize the back-off in the active constraints and the consequent economic loss, a simple strategy of moving the throughput manipulator to the next active constraint is used. The economic performance of the plantwide control structure (including supervisory active constraint controllers) so obtained (CS1) is compared with three other reasonable control structures (CS2−CS4). The quantitative results on the back-off necessary to avoid constraint violation due to a worst-case disturbance and the consequent economic loss are presented to demonstrate the significance of a proper plantwide control system design for economically optimal process operation. The article ends with the conclusions from the work.

2. PROCESS AND OPTIMAL OPERATION

2.1. Process Description. The process consists of a liquid-phase continuous stirred tank reactor (CSTR) followed by two distillation columns. The exothermic reactions A + B → C (main reaction) and C + B → D (side reaction) occur in the cooled CSTR. The reactor effluent is distilled in the recycle column to recycle the light reactants (A and B) back to the CSTR. The column bottoms is further distilled in the product column to produce nearly pure C as the overhead product with side product D leaving from the bottoms. The reaction chemistry necessitates reactor operation in excess A environment to suppress the side reaction. Figure 2 shows a schematic of the process along with salient design and base-case operating conditions for processing 100 kmol/h fresh A to produce 99 mol % pure C. The reaction kinetics and hypothetical component properties for modeling in Hysys are reported in Table 1. The process, though hypothetical, is realistic in that it includes essential features of most chemical processes such as the presence of an undesirable side reaction, a reaction section followed by a reactant−product separation train, and recycle of precious reactants. The chemistry used here is the same as for alkylation processes and the basic flow sheet configuration is very similar (see for example, the cumene process recently studied by Luyben[10]).

The base-case process design is a reasonable one, but not the strictly economically optimum design for F_A = 100 kmol/h. This is acceptable as the focus of this work is plantwide control system design for an *existing* process. This is a commonly encountered scenario, for example, when the control system of an operational plant is revamped in its entirety or upgraded to implement a supervisory layer on top of an existing regulatory layer. For the prevailing market conditions and desired throughput, both of which are likely to be different from when the process was originally designed, the existing process design would almost always be reasonable but not strictly optimum.

2.2. Optimal Steady-State Solutions. For the process, there are a total of eight steady-state operational degrees of freedom: two for the feeds (two feed rates), two for the reactor (temperature and holdup), and two each for the two distillation columns. The following variables are chosen as steady-state degrees of freedom (any independent set may be chosen) for optimization: the fresh A feed rate (F_A), the reactor feed A to B excess ratio ($[x_A/x_B]^{\mathrm{RxrIn}}$), the reactor level ($V_{\mathrm{rxr}}$) and temperature ($T_{\mathrm{rxr}}$), the recycle column reflux rate (L_1) and bottoms B to C mole ratio ($[x_B/x_C]^{\mathrm{Bot1}}$), and the product column distillate D loss ($[l_D]^{\mathrm{Dist2}}$) and bottoms C loss ($[l_C]^{\mathrm{Bot2}}$). The loss in a column product stream is defined as the ratio of the product stream impurity component flow rate to the corresponding feed component flow rate.

The desired product purity ($[x_C]^{\mathrm{Dist2}}$) is 99 mol % C, and as this is the valuable product, it will always be an active constraint. Since the final product separation (column 2) is an easy one, the

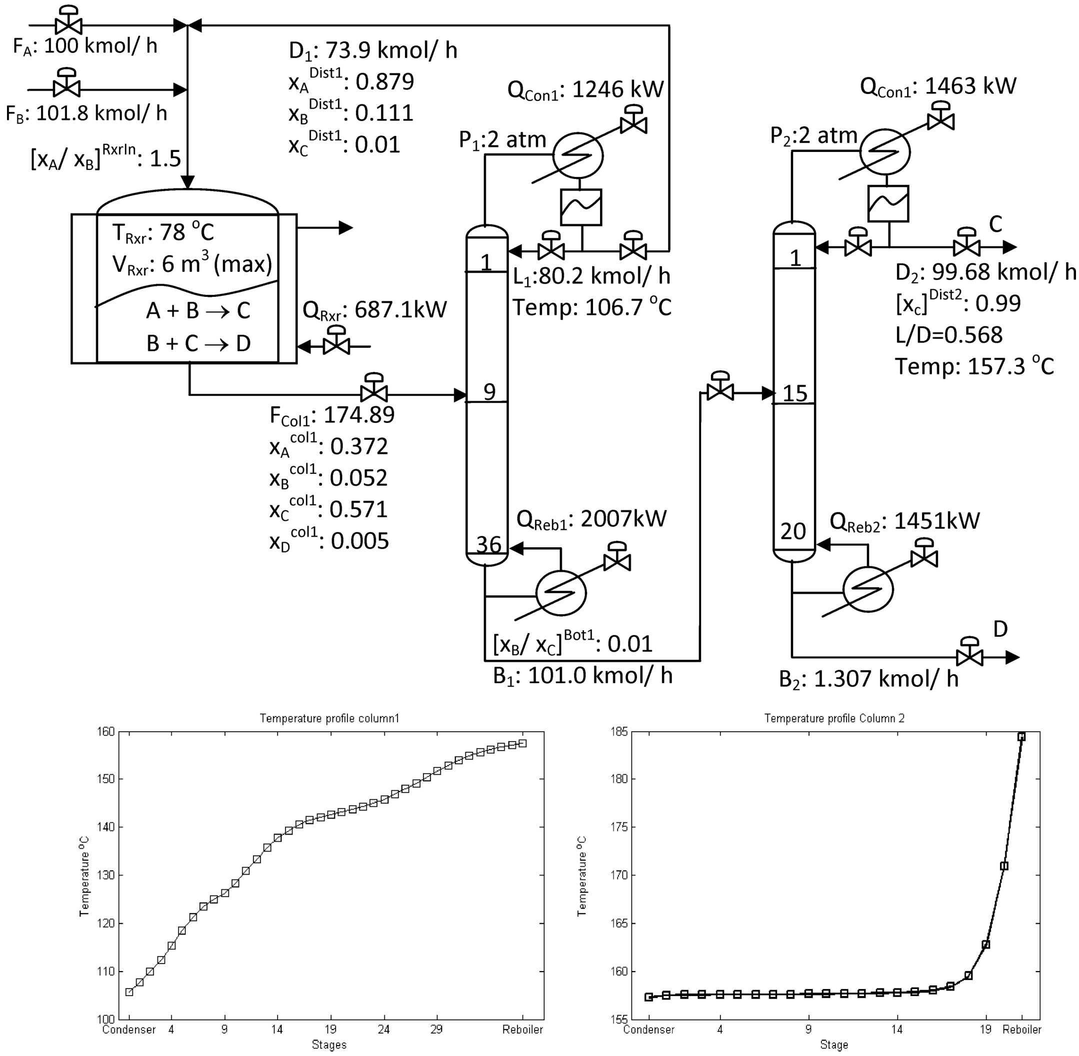

Figure 2. Schematic of recycle process studied.

Table 1. Modeling Details of Recycle Process[a]

			kinetics	
A + B → C			$r_1 = k_1 x_A x_B$	$k_1 = 2 \times 10^8 \exp(-60000/RT)$
B + C → D			$r_2 = k_2 x_B x_C$	$k_2 = 1 \times 10^9 \exp(-80000/RT)$
	hypotheticals			
	MW	NBP (°C)		
A	50	80	hydrocarbon estimation procedure used to estimate	
B	80	100	parameters for thermodynamic property calculations	
C	130	130		
D	210	180		
VLE			Soave−Redlich−Kwong	

[a] Reaction rate units, kmol·m^{-3}·s^{-1}.

total reboiler energy consumption (in columns 1 and 2) is minimized by allowing B to leak out to the maximum extent possible without violating the product purity specification (in the top of column 2). This requires fixing the B to C mole ratio in the recycle column (column 1) bottoms ($[x_B/x_C]^{Bot1}$) to be 0.01. Also, to minimize the loss of precious C in the byproduct stream, the C (light key) loss in the product column bottoms is specified to be low at 0.5%. The D loss in the distillate ($[l_D]^{Dist2}$) is kept small at 1%. Such a choice of specifications gives a distillate C purity of 99 ± 0.001% over the entire range of fresh A processing rate considered, implying a negligible quality/product giveaway. The particular choice of specifications is used as it gives robust flow sheet convergence using the Hysys steady-state solver for the entire throughput range in contrast to the case where $[x_C]^{Dist2}$ is directly specified. The common-sense approach fixes three specifications ($[l_D]^{Dist2}$, $[l_C]^{Bot2}$, and $[x_B/x_C]^{Bot1}$) for on-spec product quality while minimizing energy consumption and product loss, leaving five degrees of freedom for optimizing the process operation.

The remaining five degrees of freedom should be adjusted to optimize an economic criterion such as plant operating profit or energy consumption subject to process constraints on maximum/minimum allowable flows, pressures, temperatures, etc. In this case, the objective is to maximize the profit, where

$$\text{operating profit} = [\text{product value} - \text{raw material cost} - \text{energy cost}] \quad \text{per year}$$

dx.doi.org/10.1021/ie1024358 |Ind. Eng. Chem. Res. 2011, 50, 8571–8584

Table 2. Process Optimization Results

objective function	cases Ia/Ib/Ic and IIa: product cost − (reactant cost + energy cost)	
	case IIb: fresh A processing rate	
cost data	cost of fresh A: 20 \$/kmol	cost of fresh B: 40 \$/kmol
	cost of product C: 65 \$/kmol	steam: 4.7 \$/GJ
	cooling water: 0.47 \$/GJ	
process constraints	60 °C $\leq T_{rxr} \leq$ 100 °C	$0 \leq Q_{reb1} \leq 1.5$ (base case)
	$0 \leq$ material flows ≤ 2 (base case)	$0 \leq Q_{reb2} \leq 2$ (base case)
	$0 \leq$ recycle flow ≤ 3 (base case)	$[x_B/x_C]^{Bot1} = 0.01$
	$0 \leq$ energy flows ≤ 2 (base case)	$[r_C]^{Dist2} = 99.5\%$
	$0 \leq V_{rxr} \leq 6$ m^3	$[r_D]^{Bot2} = 99.0\%$

	case Ia, given F_A	case Ib, given F_A	case Ic, given F_A	case IIa, optimum F_A	case IIb, maximum F_A
throughput (F_A)	70 kmol/h[a]	100 kmol/h[a]	170 kmol/h[a]	182.1 kmol/h[b]	188.7 kmol/h[c]
V_{rxr}	6 m^3 (max)	6 m^3 (max)	6 m^3 (max)	6 m^3 (max)	6 m^3 (max)
T_{rxr}	63.66 °C	70.3872 °C	100 °C (max)	100 °C (max)	100 °C (max)
$[x_A/x_B]^{RxrIn}$	2.274	2.3378	1.831	1.655	1.564
L_1	~0 kmol/h	~0 kmol/h	~0 kmol/h	~0 kmol/h	~0 kmol/h
yield (A → C)	99.21%	99.17%	98.49%	98.30%	98.17%
profit per year	\$1.94 × 10^6	\$2.876 × 10^6	\$4.237 × 10^6	\$4.382 × 10^6	\$4.354 × 10^6
active constraints	V_{rxr}^{MAX}	V_{rxr}^{MAX}, Q_{reb1}^{MAX}	V_{rxr}^{MAX}, Q_{reb1}^{MAX}, T_{rxr}^{MAX}	V_{rxr}^{MAX}, Q_{reb1}^{MAX}, T_{rxr}^{MAX}	V_{rxr}^{MAX}, Q_{reb1}^{MAX}, T_{rxr}^{MAX}, Q_{reb2}^{MAX}
unconstrained degrees of freedom	2	1	0	1	0
self-optimizing controlled variables	T_{rxr}, $[x_B]^{RxrIn}$	$[x_B]^{RxrIn}$	–	$[x_B]^{RxrIn}$	–

[a] F_A is specified. [b] F_A is also optimized for maximum operating profit. [c] Maximum achievable throughput.

We consider two main modes of operation: mode I, with a given throughput (given fresh A feed processing rate), and mode II, where the throughput is a degree of freedom. Optimization is first performed for three cases of mode I with specified fresh A feed processing rates (F_A) of (a) 70, (b) 100, and (c) 170 kmol/h. The process operation is also optimized for mode II with F_A also being an optimization variable for (a) maximum operating profit and (b) maximum fresh A processing rate (i.e., maximum F_A). Case b in mode II (maximum throughput) is generally economically optimal for chemical processes operating in a "seller's market" with high demand and high product prices. The optimization is performed using the fmincon subroutine in Matlab with Hysys as the steady-state flow sheet solver.

The optimization problem including cost data and process constraints along with results for the five cases is summarized in Table 2. A maximum reactor temperature constraint is imposed due to practical considerations of catalyst deactivation or excessive vaporization, etc. In all cases, the maximum reactor holdup constraint (V_{rxr}^{MAX}) is active and the recycle column reflux is close to zero. In case b (F_A = 100 kmol/h), in addition, the maximum boilup for the recycle column (Q_{reb1}^{MAX}) is active. In case c with F_A = 170 kmol/h, the maximum reactor temperature constraint (T_{rxr}^{MAX}) further becomes active. With F_A as an optimization variable for maximizing profit, the T_{rxr}^{MAX}, Q_{reb1}^{MAX}, and V_{rxr}^{MAX} constraints remain active, and the optimum processing rate of F_A is 182.1 kmol/h (mode II, optimum profit). Increasing the feed rate beyond this value reduces the profit for the given prices. This occurs because the relative increase in side product D formation dominates over main product C formation so that the raw material consumption goes up without a commensurate increase in the product rate. This is an example of a process where the market conditions are such that maximizing production is not equivalent to maximizing economic profit. The market, however, is dynamic and may change toward a substantially higher product price or byproduct credit, in which case the optimal processing rate would increase. Nevertheless, even with infinite product prices there is a maximum achievable throughput as given by the operational constraints. This occurs when the maximum product column boilup (Q_{reb2}^{MAX}) constraint becomes active and there are no remaining unconstrained degrees of freedom. The resulting maximum achievable fresh A processing rate (F_A) for the process is 188.7 kmol/h (mode II, maximum throughput).

From the set of active constraints over the complete range of F_A processing rates, the process operation may be divided into low processing rates (only V_{rxr}^{MAX} active), intermediate processing rates (V_{rxr}^{MAX} and Q_{reb1}^{MAX} active), high processing rates (V_{rxr}^{MAX}, Q_{reb1}^{MAX}, and T_{rxr}^{MAX} active), optimal processing rate ((V_{rxr}^{MAX}, Q_{reb1}^{MAX}, and T_{rxr}^{MAX} active), and maximum processing rate (V_{rxr}^{MAX}, Q_{reb1}^{MAX}, T_{rxr}^{MAX}, and Q_{reb1}^{MAX} active). These operating regions have been termed as mode Ia, mode Ib, mode Ic, mode IIa, and mode IIb, respectively. Also, mode IIa (optimum processing rate) lies in the throughput range for mode Ic (high processing rates), whereas mode IIb (maximum processing rate) corresponds to the maximum rate for mode Ic. Also, the active constraint set at the economic optimum remains unaltered for small variations in the price data, for example, a waste disposal penalty on the byproduct stream or fluctuations in energy prices (energy prices used here are on the lower side).

The results in Table 2 may be interpreted as follows. The V_{rxr}^{MAX} active constraint in all modes maximizes the reactor single-pass conversion for a given T_{rxr}. The maximum recycle

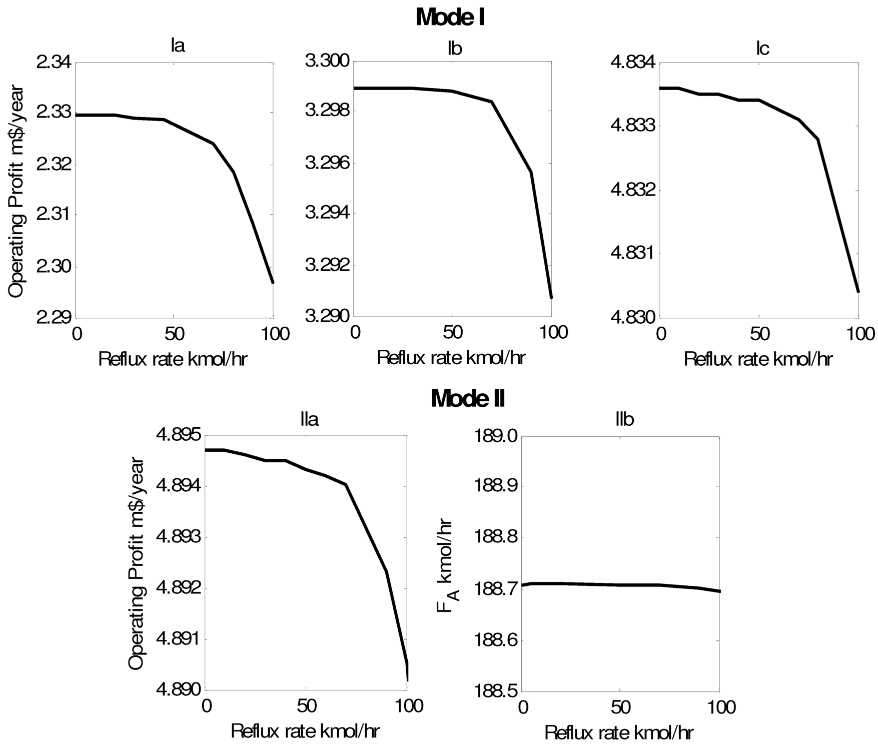

Figure 3. Sensitivity of economic criterion to recycle column reflux.

column boilup (Q_{reb1}^{MAX}) constraint in mode Ib/Ic and mode II maximizes the recycle rate (mostly component A) to suppress the side reaction for increased yield to desired product. In mode Ia/Ib, the reactor temperature is unconstrained. A decrease in temperature causes the single-pass reactor conversion to decrease so that the recycle energy cost increases in mode Ia (Q_{reb1}^{MAX} not active) while in mode Ib (Q_{reb1}^{MAX} active) the recycle stream contains more unreacted B adversely affecting the yield. On the other hand, an increase in reactor temperature causes the throughput to increase at the expense of a lower yield in both mode Ia and mode Ib. The penalty due to the decreased yield is, however, offset by the increased production of the value-added product C. In mode Ic, the T_{rxr}^{MAX} constraint is active and an increase in throughput requires an increase in the reactor limiting reactant composition so that the throughput increase is again at the expense of a lower yield. For the specific cost data used, the decrease in yield causes the maximum throughput solution (F_A = 188.7 kmol/h) to be slightly less profitable than the optimum throughput solution (F_A = 182.1 kmol/h).

The optimization results in Table 2 also show that the liquid reflux in the first column is close to zero in all operating modes. This is further illustrated in Figure 3, which explores the variation in the economic criterion as the reflux rate specification in the recycle column (L_1) is varied around the optimum for each operating mode. The economic criterion is close to maximum and relatively insensitive to changes in L_1 for L_1 < 20 kmol/h. The simplest choice of no reflux (i.e., L_1 = 0) appears close to optimal regardless of the operating mode. This choice is equivalent to recycle column operation as a stripper with no rectification, which takes away one degree of freedom. The flatness of the profit curve as the recycle column reflux is decreased is due to two opposing effects. For a fixed recycle column boilup (maximum in modes Ib/Ic and II), as the reflux rate is reduced, the recycle rate (mostly A) increases, which causes the reactor feed A/B ratio to increase, suppressing the side reaction. On the other hand, the C recycle rate increases, promoting the side reaction. For the kinetics and base-case design used in this work, it turns out that the two opposing effects cancel each other so that the plant operating profit remains about the same as the recycle column approaches the stripper limit. This may not be the case if the reaction rate constant ratio of the main and side reactions is significantly lower.[11]

2.3. Unconstrained Degrees of Freedom and Choice of Economic Controlled Variables (CVs). For every constraint that becomes active, a steady-state degree of freedom gets exhausted to drive the constraint to its limit. There are originally eight degrees of freedom, but four of these are needed to satisfy the chosen specifications on the columns, including recycle column operation as a stripper (L_1 = 0). In mode Ia, the V_{rxr}^{MAX} active constraint and F_A specification imply two remaining unconstrained degrees of freedom. In mode Ib, the additional Q_{reb1}^{MAX} active constraint implies one unconstrained degree of freedom. In mode Ic, the three active constraints (V_{rxr}^{MAX}, T_{rxr}^{MAX}, and Q_{reb1}^{MAX}) along with the F_A specification consume all four degrees of freedom. In mode IIa, the three active constraints (V_{rxr}^{MAX}, T_{rxr}^{MAX}, and Q_{reb1}^{MAX}) leave one unconstrained degree of freedom, which is the optimal value of F_A. Finally, in mode IIb, there are four active constraints (V_{rxr}^{MAX}, T_{rxr}^{MAX}, Q_{reb1}^{MAX}, and Q_{reb2}^{MAX}) and no degrees of freedom are left (F_A depends on the values of the active constraints).

In terms of control, we need to identify controlled variables (CVs) associated with each of the eight steady-state degrees of freedom. Clearly, the active constraints should be selected as CVs with the goal of keeping them close to their limiting values. For the unconstrained degrees of freedom there is no obvious choice, but in each operation mode the associated CVs should be chosen

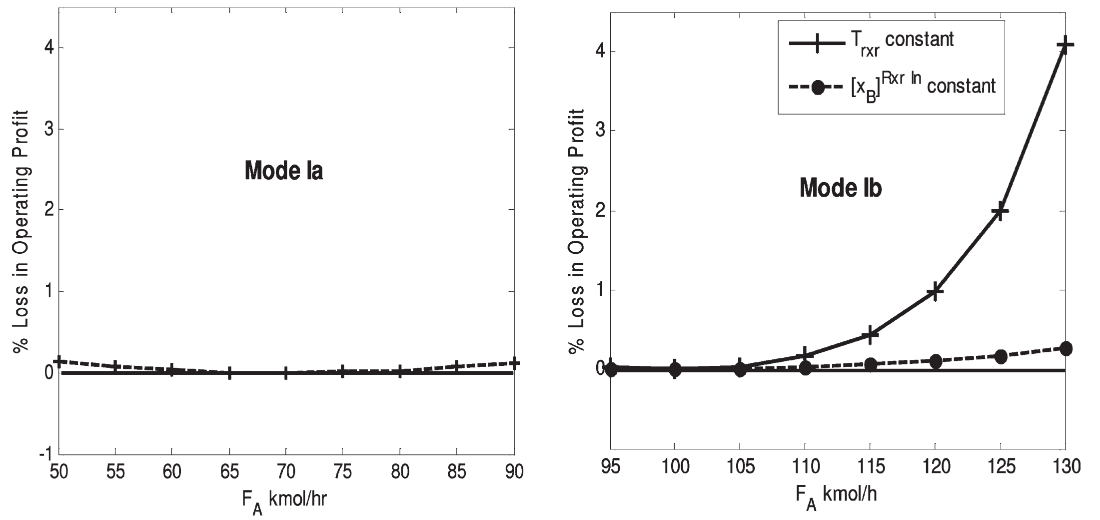

Figure 4. Percentage loss in profit for process operation at constant T_{rxr} and/or constant $[x_B]^{RxrIn}$. (left) Mode Ia: loss with both T_{rxr} and $[x_B]^{RxrIn}$ constant. (right) Mode Ib: loss with either T_{rxr} constant or $[x_B]^{RxrIn}$ constant.

with the goal of driving the economic criterion toward optimality. For example, the choice should be such that the economic criterion is relatively insensitive to a change in its specification. A more rigorous approach is to consider different disturbance scenarios and reoptimize the unconstrained degree of freedom with the disturbance. For different choices of the unconstrained independent variable, a comparison of the economic performance with and without reoptimization would reveal variable choices that are "self-optimizing", where the economic loss is negligible or acceptable with the variable held constant (i.e., not reoptimized). Self-optimizing variables significantly simplify process operation, obviating the need for a real-time optimizer to specify the unconstrained independent variable.

In mode I (a/b), there are (two/one) unconstrained degrees of freedom and we need to identify (two/one) "self-optimizing" controlled variables (CVs). Intuitively, the reactor temperature and the composition of the reactor feed may be good self-optimizing variables. For a quantitative analysis, Figure 4(left) plots the percentage profit loss as F_A is varied over the mode Ia throughput range from 50 to 90 kmol/h while holding the reactor feed composition $[x_B]^{RxrIn}$ and the reactor temperature T_{rxr} at the calculated optimum for F_A = 70 kmol/h. The profit loss is calculated from the fully optimized solution (both T_{rxr} and $[x_B]^{RxrIn}$ are reoptimized). The loss in profit as F_A is varied by $\pm$20 kmol/h around 70 kmol/h is less than 0.2%, confirming that T_{rxr} and $[x_B]^{RxrIn}$ are indeed good self-optimizing variables for the two unconstrained degrees of freedom in mode Ia.

In mode Ib, there is only one unconstrained degree of freedom. To choose between $[x_B]^{RxrIn}$ and T_{rxr}, Figure 4(right) plots the percentage profit loss as F_A is varied over the mode Ib throughput range with the recycle column boilup at its constraint value (Q_{reb1}^{MAX}) holding $[x_B]^{RxrIn}$ at its calculated optimum for F_A = 100 kmol/h and, complementarily, holding T_{rxr} at its calculated optimum for F_A = 100 kmol/h. The loss in profit when T_{rxr} is held constant blows up much faster than when $[x_B]^{RxrIn}$ is held constant. Specifically, as F_A is increased to 130 kmol/h, the loss in profit is only 0.3% when $[x_B]^{RxrIn}$ is held constant while the corresponding value when T_{rxr} is held constant is 4%. $[x_B]^{RxrIn}$ is therefore the better self-optimizing variable and is used to exhaust the one remaining degree of freedom for mode Ib.

With regard to mode II operation where F_A itself is a degree of freedom, all degrees of freedom are exhausted for process operation at maximum throughput (mode IIb) while one degree of freedom remains for maximum profit process operation (mode IIa). The reactor feed B composition ($[x_B]^{RxrIn}$) is considered a reasonable self-optimizing variable for mode IIa with only a 0.2% profit loss for a 5 mol % heavy impurity, *S*, in the fresh B feed. Other choices for the self-optimizing variable are the yield to desired product (selectivity) and reactor A/B excess ratio, which result in a much lower profit loss (<0.02%) for the same disturbance. These are, however, more complex measurements and are therefore rejected in favor of $[x_B]^{RxrIn}$.

3. PLANTWIDE CONTROL STRUCTURES

3.1. Interaction between Regulatory and Supervisory Control Layers. The main objective of the regulatory control layer is to ensure stable and safe process operation. Ideally it should be designed independent of the economic control objectives which may vary depending on disturbances and market conditions. However, it is well established that the regulatory control layer configuration can significantly impact the transients in active constraint variables as well as the tightness of active constraint control by forcing certain input−output pairings in the supervisory layer. This then translates to the need for a regulatory structure dependent back-off from the constraint limit to avoid hard constraint violation during transients. How close the process can be driven to the active constraint limit thus depends on the regulatory control system which in turn determines the achievable profitability. A priori knowledge of the active constraints at economic optimum may be exploited for "top-down" design of a regulatory control structure that minimizes the back-off in the economically dominant active constraints.

In our example, as the throughput is increased, economic considerations cause a progressive increase in the number of active constraints. Based on the desired throughput, the process must be operated to drive it as close as possible to these active constraints for maximum profitability (mode Ia/Ib/Ic and mode IIa/IIb in the present case study). The required switching of controlled variables and pairings is the task of the supervisory

dx.doi.org/10.1021/ie1024358 |*Ind. Eng. Chem. Res.* 2011, 50, 8571–8584

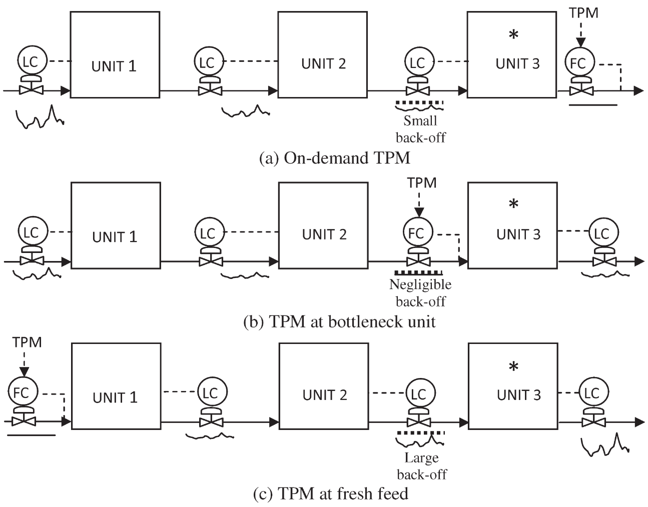

Figure 5. Orientation of inventory control loops around TPM and propagation of flow transients. An asterisk (∗) indicates a bottleneck unit.

layer. Note that the dimensionality of this supervisory task is set by the number of active constraints (operating mode).

3.2. Throughput Manipulator (TPM). A very important decision for plantwide control is the location of the throughput manipulator (TPM).[12] Aske and Skogestad[13] define the TPM as "a degree-of-freedom that affects the network flow which is not directly or indirectly determined by the control of the individual units, including their inventory control". Normally, the throughput is set by the operator, and the TPM set point is the degree of freedom adjusted to achieve the desired throughput (e.g., to get F_A = 70 kmol/h in mode Ia). A fresh feed flow set point is preferred by operators for throughput manipulation as it directly fixes the feed processing rate (throughput). Other than operator preference and specific processing requirements that fix the TPM location at say the product stream for on-demand operation or at the feed stream due to upstream supply constraints, there is no restriction on the TPM location and it may be chosen anywhere inside the plant. The location is important, first due to its effect on economics as demonstrated later in the case study and, second, because it dictates the orientation of the inventory (level and pressure) control loops to radiate around the TPM[13] (see Figure 5), directly affecting the rest of the control system. Note that an explicit throughput manipulator (TPM) is necessary in mode I operation for holding the fresh A processing rate at the desired value. In mode II operation, there is no explicit TPM with the production rate being set by optimal economics.

Which variable should be used as the TPM? In the plantwide control literature, it is recommended the TPM be located close to and, where possible, at the bottleneck/economically dominant active constraint for economic operation.[9,14] As illustrated in Figure 5, the regulatory control system then propagates flow transients away from the constraint due to the orientation of the inventory loops radiating outward from TPM. This naturally propagates the transients away from the bottleneck for a reduced back-off and consequent economic loss.

In our example, an extension of this insight is necessary for the multiple constraints that successively become active as the throughput is increased. *A simple guideline to minimize the back-off is to locate the TPM at the next constraint to become active as the throughput is increased.* If the next active constraint is a controlled variable (CV), then its associated manipulated variable (MV) must be located "close" such that tight control is possible. However, moving the TPM generally requires rearranging inventory loops because of the radiation rule, unless it is moved to an unconstrained CV that is given up on reaching the constraint, which is the case in the example considered here.

The guideline is based purely on economic back-off considerations, and the idea is to set up a control strategy that is "ready" to achieve tight control of the active constraint when it becomes active. Implementation necessarily requires the TPM location to move as the active constraint set changes, which may not be appreciated by operators. In general, however, the choice of the TPM location is flexible and this flexibility is gainfully exploited in the guideline for economic benefit. The economic benefit should justify the change in TPM location, and due care must be exercised to confirm that the regulatory control performance of the resulting control structure is acceptable. Instead of moving the TPM, the possibility of configuring a loop for tight control of the constraint that becomes active should also be explored.

3.3. Regulatory Control Issues. The purpose of the regulatory layer is to "stabilize" the plant using a simple control structure with single-loop proportional integral derivative controllers. Preferably, the regulatory layer should be independent of the economic control objectives and operating modes. First, one must identify the "stabilizing" CVs and next choose the pairing, i.e., the MVs used to control these. The pairing issue is not always simple due to possible conflicting objectives that need to be taken into account. First, the TPM cannot be used for regulatory control. Next, we need a radiating inventory control system around the TPM to have local consistency. Third, we should avoid using variables that may become active (for a disturbance) for regulatory tasks, because otherwise (1) back-off would be required to maintain control or (2) the regulatory loops would have to be reconfigured.

For our process, the reactor level and temperature along with the operating pressure, condenser level, reboiler level, and sensitive temperature for the two columns are identified as the stabilizing variables. Note that the set points of these CVs generally are degrees of freedom for economic (steady-state) operation, with the exception of the levels in the columns, which have no steady-state effect, and the column pressures, which are assumed to be slightly above atmospheric. The set points of the column temperature controllers may be used for composition control. The details of the control structures depend strongly on the location of the TPM, and four alternatives for mode Ia are discussed below.

3.4. Alternative Regulatory Control Structures (Mode Ia). The choice of the TPM is central to the design of a consistent regulatory control system for a process. To ensure consistency, a proper understanding of the adjustment (direct/indirect) necessary in the reactor operating conditions to effect a throughput change is a must as the reactor is where the reactants are consumed and the value-added product is generated. For the reactor, its holdup, temperature, and A and B compositions are the four independent variables (corresponding to the four steady-state degrees of freedom for the process, excluding columns) that determine the reaction rate(s) inside the reactor. The V_{rxr} and T_{rxr} set points of the respective stabilizing reactor control loops are possible TPMs that effect an immediate change in the production rate inside the reactor. The other option is to alter the reactor A and/or B composition. This may be done by altering the two fresh feeds directly or one fresh feed and another process flow stream or two process flow streams inside the process. Assume that one of the fresh feeds gets used to maintain the two fresh feeds in ratio as dictated by the main reaction stoichiometry, with the ratio set point being adjusted to maintain $[x_B]^{RxrIn}$ (mode Ia/Ib self-optimizing variable), which is the most direct and dynamically fastest way of regulating the same. The wild fresh feed flow controller set point is then a possible TPM. The $[x_B]^{RxrIn}$ set point is also a possible TPM.

Of the various TPM possibilities in mode I, the V_{rxr} set point is not available since economic considerations dictate reactor operation at maximum holdup in all operation modes. The T_{rxr} set point can only be used as the TPM in mode Ib as it is a self-optimizing variable for mode Ia and is an active constraint in mode Ic. Similarly, the $[x_B]^{RxrIn}$ set point can only be used as a TPM in mode Ic (self-optimizing in mode Ia/Ib).

Based on the TPM guideline given above, a good choice for the TPM in mode Ia is the recycle column steam flow controller set point since the recycle column boilup (Q_{reb1}) reaching its maximum is the next constraint to become active. Consequently, as throughput is increased to transition to mode Ib, no back-off from the Q_{reb1}^{MAX} limit is needed. Also, no back-off is required in the other modes (mode Ic and mode II) where the Q_{reb1}^{MAX} constraint is active.

In addition to Q_{reb1} as the regulatory layer TPM, three other alternative TPM choices are considered here, which are the feed to the recycle column (F_{col1}), the total flow to the reactor (F_{rxr}), and the fresh A feed (F_A), the latter being preferred by operators as the most direct way of setting the process throughput. The former two correspond to fixing a flow inside the recycle loop recommended by Luyben[15] as a means of mitigating snowballing and using the flow set point as the TPM. For each choice of the TPM, the regulatory control system is designed around it to achieve consistent inventory control.[13] The resulting control structures are shown in Figure 6 and labeled, in order, CS1−CS4 and are suitable for operating the process in the feasible operating space away from process constraint limits without any supervisory controllers. Note that snowballing is not an issue in CS4, where the fresh feed is set with the maximum recycle column boilup (Q_{reb1}^{MAX}) fixing the recycle flow rate. Similarly, flow controlling Q_{reb1}, the TPM in CS1, is equivalent to fixing the recycle flow rate.

In CS1, the use of the recycle column steam as the TPM makes it unavailable for column temperature control, forcing the column fresh feed (F_{col1}) to be used for the purpose. This temperature controller prevents excess B leakage down the bottoms which would end up contaminating the product stream. The column tray temperature controller set point is adjusted to maintain the B impurity in the product stream in a cascade arrangement. The CSTR level is controlled by adjusting the fresh B stream (F_B) and F_A is maintained in ratio with F_B. The ratio set point is adjusted by a composition controller that maintains $[x_B]^{RxrIn}$. The reactor temperature is controlled by adjusting the reactor cooling duty. The condenser level in the two columns is maintained by manipulating the respective distillate streams, and the condenser pressure is maintained by adjusting the condenser duty. The sump level in the recycle column is maintained by adjusting the bottoms flow. The control structure for the product column is largely independent of the rest of the process. Its sump level is maintained by adjusting the boilup since the bottoms byproduct stream has a very small flow rate, making it less suitable for level control. An average temperature of three sensitive trays in the stripping section is maintained by adjusting the bottoms rate. This temperature set point is adjusted to hold the C recovery in the bottoms constant. The reflux in the product column is maintained in ratio with the column feed. This ratio set point is adjusted to maintain the D impurity mole fraction in the distillate product.

In CS2, the use of flow to the recycle column (F_{col1}) as the TPM allows for conventional single ended temperature control using the reboiler duty in the recycle column. The remainder of the control structure is very similar to CS1. In CS3, since the total flow to the reactor (F_{rxr}) is held constant by adjusting F_B with the flow set point acting as the TPM, the reactor level controller is in the direction of process flow and manipulates the recycle column feed. The remainder of the control structure is very similar to CS2. In the last "conventional" control structure, CS4, with F_A set point as the TPM, F_B is maintained in ratio with F_A with the ratio set point being adjusted by the reactor feed composition controller. The reactor level controller manipulates the recycle column feed, and the remaining control structure is similar to CS3.

3.5. Supervisory Control: Extension of the Control Structures to Other Modes. Each of the regulatory control structures (CS1−CS4) is suitable for process operation in mode Ia (low throughput), where only the V_{rxr}^{MAX} constraint is active. Economic considerations, however, dictate that the process be driven toward additional "active" constraints as the throughput is increased, eventually exhausting the available steady-state operating degrees of freedom at maximum throughput. This requires switching of controlled variables, reassignment of input pairings, and, in some cases, moving the location of the throughput manipulator (TPM). These are some of the main tasks of the supervisory control layer.

The first additional constraint to become active as the throughput is increased to transition from mode Ia to mode Ib is the reboiler duty in the recycle column (Q_{reb1}^{MAX}). In CS1, this corresponds to simply setting the Q_{reb1} set point at Q_{reb1}^{MAX} with no back-off needed, so there is no economic loss. However, Q_{reb1} cannot be the TPM any more and we need to find a new TPM in mode Ib. Since T_{rxr} is the next constraint to become active (transition to mode Ic) and it is in fact the unconstrained CV that is given up on reaching the Q_{reb1}^{MAX} constraint, the T_{rxr} set point is available for throughput manipulation. It is therefore chosen as the mode Ib TPM. The throughput manipulation task is thus taken over by T_{rxr} with Q_{reb1} fixed at its maximum.

In CS2, Q_{reb1} is used for stabilizing control of the recycle column temperature. As the throughput is increased and Q_{reb1} approaches its maximum limit, we still need to maintain control of this temperature. The closest available degree of freedom is the column feed rate F_{col1}, which is the TPM in mode Ia. In mode Ib, either we can set Q_{reb1} at its maximum and use F_{col1} for controlling the column temperature (identical to CS1), or we can use F_{col1} as the manipulated variable to hold Q_{reb1} close to the maximum constraint. The first option gives back structure CS1, so the latter option is chosen. This option avoids the need to reassign the temperature loop but requires back-off for the duty. Given the closeness of the manipulation to the active constraint location, the open loop dynamics would be fast, allowing for tight recycle column boilup control with a consequently small back-off. Similar to CS1, F_{col1} is no longer available for throughput manipulation, so the reactor temperature T_{rxr} is selected as the TPM in mode Ib.

As in CS1 and CS2, F_{rxr} ceases to be the mode Ib TPM for CS3. It is then manipulated to maintain Q_{reb1} (active constraint) close to its maximum and T_{rxr} is used as the mode Ib TPM.

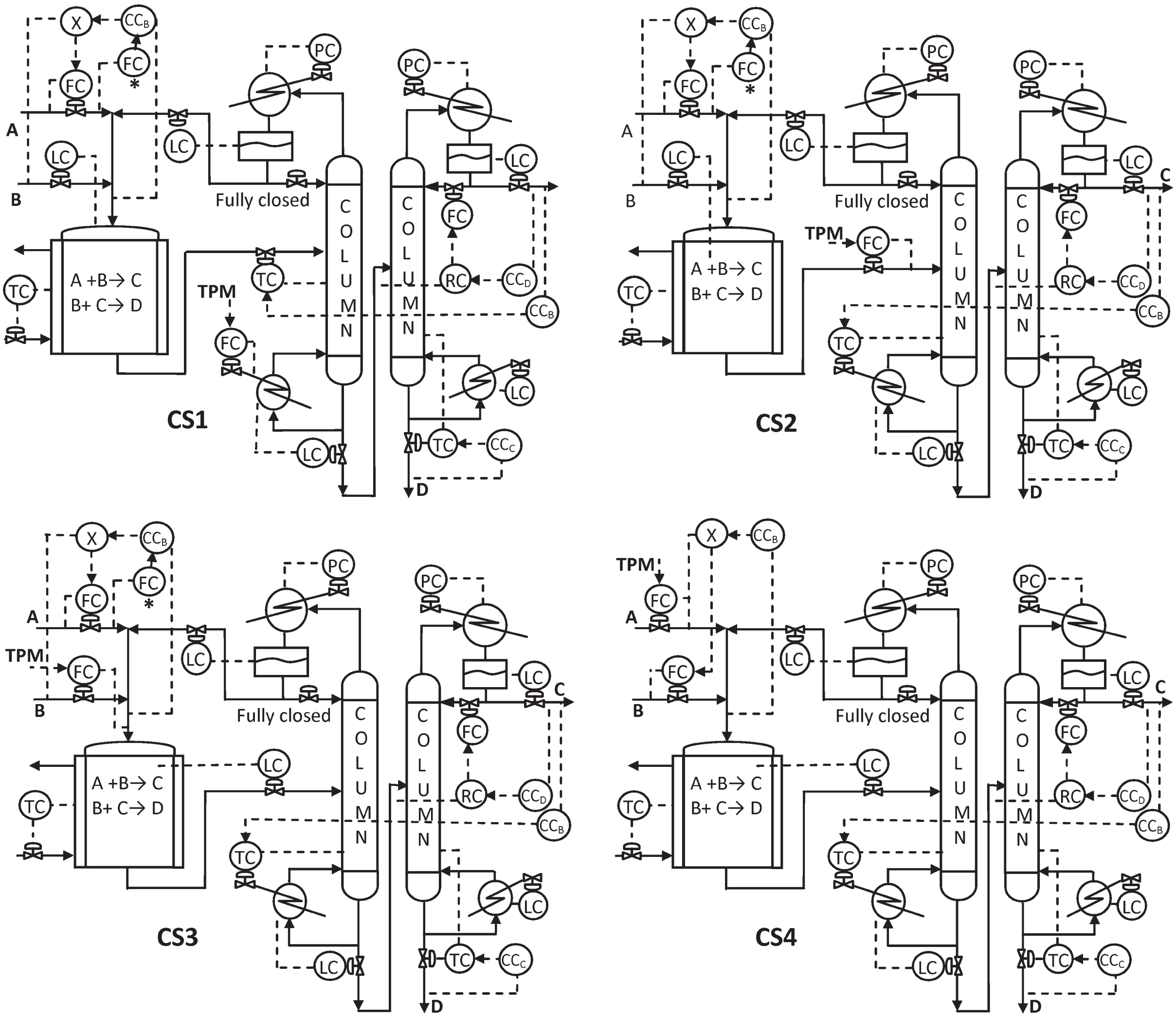

Figure 6. Plantwide regulatory control structures studied (for mode Ia operation). An asterisk (∗) indicates FC adjusting CC_B set point to get desired F_A processing rate.

In CS4, the feed rate F_A is the throughput manipulator. We would like to keep it as the TPM also in mode Ib to evaluate economic process operation using the traditional scheme of keeping the TPM fixed at a fresh feed regardless of the active constraint set (operating mode). In addition, since F_A is quite far removed from the recycle column, it would not be suitable for taking over column control tasks when the reboiler duty saturates in mode Ia. Instead, T_{rxr} is manipulated to maintain Q_{reb1} close to its maximum in mode Ib.

As the throughput is increased in mode Ib, T_{rxr} approaches its maximum limit. A further increase in T_{rxr} is then not possible, and a new throughput manipulator needs to be identified for structures CS1−CS3 in mode Ic. Even as Q_{reb2} is the next constraint to become active, shifting the TPM to Q_{reb2} would require significant reconfiguration of loops as Q_{reb2} is already used for maintaining the product column bottoms purity (indirectly through the action of the level loop). The simplest choice, in terms of avoiding reconfiguration of loops, is to use the $[x_B]^{RxrIn}$ set point as the TPM, controlling which in mode Ic must be given up with all degrees of freedom exhausted. Changing the $[x_B]^{RxrIn}$ set point changes the feed rate F_A, which could alternatively have been chosen as the TPM in mode Ic. However retaining the composition loop for $[x_B]^{RxrIn}$ requires less change with the additional advantage of better regulation of the reactor conditions.

In CS4, since T_{rxr} is no longer available for maintaining Q_{reb1} close to maximum, one may manipulate $[x_B]^{RxrIn}$ for this purpose. This ensures that the TPM location remains fixed at F_A over the entire throughput range (mode Ia/Ib/Ic), the main motivation behind considering CS4.

Further increasing the throughput in mode Ic causes the product column maximum reboiler duty constraint (Q_{reb2}^{MAX}) to be eventually approached, exhausting all the available degrees of freedom. The process then operates at the maximum achievable throughput (mode IIb). To drive the Q_{reb2} close to its maximum constraint without altering supervisory loop configurations for controlling the other active constraints, $[x_B]^{RxrIn}$ is the only adjustable regulatory layer set point. Even as this Q_{reb2}−$[x_B]^{RxrIn}$ loop is a long and slow one, the transients in Q_{reb2} are likely to be mild as the tray temperature is controlled by adjusting the bottoms flow rate, which is a very small stream. The bottoms level would thus change slowly and the change in Q_{reb2} to maintain the bottom level would be slow, implying mild transients in Q_{reb2} so that the back-off is likely to be not very large. The long Q_{reb2}−$[x_B]^{RxrIn}$ loop is thus deemed acceptable. By maintaining Q_{reb2}

Table 3. Supervisory Layer Control Loop Configuration for Different Operating Modes for CS1−CS4[a]

	mode Ia	mode Ib	mode Ic	mode IIa	mode IIb
active constraint set	V_{rxr}^{MAX}	V_{rxr}^{MAX} Q_{reb1}^{MAX}	V_{rxr}^{MAX} Q_{reb1}^{MAX} T_{rxr}^{MAX}	V_{rxr}^{MAX} Q_{reb1}^{MAX} T_{rxr}^{MAX}	V_{rxr}^{MAX} Q_{reb1}^{MAX} T_{rxr}^{MAX} Q_{reb2}^{MAX}
F_A (kmol/h)	50−95	95−165	>165	optimal:182.1	maximum: 188.7
Supervisory Layer Control Loops (CV−MV): Changes Compared to Figure [6]					
CS1	F_A-Q_{reb1}	F_A-T_{rxr}	$F_A-[x_B]^{RxrIn}$	$[x_B]^{RxrIn}-F_A$	$Q_{reb2}-[x_B]^{RxrIn}$
CS2	F_A-F_{col1}	$Q_{reb1}-F_{col1}$ F_A-T_{rxr}	$Q_{reb1}-F_{col1}$ $F_A-[x_B]^{RxrIn}$	$Q_{reb1}-F_{col1}$ $[x_B]^{RxrIn}-F_A$	$Q_{reb1}-F_{col1}$ $Q_{reb2}-[x_B]^{RxrIn}$
CS3	F_A-F_{rxr}	$Q_{reb1}-F_{rxr}$ F_A-T_{rxr}	$Q_{reb1}-F_{rxr}$ $F_A-[x_B]^{rxrIn}$	$Q_{reb1}-F_{rxr}$ $[x_B]^{RxrIn}-F_A$	$Q_{reb1}-F_{rxr}$ $Q_{reb2}-[x_B]^{RxrIn}$
CS4		$Q_{reb1}-T_{rxr}$	$Q_{reb1}-[x_B^{RxrIn}]$	$Q_{reb1}-[x_B^{RxrIn}]$ $[x_B]^{RxrIn}-F_B/F_A$	$Q_{reb1}-[x_B^{RxrIn}]$ $Q_{reb2}-F_A$
set points	V_{rxr}: $V_{rxr}^{MAX}-\Delta$	V_{rxr}: $V_{rxr}^{MAX}-\Delta$ Q_{reb1}: $Q_{reb1}^{MAX}-\Delta$	V_{rxr}: $V_{rxr}^{MAX}-\Delta$ Q_{reb1}: $Q_{reb1}^{MAX}-\Delta$ T_{rxr}: $T_{rxr}^{MAX}-\Delta$	V_{rxr}: $V_{rxr}^{MAX}-\Delta$ Q_{reb1}: $Q_{reb1}^{MAX}-\Delta$ T_{rxr}: $T_{rxr}^{MAX}-\Delta$	V_{rxr}: $V_{rxr}^{MAX}-\Delta$ Q_{reb1}: $Q_{reb1}^{MAX}-\Delta$ T_{rxr}: $T_{rxr}^{MAX}-\Delta$ Q_{reb2}: $Q_{reb2}^{MAX}-\Delta$

[a] Δ, back-off to avoid transient constraint violation. TPM = MV used for controlling F_A (TPM = F_A for CS4).

as close as possible to its maximum, the process operates at the maximum achievable throughput and there is no explicit TPM in mode IIb.

Normally, the profit increases as we increase the throughput because of the price difference between products and feeds. However, because of constraints, the operation tends to become less efficient. With the throughput as a degree of freedom (mode II), we found an optimal feed rate that gives maximum steady-state profit (mode IIa). To exhaust the one unconstrained degree of freedom in mode IIa, $[x_B]^{RxrIn}$ was found to be a reasonable self-optimizing variable. Since the optimum throughput lies in the throughput range for mode Ic, the only alteration necessary compared to mode Ic is to close a loop that involves adjusting the TPM set point to keep $[x_B]^{RxrIn}$ constant. The action of this loop ensures that the process throughput adjusts to near optimum.

The supervisory loops and reactor holdup/temperature set point that must be implemented on top of the regulatory control structures CS1−CS4 for each of the four operation modes are summarized in Table 3. Table 3 also shows how the throughput manipulator (TPM) is moved depending on the control structure and operation modes.

From Table 3, notice that, to transition between the different operating regions in mode I, only the TPM location is moved in CS1 and no additional supervisory active constraint control loops need to be implemented. In contrast, for CS2−CS3, in addition to moving the TPM, a supervisory active constraint control loop needs to be configured when Q_{reb1}^{MAX} constraint becomes active. In CS4, the TPM is kept fixed at F_A regardless of the active constraint set and a Q_{reb1} active constraint control loop is implemented. Thus, in terms of mode I supervisory loop reconfigurations, CS1 is the simplest. In mode IIb, an additional Q_{reb2} active constraint control loop needs to be implemented in all the structures. For reasons of simplicity, one can always choose not to implement these additional supervisory active constraint controllers. The worst-case transients in the uncontrolled active constraints would then be more severe, necessitating a higher back-off and a consequent economic loss.

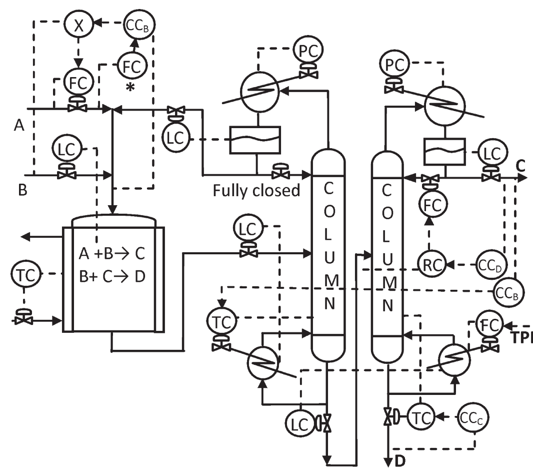

Figure 7. Regulatory control structure with Q_{reb2} as TPM. The asterisk (∗) indicates FC adjusting CC_B set point to get desired F_A processing rate.

3.6. Other Control Structure Possibilities. It is worth highlighting that a regulatory control system may be designed using the last constraint to become active, the product column boilup, as the TPM as shown in Figure 7 (CS5). This requires the inventory control system for the rest of the plant to be in the opposite direction of flow. With the product column boilup under flow control, the column base level is controlled using the feed to the column. The recycle column base level is then controlled using its feed, and the column temperature is controlled using the boilup. The reactor level is controlled using F_B with F_A being maintained in ratio with F_B. The ratio set point is adjusted to maintain $[x_B]^{RxrIn}$. In mode Ib, T_{rxr} is adjusted to maintain Q_{reb1} near maximum while, in mode Ic, $[x_B]^{RxrIn}$ is adjusted for the same. In either case, in particular the latter one with its long loop, a back-off from Q_{reb1}^{MAX} would be necessary, adversely affecting the process yield and hence economics. Holding both Q_{reb1} and Q_{reb2} at their respective maximum constraints thus appears

Table 4. Regulatory Layer Controller Tuning[a,b,c]

controlled variable	K_C	τ_i (min)	τ_d (min)	sensor span
$[x_B]^{RxrIn}$	2	400	–	0−1
T_{rxr}	4	10	2	60−130 °C
T_{col1}	0.5	10	–	100−160 °C
T_{col2}	2	20	–	120−200 °C
reboiler 2 level	1.5	20	–	0−100%
$[x_B]^{Dist2}$	0.1	40	–	0−0.02
$[x_D]^{Dist2}$	0.1	30	–	0−0.0004

[a] All compositions have a 6 min dead time and sampling time. All temperature measurements are lagged by 2 min. [b] All level loops use K_C = 2 unless otherwise specified. [c] Pressure/flow controllers tuned for tight control.

impractical for this process. For the price data used, since the maximum throughput (mode IIb) solution is less profitable than the most profitable solution (mode IIa), and also because the severity of the transients in Q_{reb2} is mild, holding Q_{reb1} at its constraint value is deemed more important and CS1 may be considered as the best overall structure. Of course, should the economic conditions change toward a much higher product−raw material (including energy) price differential, the maximum throughput solution would be the most profitable and this on-demand control structure would likely be the best in terms of minimizing the economic loss.

4. SIMULATIONS AND INTERPRETATION

Rigorous dynamic simulation of the process for the different plantwide control structures (CS1−CS4, including supervisory layer) is performed in Hysys. A small inert N_2 stream is provided to the CSTR for stabilizing the reactor pressure to prevent the Hysys pressure flow solver from crashing in dynamics. The inlet N_2 is flow controlled while the outlet is adjusted for CSTR pressure control. The N_2 that leaks with the CSTR liquid outlet is taken out as vapor distillate from the recycle column. This purge also provides a way out for other light components that would otherwise accumulate. All controllers except the composition controller are continuous. The composition controller is sampled every 6 min and has a 6 min dead time to represent typical analytical instruments. Temperature measurements are lagged by 2 min to account for typical sensor dynamics. All pressure controllers are tuned for tight pressure control. All level controllers are Proportional only with a gain of 2 (unless noted otherwise). The temperature and composition loops are tuned heuristically for a not-too-oscillatory servo response. The tuning parameters implemented for salient loops in the regulatory layer are reported in Table 4 for CS1−CS4. The tuning parameters used in the supervisory control loops are also reported in Table 5. Before proceeding with a quantitative economic comparison of the different control structures, rigorous dynamic simulations for ±10% changes in the TPM set point in mode Ia show that all the structures work effectively with a similar plantwide response settling time of 25−30 h. These structures are therefore deemed comparable from the regulatory performance standpoint.

4.1. Quantitative Back-Off and Economic Performance Comparison. For an active constraint, the back-off is the difference between its set point and the constraint limit. Any back-off will result in an economic penalty. For each regulatory control structure with a supervisory control system on top to drive process operation close to the appropriate active constraint set, a back-off

Table 5. Supervisory Layer Control Loop Tuning Parameters

	CS1		CS2		CS3		CS4	
controlled variable	K_C	τ_i (min)	K_C	τ_i (min)	K_C	τ_i (min)	K_C	τ_i (min)
Q_{reb1}	–	–	0.3	20	0.2	30	0.2	40
Q_{reb2}	0.2	80	0.2	80	0.2	80	0.2	80
F_A	0.1	60	0.1	60	0.1	60	–	–
$[x_B]^{RxrIn}$	2	400	2	400	2	400	2	400

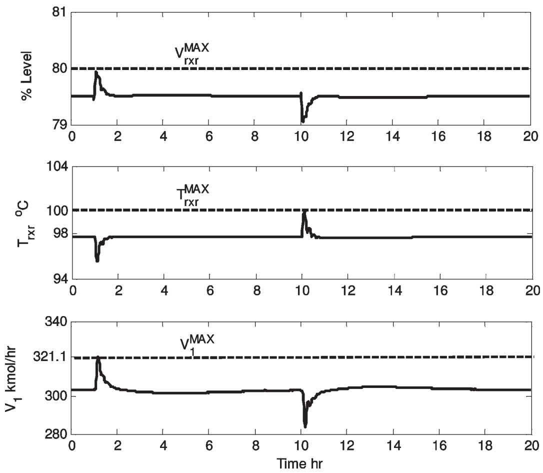

Figure 8. Illustration of back-off for CS3 (F_A = 170 kmol/h, mode Ic).

is necessary in the supervisory active constraint controller set point to avoid hard constraint violation due to transients caused by a disturbance. For the purpose of this study, all active constraint variables are considered as hard (i.e., a transient constraint violation is unacceptable). A 5 mol % heavy impurity pulse of 10 h duration in the fresh B stream is considered the worst-case disturbance. The heavy impurity ends up in the bottoms byproduct stream from the product column. The back-off in an active constraint controller set point for a particular operation mode is obtained via hit and trial so that the constraint variable just touches the constraint limit during the transient. This is illustrated in Figure 8 for CS3 for mode Ic (F_A = 170 kmol/h) operation. Notice that a back-off in recycle column boilup and reactor level is due to the transient rise when the feed B impurity level goes up. On the other hand, a back-off in the reactor temperature is necessitated due to the transient temperature rise caused by a more concentrated limiting reactant B feed when the impurity level goes back down at 10 h.

Table 6 reports for the four control structures CS1−CS4 the process parameters and steady-state yearly profits for chosen F_A values of 70 (mode Ia), 100 (mode Ib), and 170 kmol/h (mode Ic) and the optimal and maximum rates (mode IIa and mode IIb). The back-off in the active constraint variables can be read off as the difference from the maximum value. The corresponding fresh B feed rates and process yields are also given. For comparing the economic loss, the optimal solution corresponding to no back-off in any constraint variable is also reported.

In mode Ia, a small back-off occurs from V_{rxr}^{MAX}, the only active constraint, in all the control structures, which causes a negligible economic loss. Notice that F_B is slightly less than F_A in mode Ia/Ib. This is attributed to the small but relatively higher

Table 6. Salient Parameters for Backed-Off Process Operation for CS1−CS4

	F_A (kmol/h)	F_B (kmol/h)	% yield (A → C)	$[x_A/x_B]^{RxrIn}$	col 1 boilup (kmol/h)	col 2 boilup (kmol/h)	V_{rxr} (%)	T_{rxr} (°C)	profit (×10^6 \$/year)
					Mode Ia				
optimum	70	69.48	97.72	2.275	230.7	90.23	80.0[a]	63.66	1.942[b]
CS1	70	69.48	97.72	2.275	232	90.21	78.5	63.66	1.941
CS2	70	69.47	97.72	2.275	232.2	90.21	78.2	63.66	1.942
CS3	70	69.48	97.72	2.275	231.2	90.22	79.5	63.66	1.943
CS4	70	69.48	97.71	2.275	231.3	90.22	79.3	63.66	1.942
					Mode Ib				
optimum	100	99.660	97.71	2.338	321.1[a]	122.5	80.0[a]	70.39	2.876[b]
CS1	100	99.676	97.71	2.337	321.1	122.5	79.0	70.55	2.875
CS2	100	99.690	97.68	2.334	314.0	122.2	78.7	71.63	2.875
CS3	100	99.687	97.67	2.333	308.3	122.0	79.5	72.43	2.873
CS4	100	99.710	97.64	2.333	307.2	121.9	79.2	72.65	2.874
					Mode Ic				
optimum	170	171.5	96.27	1.831	321.1[a]	199.8	80.0[a]	100[a]	4.237[b]
CS1	170	171.6	96.26	1.763	321.1	199.9	78.3	97.6	4.229
CS2	170	171.8	96.12	1.707	313.3	200.0	77.2	97.6	4.143
CS3	170	172.1	95.90	1.651	303.3	200.2	79.5	97.7	4.026
CS4	170	172.2	95.84	1.621	299.5	200.3	79.1	97.6	3.966
					Mode IIa				
optimum	182.1	184.9	95.88	1.655	321.1[a]	209.2	80[a]	100[a]	4.382[b]
CS1	176.9	179.5	96.01	1.659	321.1	203.1	78.6	97.7	4.370
CS2	174.4	177.0	95.99	1.659	315.4	200.2	78.3	97.8	4.294
CS3	173.0	175.6	95.96	1.659	310.1	198.7	79.5	98.2	4.238
CS4	171.1	173.6	95.96	1.659	306.6	196.4	79.2	98.1	4.193
					Mode IIb				
optimum	188.7[b]	192.3	95.55	1.564	321.1[a]	215.8[a]	80.0[a]	100[a]	4.354
CS1	185.4	188.9	95.59	1.526	321.1	212.0	79.0	97.3	4.307
CS2	184.8	188.5	95.43	1.492	314.2	211.6	78.3	97.6	4.158
CS3	183.1	186.8	95.39	1.500	309.2	209.7	79.6	98.0	4.113
CS4	179.9	183.2	95.24	1.545	307.5	205.7	79.1	98.4	4.156

[a] Maximum limit. [b] Optimum value.

loss of component A (lighter than B) in the N_2 purge streams from the CSTR and the recycle column vent.

In mode Ib, the value of T_{rxr} increases from its optimal value of 70.39 °C (with no back-off) to between 70.55 (CS1) and 72.65 °C (CS4) to compensate for the back-off in reactor volume (CS1−CS4) and reboiler duty (CS2−CS4). The lower recycle from the lower reboiler duty implies a higher single-pass reactor conversion which is achieved by the higher reactor temperature. The effect of the back-off from V_{rxr}^{MAX} and Q_{reb1}^{MAX} on profit is almost negligible in mode Ib; the profit drops only slightly from its optimal value.

Once the T_{rxr}^{MAX} constraint also becomes active in mode Ic and mode II, the economic loss due to back-off becomes higher and is no longer negligible. In these modes, the back-off in V_{rxr} and T_{rxr} is in the range 0.4−1.7% and 2−3 °C, respectively. The economic loss due to the back-off in these variables is small as reflected in the small difference in the maximum mode Ic operating profit of \$4.237 × 10^6 per year (no back-off) and the mode Ic CS1 operating profit of \$4.229 × 10^6 per year (no back-off in Q_{reb1} and T_{rxr}/V_{rxr} backed off). The back-off in the recycle column boilup (Q_{reb1}) increases in order from CS1 to CS4 in the mode Ib/Ic and mode II, varying between 4.3 and 6.6% for CS4. This large decrease in recycle column boilup (i.e., lower recycle rate) translates to a noticeably lower reactor feed A/B ratio with a corresponding decrease in the process yield and hence profit. In quantitative terms, the yearly profit difference between CS1 and CS4 for mode Ic is \$0.257 × 10^6, which is a significant loss of about 6%. This loss in profit is directly attributable to the back-off in Q_{reb1}. In mode IIa (optimal throughput), the CS4 yearly profit is about \$0.19 × 10^6 less than in CS4, which is a difference of more than 4%.

The back-off in Q_{reb2} for mode IIb (maximum throughput) operation increases in order from CS1 to CS4 and is between 1.7 and 3.1%. The values are about half the back-off in Q_{reb1} due to the relatively milder transients in Q_{reb2}. The mode IIb yearly profit loss in CS4 over CS1 is about \$0.359 × 10^6, which is again significant at about 7%.

To interpret the trend in active constraint back-off (and consequently profit/throughput), notice that the original mode Ia TPM location progressively moves away from the recycle column boilup from CS1 to CS4. It is therefore not surprising that the recycle column boilup back-off increases in the order CS1 < CS2 < CS3 < CS4 in mode Ib/Ic and mode IIa/IIb. This also explains the back-off trend in Q_{reb2} for mode IIb

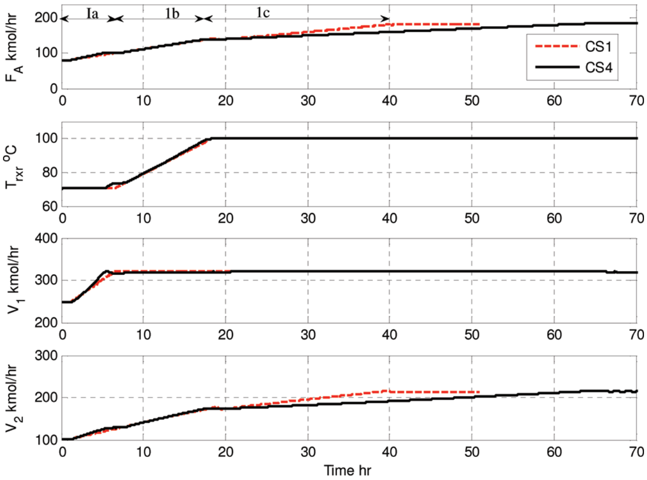

Figure 9. Smooth throughput transition using supervisory layer control configuration switching.

operation with the regulatory layer TPM location moving progressively away from the recycle column boilup in the order from CS1 to CS4.

4.2. Transition between Operating Modes. The entire throughput range from low throughputs to maximum throughput witnesses constraints progressively becoming active to exhaust all degrees of freedom at maximum throughput. Since this set of constraints is unlikely to change for a given process, a simple supervisory controller switching scheme can be implemented to transition the process throughput from low (mode Ia) to intermediate (mode Ib) to high (mode Ic) values and finally to the maximum achievable throughput (mode IIb). This simple mode transition scheme, which can be obtained directly from the supervisory controllers in Table 3 for the different modes, is briefly described for CS1 (economically best control structure) and CS4 (conventional control structure). The gradual increase in throughput is accomplished with a supervisory fresh A flow controller that adjusts the operating mode dependent regulatory layer TPM.

In CS1, the transition from mode Ia to mode Ib corresponds to moving the TPM (i.e., switching the MV for the supervisory F_A flow controller) from Q_{reb1} to the reactor temperature, T_{rxr}, when Q_{reb1} approaches its maximum limit. As the F_A set point is further increased, the T_{rxr} set point increases approaching its maximum limit (mode Ic), at which point the TPM (MV of the F_A flow controller) is switched to the reactor feed B composition set point. As the F_A set point is further increased, Q_{reb2} approaches its maximum and we have maximum throughput (mode IIb), whereby the F_A flow controller is taken offline and the reactor feed B composition set point is used as an MV to maintain Q_{reb2} close to maximum (mode IIb).

In CS4, the set point of the fresh A feed flow controller (F_A) is the TPM across the complete mode I throughput range. As the set point is increased from low F_A values (mode Ia), Q_{reb1} approaches its maximum, whereby the reactor temperature set point is used as the MV to maintain Q_{reb1} close to maximum (mode Ib). As the F_A set point is further increased, T_{rxr} approaches its maximum so that Q_{reb1} is controlled by adjusting the reactor feed B composition. As the F_A set point is further increased, Q_{reb2} approaches its maximum and the F_A set point is adjusted to maintain it near maximum for process operation at maximum throughput (mode IIb).

Figure 9 illustrates the throughput transition from low to maximum achievable using the switching scheme described above with the PI constraint controller tuning as in Table 5. The F_A set point is ramped up at a constant (but different) rate in each operating mode. The simple switching scheme accomplishes a smooth transition between the different operating modes from low to maximum throughput. It is highlighted that, in more complex cases when the active constraint set itself is uncertain, a coordinator model predictive controller[16] may be the more appropriate choice for managing the transition from a set of active constraints to the other.

A complementary logic can be applied for a throughput decrease. For example, in CS1, to transition from mode IIb (maximum throughput) to mode Ic, the Q_{reb2} controller is put on manual mode and the $[x_B^{RxrIn}]$ set point is reduced. The throughput would decrease (mode Ic) and the $[x_B^{RxrIn}]$ set point would eventually approach its mode Ib optimum, at which point the TPM is shifted to T_{rxr} with its set point being decreased to transition to mode Ib ($[x_B^{RxrIn}]$ held at its mode Ib optimum value). The throughput would decrease, and when T_{rxr} approaches its mode Ia optimum value, the TPM is shifted to Q_{reb1} (T_{rxr} held at mode Ia optimum value). Decreasing the Q_{reb1} set point would cause the transition into mode Ia operating region. A similar logic can also be devised for the other control structures.

The synthesized plantwide control structures provide a smooth transition over a large throughput range (F_A, 70 to ~187 kmol/h). With appropriate back-off in the active constraints, a change in the feed composition is also handled in all the operation modes. For most processes, throughput and feed composition changes are the primary disturbances with a "global" plantwide effect and both CS1 and CS4 are effective in terms of disturbance rejection. The far superior economic performance of CS1 due to tight control of the dominant economic constraint, (Q_{reb2}^{MAX}) serves to illustrate the close coupling between plantwide control system design and plant economics.

5. CONCLUSIONS

In conclusion, this case study on the economically optimum operation of a recycle process demonstrates that economic operation requires driving the process to the active constraints active at the optimum. For the example process, the number of active constraints at economic optimum increases progressively as the process throughput is increased until all the steady-state degrees of freedom are exhausted at maximum throughput. Supervisory constraint controllers may be used to drive the process operation as close as possible to the limits of the active constraint set. A control system, CS1, was designed for economic operation by exploiting the flexibility in TPM location to move it to the next constraint to become active as the throughput is increased. Quantitative results for the four evaluated control structures show that CS1 gives the best economic performance. Conventionally, the TPM is located at the feed and is not moved as the active constraints change. For the case study, this results in large back-off and poor economic performance, and the best choice was to locate the TPM away from the feed and also let its location vary depending on the operating region. The case study shows that proper choice of the regulatory layer TPM is the key to economical process operation. In contrast to the process studied here, work in the near future will focus on the economic plantwide control of real processes with no hypothetical components.

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Notes

†A preliminary version of this paper was presented at the 20th European Symposium on Computer Aided Process Engineering, June 6−9, 2010, Ischia, Naples, Italy.

ACKNOWLEDGMENT

The financial support from the Department of Science and Technology, Government of India, and the Erasmus EU−India exchange program is gratefully acknowledged.

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