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Plantwide Control to Economic Optimum of a Recycle Process with Side Reaction[#]

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Abstract

Plantwide control system design for economically optimum operation of a recycle process with side reaction, consisting of a 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 till all steady state degrees of freedom are exhausted at the maximum throughput. A simple strategy of moving the throughput manipulator to the next constraint to become active as throughput is increased is used to minimize the variability and hence back-off in the active constraint variables for economically optimal operation. The plantwide control system, CS1, so obtained is quantitatively compared with three other reasonable control systems (CS2-CS4) for the back-off necessary to avoid hard constraint violation for a worst case disturbance. Results show that the most economical operation is achieved using CS1 and the conventional scheme of fixing throughput at the feed (CS4) gives significantly higher economic loss. A simple switching scheme to transition from low to maximum throughput is demonstrated.

Keywords: Plantwide control, control system design, optimal operation

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1. Introduction

The plantwide control system for chemical processes typically consists of a regulatory layer that ensures safe and stable operation and an "economic" control layer on top for ensuring economically optimal operation. The 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 to drive them as close as possible to their limiting values. Model predictive control (MPC) is often used for the control function in the economic layer. In addition to these two layers, a real-time optimization layer may be further added to adjust key unconstrained setpoints 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 (Skogestad, 2000) 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 considerations are inadvertently ignored. 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 operation. Based on this concept, a systematic "top-down bottom-up" design procedure that uses *apriori* knowledge of active constraints at the economic optimum to synthesize the regulatory control system has been proposed [2,3]. Skogestad [4] has also proposed the idea of "self-optimizing" controlled variables which are chosen or designed such that holding these constant (i.e. at setpoint) causes negligible / 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 [5-7].

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 appropriate supervisory and regulatory control system 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 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[8] show that both the choice of the regulatory control structure and 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.

In this work, plantwide control for economically optimum operation of a more realistic recycle process with side reaction is considered. 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 till at maximum throughput, all steady state degrees of freedom get 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 proper plantwide control system design for economically optimal process operation. A simple supervisory controller switching scheme for process operation transition from low to maximum achievable throughput is also demonstrated. 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 CSTR followed by two distillation columns. The exothermic reactions $A + B \rightarrow C$ (main reaction) and $C + B \rightarrow D$ (side reaction) occur in the jacketed 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 1 shows a schematic of the process along with salient design and base-case operating conditions for processing 100 kmol/h of fresh *A* to produce 99 mol% pure C. The reaction kinetics and hypothetical component properties for modeling in Hysys are reported in Table 1.

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 ($[x_A/x_B]^{RxrIn}$), the reactor level (V_{rxr}) and temperature (T_{rxr}), the recycle column reflux rate (L_1) and bottoms *B* to *C* mol ratio ($[x_B/x_C]^{Bot1}$) and the product column distillate *D* loss ($[l_D]^{Dist2}$) and bottoms *C* loss ($[l_C]^{Bot2}$). The loss in a column product stream is defined as the ratio of the product stream impurity component flow rate to the feed component flow rate. The desired product purity ($[x_C]^{Dist2}$) is 99 mol% *C* and as this is the valuable product it will always be an active constraint. Since all of the *B* that leaks out the bottoms of the recycle column must necessarily end up in the product stream, the energy consumption in the recycle column is minimized by allowing *B* to leak out to the maximum extent possible without violating the product purity specification. This requires fixing the *B* to *C* mol ratio in the recycle column 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%. Lastly, given the relatively easy separation in the product column, 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 give-away. The particular choice of specifications is used as it gives robust flowsheet convergence using the Hysys steady state solver for the complete 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 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 and temperatures etc. In this case, the objective is to maximize the profit, where

Operating Profit = Product Value – Feed Cost - Raw Material Cost – Energy Cost

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 a specified fresh *A* feed processing rate (F_A) of (a) 70 kmol/h, (b) 100 kmol/h 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 (ie maximum F_A). Case (b) in Mode II (maximum throughput) is generally economically optimal for chemical processes operating in a "sellers market" with high demand and high product prices. The optimization is performed using the *fmincon* subroutine in Matlab with Hysys as the steady state flowsheet solver.

The optimization problem including cost data and process constraints along with results for the five cases, are 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 hold-up constraint (V_{rxr}^{MAX}) is active. 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. However, the market may change and with a higher product price the optimal processing rate increases. 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 rate, 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. Note that 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.

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 column boilup (Q_{reb1}^{MAX}) constraint in Mode Ib/c and Mode II maximizes the recycle rate (mostly component *A*) to suppress the side reaction for increased yield to desired product. In

Mode Ia/b, 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 2 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 (ie $L_1 = 0$) 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.

2.3 Unconstrained Degrees of Freedom and Choice of Economic 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 the 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 to keep 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 with the goal to drive the economic criterion towards 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 3(a) plots the percentage profit loss as F_A is varied over Mode Ia throughput range from 50 kmol/h to 90 kmol/h while holding 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 ±20 kmol/h around a base value of 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 3(b) 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 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 can the process 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/b/c and Mode IIa/b in the present case study). The required switching of controlled variables and pairings is the task of the supervisory control 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) [11]. Aske and Skogestad[10] 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 setpoint is the degree of freedom adjusted to achieve the desired throughput (e.g. to get $F_A = 70$ kmol/h in Mode Ia). The fresh feed flow setpoint as preferred by operators for throughput manipulation as it directly fixes the feed processing rate (throughput). Other than operator preference, there is no restriction on the TPM location and it may be chosen anywhere inside the plant. The location is important, firstly due to its effect on economics as demonstrated later in the case study and secondly, as it dictates the orientation of the inventory (level and pressure) control loops to radiate around the TPM [11] (see Figure 4) 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 [8, 12, 13]. As illustrated in Figure 4, the regulatory control system then propagates flow transients away from the constraint due to the orientation of the inventory loops radiating outwards 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 PID 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 can not 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 will 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 setpoints of these controlled variables generally are degrees of freedom for the economic (steady-state) operation, with 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 setpoints of the column temperature controllers may be used for composition control. The details of the control structures, depends 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 for our process, 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 hold up, temperature and the A / 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} setpoints 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 setpoint being adjusted to maintain $[x_B]^{RxrIn}$ (Mode Ia/b self optimizing variable), which is the most direct and dynamically fastest way of regulating the same. The wild fresh feed flow controller setpoint is then a possible TPM. The $[x_B]^{RxrIn}$ setpoint is also a possible TPM.

Of the various TPM possibilities in Mode I, the V_{rxr} setpoint is not available since economic considerations dictate reactor operation at maximum hold-up in all operation modes. The T_{rxr} setpoint 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 $[x_B]^{RxrIn}$ setpoint can only be used as a TPM in Mode Ic (self optimizing in Mode Ia/b).

Based on the guideline given above, a good choice for the TPM in Mode Ia is the recycle column steam flow controller setpoint 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 [9] as a means of mitigating snowballing and using the flow setpoint as the TPM. For each choice of the TPM, the regulatory control system is designed around it to achieve consistent inventory control [10]. The resulting control structures are shown in Figure 5 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 recycle column boilup (Q_{reb1}) reaching its maximum limit 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 setpoint 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 setpoint 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 by-product 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 setpoint 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 setpoint is adjusted to maintain the *D* impurity mol 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 setpoint 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 setpoint as the TPM, F_B is maintained in ratio with F_A with the ratio setpoint being adjusted by the reactor feed composition controller. The reactor level controller manipulates the recycle column feed and the remaining control structure is very 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 towards 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} setpoint at Q_{reb1}^{MAX} with no back-off needed, so there is no economic loss. However, Q_{reb1} can not 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 in fact is the unconstrained CV that is given up on reaching the Q_{reb1}^{MAX} constraint, the T_{rxr} setpoint is available for 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 feedrate F_{col1} which is the TPM in Mode Ia. In Mode Ib, we can either set Q_{reb1} at its maximum and use F_{col1} for controlling the column temperature (identical to CS1), or 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 that 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.

In CS4, the feedrate 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 $[x_B]^{RxrIn}$ setpoint as the TPM, controlling which in Mode Ic must be given up with all degrees of freedom exhausted. Changing the $[x_B]^{RxrIn}$ setpoint, changes the feedrate 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/b/c), 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 setpoint. 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 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} 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 feedrate 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 setpoint 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 setpoint setpoints 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. The Table also shows how the throughput manipulator (TPM) is moved depending on the control structure and operation modes.

3.3 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 6 (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 setpoint gets adjusted to maintain $[x_B]^{RxrIn}$. In Mode Ib, T_{rxr} is adjusted to maintain Q_{reb1} near maximum while in Mode Ic, $[x_B]^{RxrIn}$ gets 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 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 towards 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 pressure controllers are tuned for tight pressure control. All level controllers are P only with a gain of 2 (unless noted otherwise). 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.

4.1 Quantitative Back-off Comparison

For an active constraint, the back-off is the difference between its setpoint 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 is necessary in the supervisory active constraint controller setpoint 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 (ie a transient constraint violation is unacceptable). A 5 mol% heavy impurity pulse of 10 hour duration in the fresh *B* stream is considered the worst case disturbance. The heavy impurity ends up in the bottoms by-product stream from the product column. The back-off in an active constraint controller setpoint 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 7 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 hours.

Table 6 reports for the four control structures CS1-CS4, the process parameters and steady-state yearly profit for chosen F_A values of 70 kmol/h (Mode Ia), 100 kmol/h (Mode Ib), 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/b. This is attributed to the small but relatively higher 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 ºC (with no back-off) to between 70.55 °C (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 requires 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 dropping 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 \$4.237x10^6 per year (no back-off) and the Mode Ic CS1 operating profit of \$4.229x10^6 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/c and Mode II, varying between 4.3% to 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 \$0.257x10^6 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 \$0.19x10^6 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 CS1-CS4 and is between 1.7 to 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 \$0.359x10^6, 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 (Mode Ia) progressively moves away from the recycle column boilup from CS1 to CS4. It is therefore not surprising that the recycle column boil-up back-off increases in order CS1 < CS2 < CS3 < CS4 in Mode Ib/c and Mode IIa/b. This also explains the back-off trend in Q_{reb2} for Mode IIb operation with the regulatory layer TPM location moving progressively away from the recycle column boilup in order 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 setpoint is further increased, the T_{rxr} setpoint 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 setpoint. As the F_A setpoint 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 setpoint is used as an MV to maintain Q_{reb2} close to maximum (Mode IIb).

In CS4, the setpoint of the fresh *A* feed flow controller (F_A) is the TPM across the complete Mode I throughput range. As the setpoint is increased from low F_A values (Mode Ia), Q_{reb1} approaches its maximum whereby the reactor temperature setpoint is used as the MV to maintain Q_{reb1} close to maximum (Mode Ib). As the F_A setpoint 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 setpoint is further increased, Q_{reb2} approaches its maximum and the F_A setpoint is adjusted to maintain it near maximum for process operation at maximum throughput (Mode IIb).

Figure 8 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 setpoint 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 [12] 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 $[x_B^{RxrIn}]$ setpoint is reduced. The throughput would decrease (Mode Ic) and the $[x_B^{RxrIn}]$ setpoint would eventually approach its Mode Ib optimum at which point the TPM is shifted to T_{rxr} with its setpoint 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} setpoint would cause the transition into Mode Ia operating region. A similar logic can also be devised for the other control structures.

6. 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 till 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.

Acknowledgments

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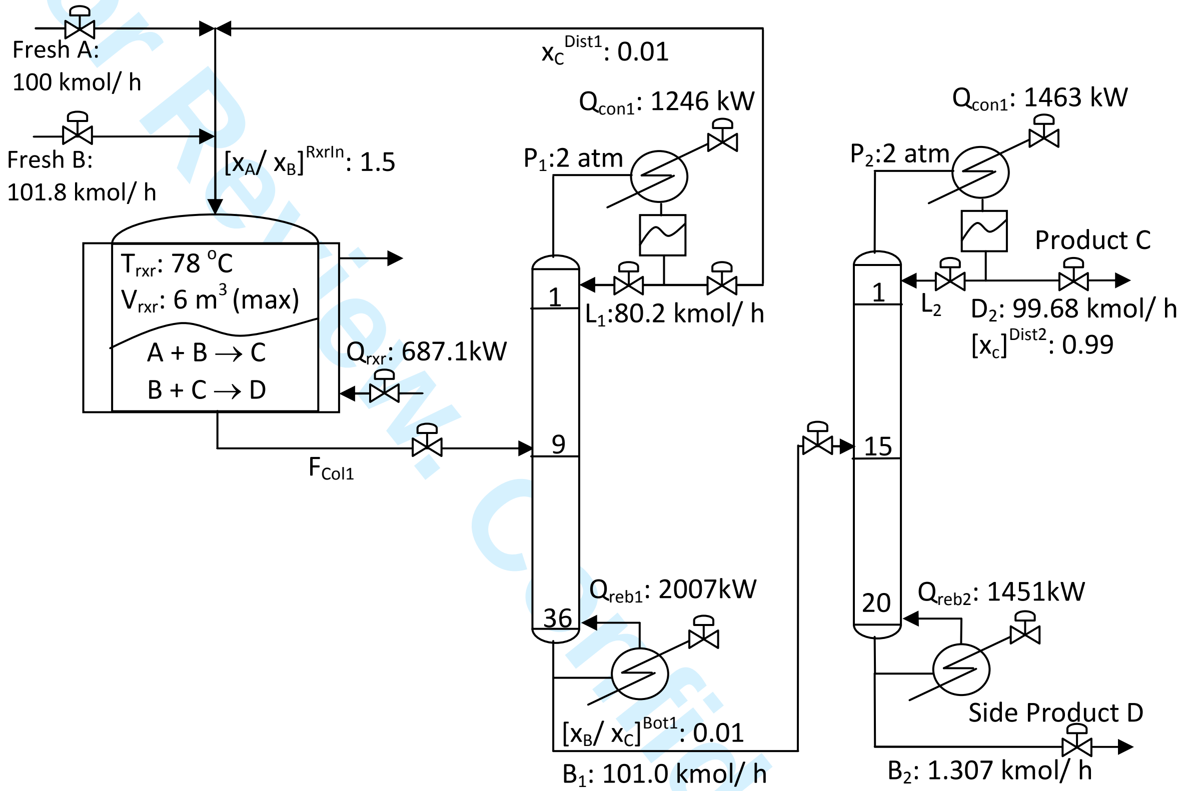

Figure 1: Schematic of recycle process studied

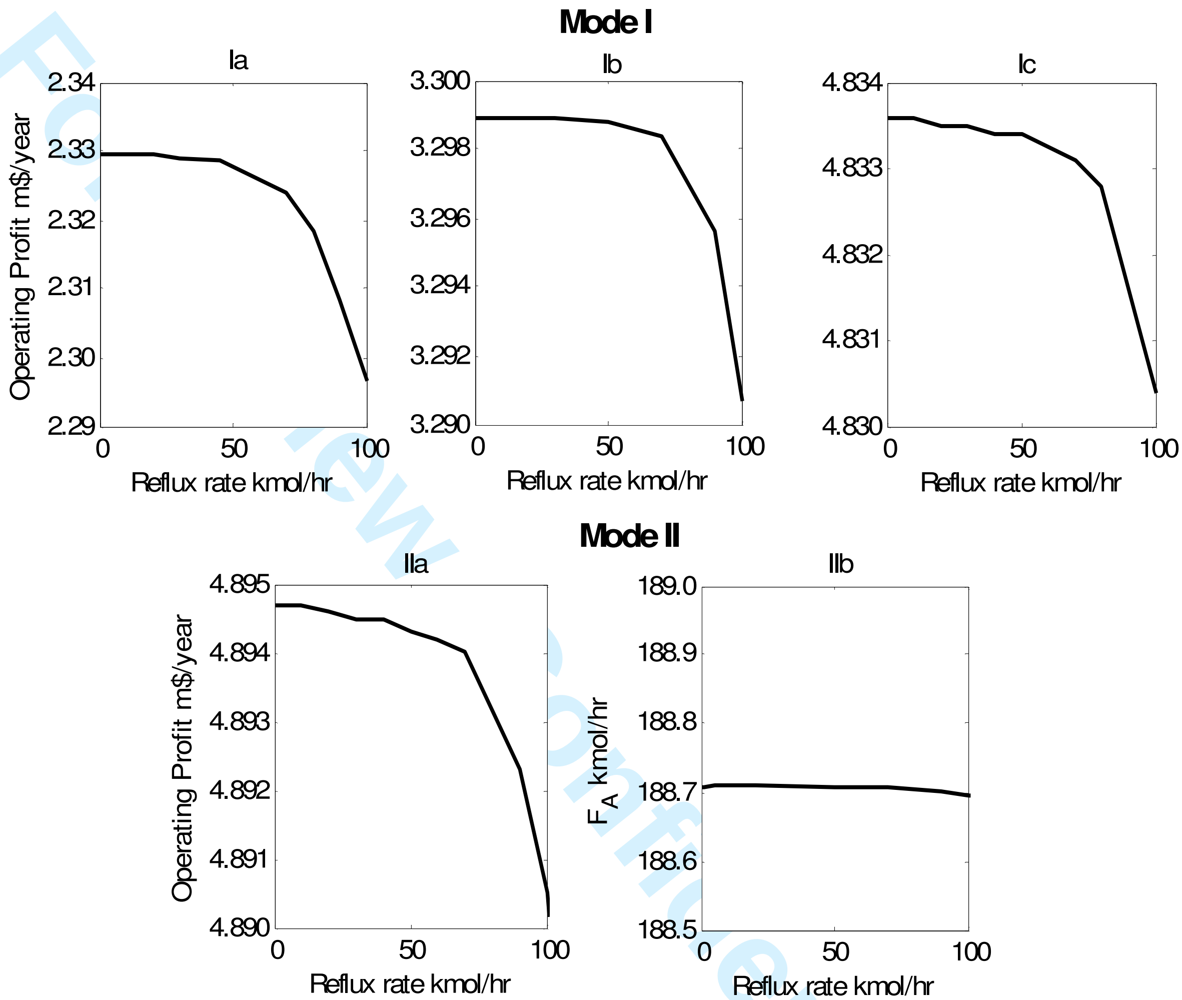

Figure 2. Sensitivity of economic criterion to recycle column reflux

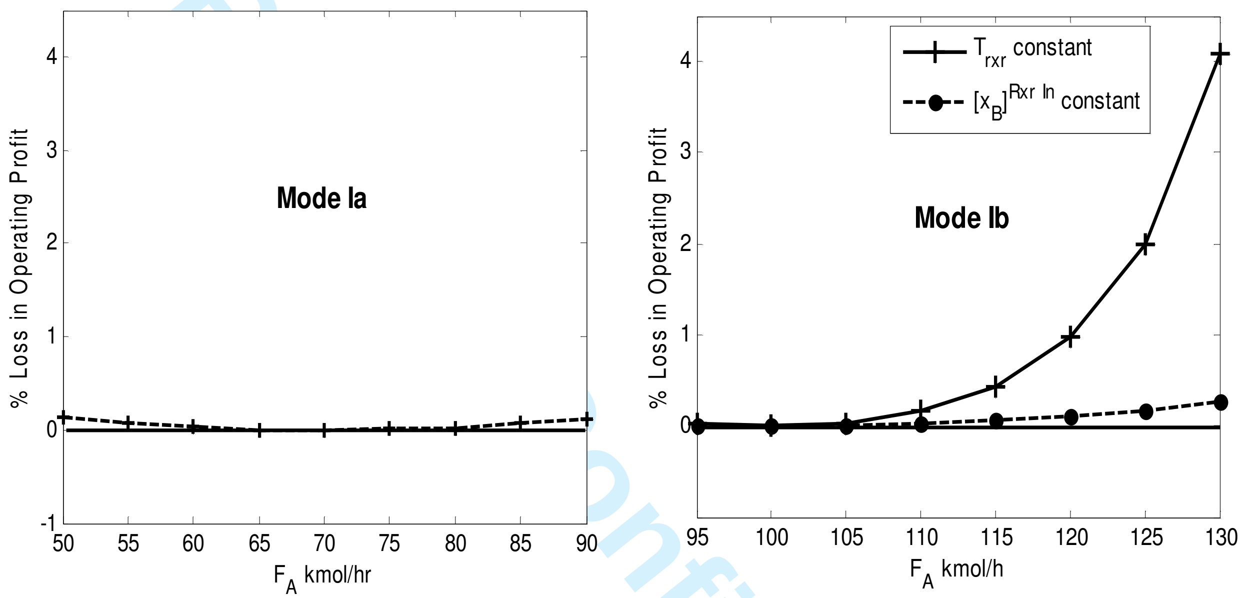

Figure 3. Percentage loss in profit for process operation at constant T_{rxr} and/or constant $[x_B]^{RxrIn.}$.
Mode Ia: Loss with both T_{rxr} and $[x_B]^{RxrIn}$ *constant.*
Mode Ib: Loss with either T_{rxr} constant or $[x_B]^{RxrIn}$ constant.

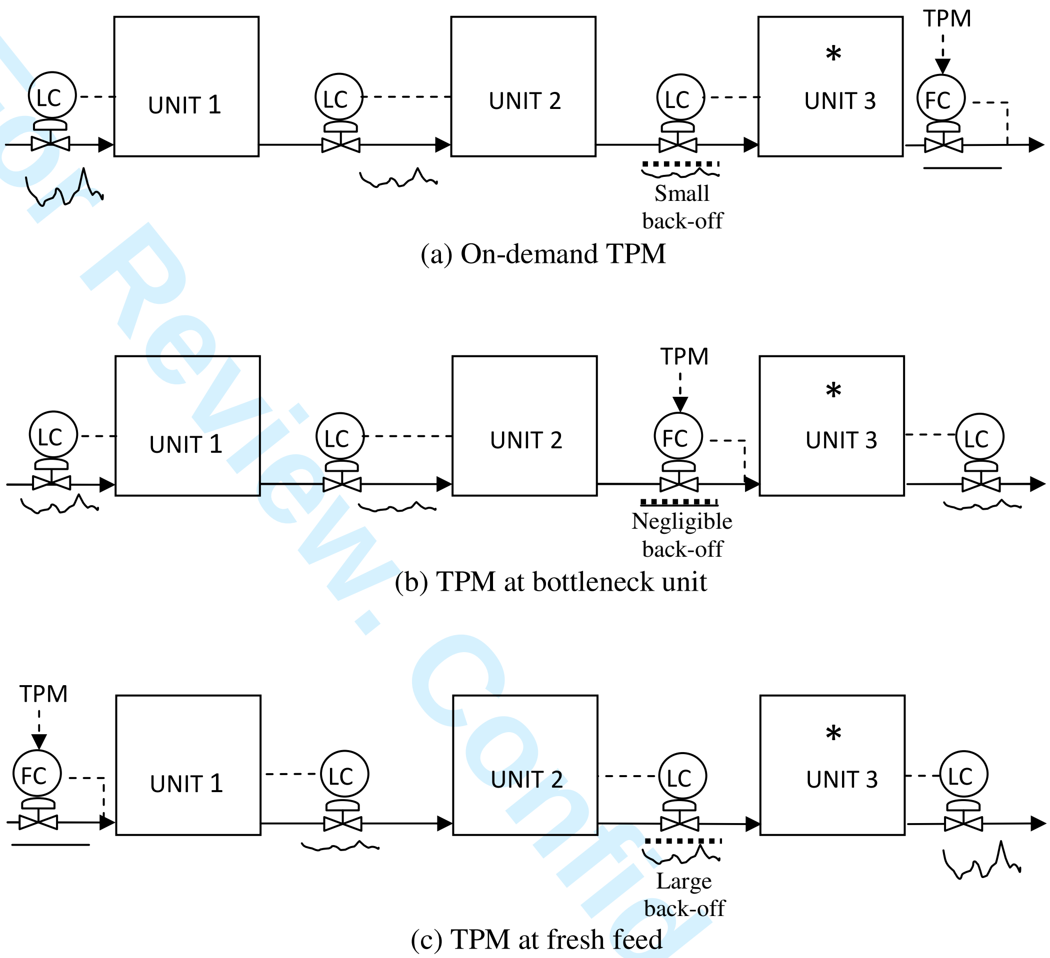

Figure 4. Orientation of inventory control loops around TPM and propagation of flow transients

*: Bottleneck unit

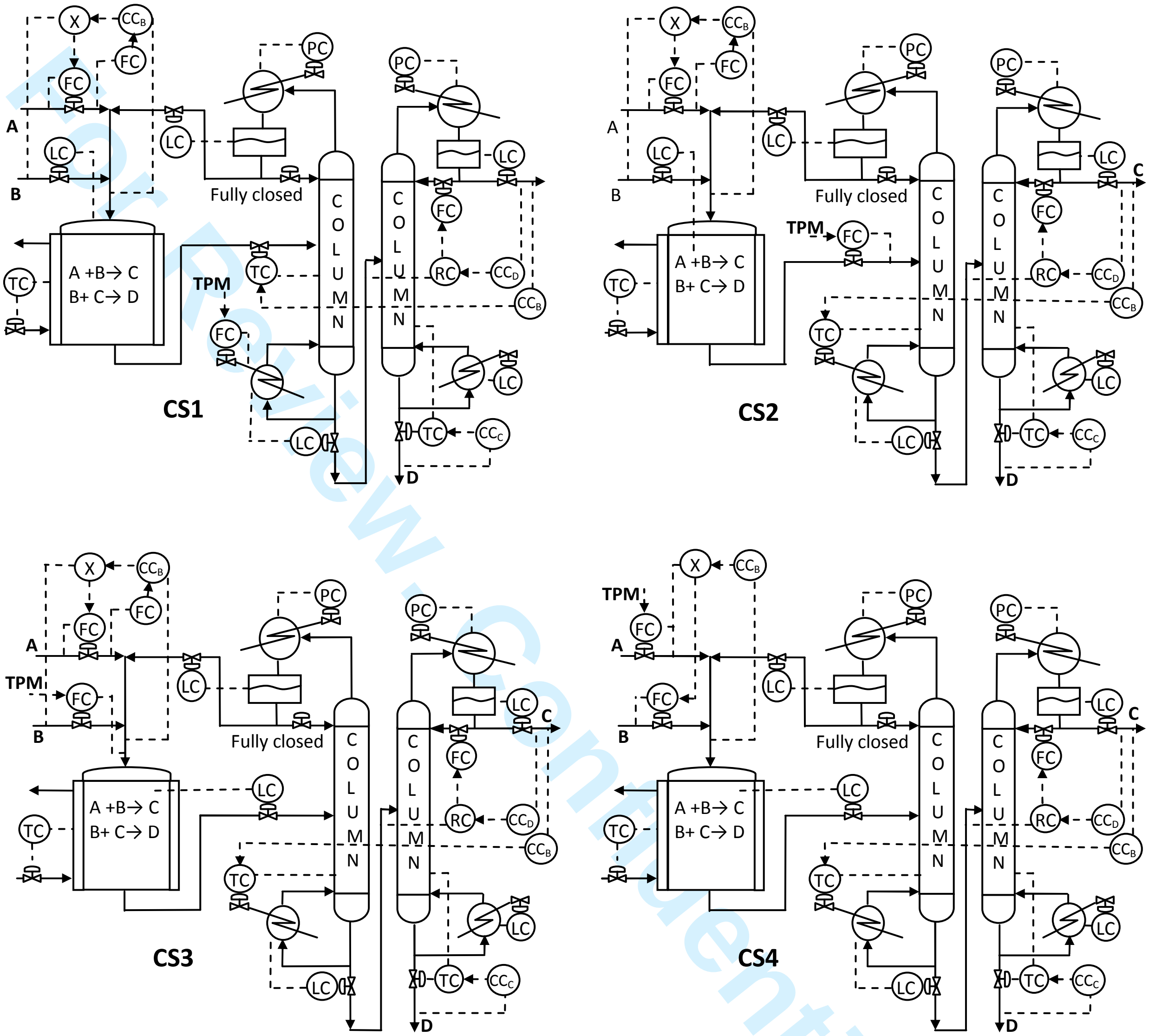

Figure 5. Plantwide regulatory control structures studied (for Mode Ia operation)

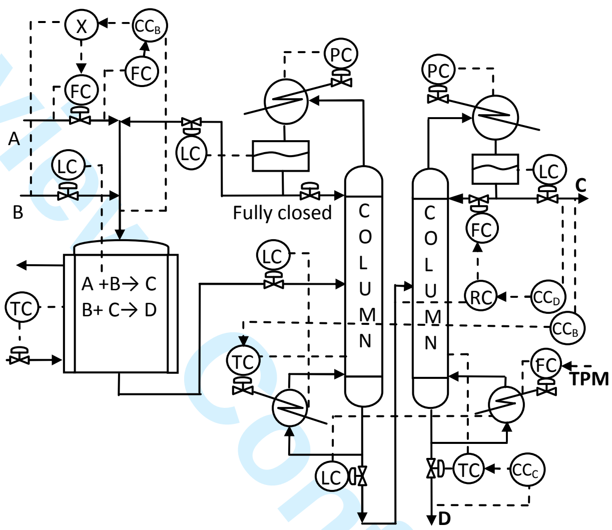

Figure 6. Regulatory control structure with Q_{Reb2} as TPM

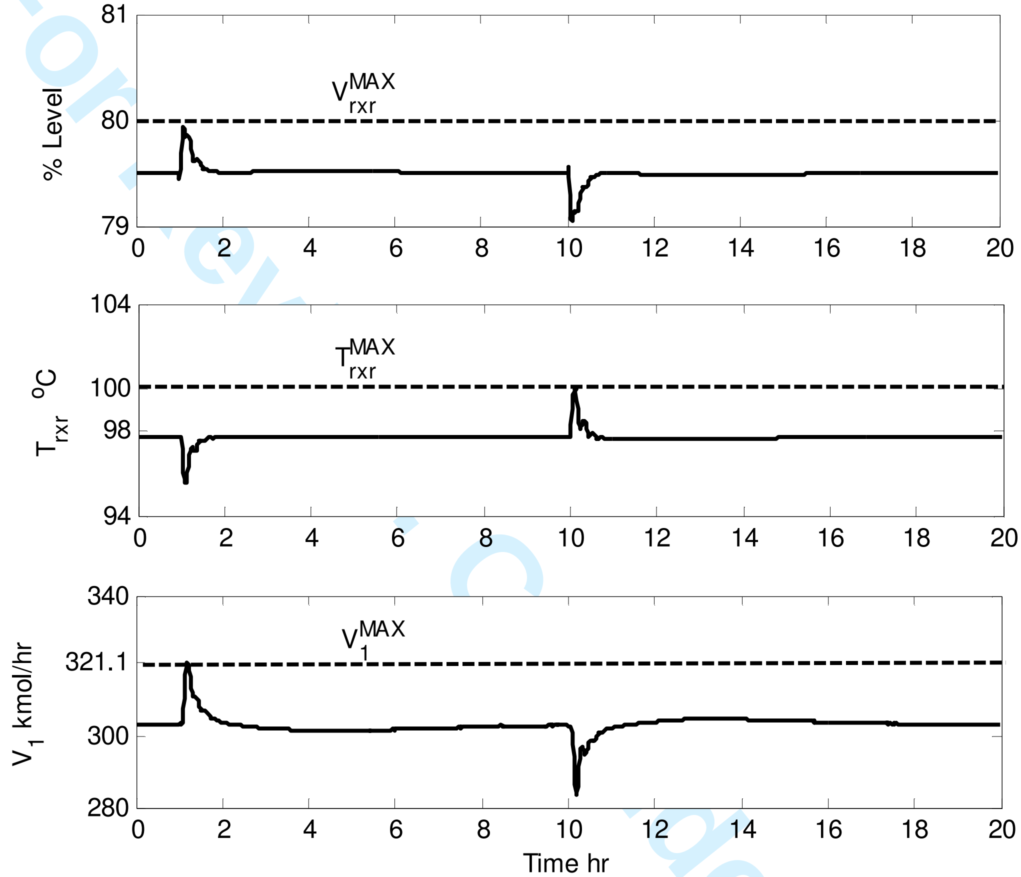

Figure 7. Illustration of back-off for CS3 (F_A = 170 kmol/h, Mode Ic)

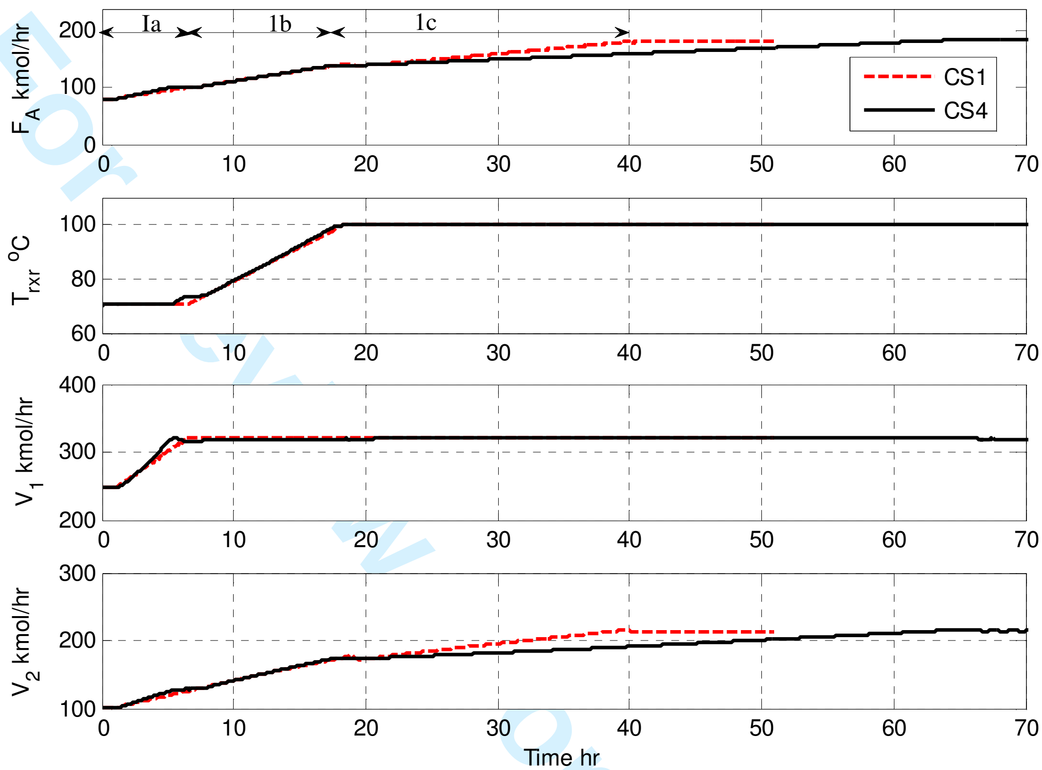

Figure 8. Smooth throughput transition using supervisory layer control configuration switching

Table 1: Modeling details of recycle process

Kinetics	$A + B \rightarrow C$ $B + C \rightarrow D$	$r_1 = k_1 x_A x_B$ $r_2 = k_2 x_B x_C$	$k_1 = 2x10^8 exp(-60000/RT)$ $k_2 = 1x10^9 exp(-80000/RT)$
Hypotheticals	MW	NBP (°C)	Hydrocarbon estimation procedure used to estimate parameters for thermodynamic property calculations
A	50	80	
B	80	100	
C	130	130	
D	210	180	
VLE	Soave-Redlich-Kwong		

Reaction rate units: $kmol.m^{-3}.s^{-1}$

Table 2: Process optimization results

Objective function	Cases Ia/b/c 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 ≤ CSTR Temperature ≤ 100 °C 0 ≤Material flows ≤ 2(base-case) 0 ≤ Recycle flow ≤ 3(base-case) 0 ≤ Energy flows ≤2(base-case) 0 ≤ Column 1 Reboiler duty ≤ 1.5(base-case) 0 ≤ Column 2 Reboiler duty ≤ 2(base-case) 0 ≤ CSTR Volume ≤ 6 m^3 $[x_B/x_C]^{Bot1} = 0.01$; $[r_C]^{Dist2} = 99.5\%$; $[r_D]^{Bot2} = 99.0\%$				
Case	Ia Given F_A	Ib Given F_A	Ic Given F_A	IIa Optimum F_A	IIa Maximum F_A
Throughput (F_A)	70 kmol/hr$^{\&}$	100 kmol/h$^{\&}$	170 kmol/h$^{\&}$	182.1 kmol/h*	188.7 kmol/h$^{\#}$
V_{rxr}	6 m^3 (max)	6 m^3 (max)	6 m^3 (max)	6 m^3 (max)	6 m^3 (max)
T_{rxr}	63.8538	70.3872°C	100 °C (max)	100 °C (max)	100 °C (max)
$[x_A/x_B]^{Rxr\ In}$	2.3299	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
Profit per year	\$ 2.042x10^6	\$2.876x10^6	\$ 4.237x10^6	\$ 4.382x10^6	\$ 4.354x10^6
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 dofs	2	*1*	*0*	*1*	*0*
Self-optimizing CVs	T_{rxr} , $[x_B]^{RxrIn}$	$[x_B]^{RxrIn}$	-	$[x_B]^{RxrIn}$	-

&: F_A is specified
*: F_A also optimized for maximum operating profit
#: Maximum achievable throughput

Table 3. Supervisory layer control loop configuration for different operating modes for CS1-CS4

	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 5					
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-$[x_B]^{rxr\ In}$	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
Setpoints	V_{rxr}: V_{rxr}^{MAX}- Δ	V_{rxr}: V_{rxr}^{MAX}-Δ Q_{reb1}: Q_{reb1}^{MAX}-Δ	V_{rxr}: V_{rxr}^{MAX}-Δ Q_{reb1}: Q_{reb1}^{MAX}-Δ T_{rxr}: T_{rxr}^{MAX}-Δ	V_{rxr}: V_{rxr}^{MAX}-Δ Q_{reb1}: Q_{reb1}^{MAX}-Δ T_{rxr}: T_{rxr}^{MAX}-Δ	V_{rxr}: V_{rxr}^{MAX}-Δ Q_{reb1}: Q_{reb1}^{MAX}-Δ T_{rxr}: T_{rxr}^{MAX}-Δ Q_{reb2}: Q_{reb2}^{MAX}-Δ

Δ: Back off to avoid transient constraint violation
TPM = MV used for controlling F_A(TPM = F_A for CS4)

Table 4: Regulatory Layer Controller Tuning*#

Controlled Variable	K_C	τ_i (min)	τ_d (min)	Sensor Span
$[x_B]^{Rxr\ In}$	2	400	-	0 – 1
T_{rxr}	4	10	2	60 – 130 ºC
T_{Col1}	0.5	10	-	100 – 160 ºC
T_{Col2}	2	20	-	120 – 200 ºC
Reb2 Level	1.5	20	-	0 – 100%
$[x_B]^{Dist2}$	0.1	40	-	0 – 0.02
$[x_D]^{Dist2}$	0.1	30	-	0 0.0004

*: All level loops use $K_C = 2$ unless otherwise specified

#: Pressure/flow controllers tuned for tight control

All composition measurements have a deadtime of 5 minutes and a sampling time of 2 mins

All temperatures measurements are lagged by 2 mins

Table 5. Supervisory layer control loop tuning parameters

	CS1		CS2		CS3		CS4	
Controlled Variable	K_C	τ_i (mins)	K_C	τ_i (mins)	K_C	τ_i (mins)	K_C	τ_i (mins)
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

Table 6: Salient parameters for backed-off process operation for CS1-CS4

	F_A kmol/hr	F_B kmol/hr	%Yield A → B	$[x_A/x_B]^{Rxr\ In}$	Col 1 Boilup kmol/hr	Col 2 Boilup kmol/hr	V_{rxr} %	T_{rxr} °C	Profit x10^6 $/year
					Mode Ia				
Optimum	70	69.48	97.72	2.275	230.7	90.23	80.0*	63.66	1.942#
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*	122.5	80.0*	70.39	2.876#
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*	199.8	80.0*	100*	4.237#
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*	209.2	80*	100*	4.382#
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#	192.3	95.55	1.564	321.1*	215.8*	80.0*	100*	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

*: Maximum limit #: Optimum value