I&EC research
Industrial & Engineering Chemistry Research

Article

Cite This: Ind. Eng. Chem. Res. 2020, 59, 2229−2241

pubs.acs.org/IECR

Systematic Design of Active Constraint Switching Using Classical Advanced Control Structures

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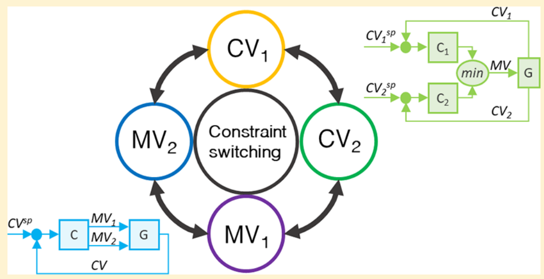
Supporting Information

ABSTRACT: An important task of the supervisory control layer is to maintain optimal operation. To achieve this, we need to change control objectives when constraints become active (or inactive) as a result of disturbances. In most process plants, the supervisory layer uses classical PID-based advanced control structures, but there is no systematic way of designing such structures. Here, we propose a systematic procedure to design the supervisory control layer using single-loop classical advanced control structures, such that the process achieves steady-state optimal operation when the active constraints change. The active constraints can be on the manipulated variable (MV, input) or on the controlled variable (CV, output). In this paper, we consider all three possible cases: CV−CV switching, which involves selectors; CV−MV switching, which does not need any special structure if we pair according to the input saturation pairing rule; and MV−MV switching, which uses split range control or some similar structure. We illustrate our methodology with two case studies.



■ INTRODUCTION

The control hierarchy typically used in process plants decomposes the overall control problem on a time scale basis, as shown in Figure 1. The upper layers are related to long-term economic optimization, whereas the two lower layers are control layers, with the objective of keeping the controlled variables (CVs) at their desired set points.

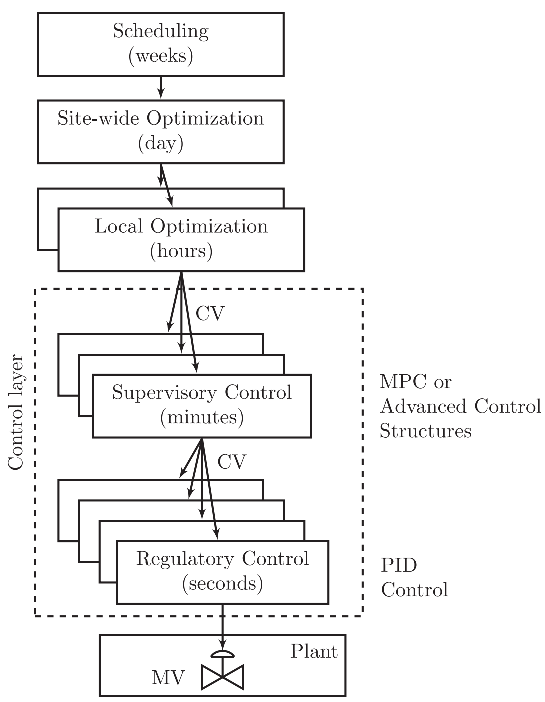


Figure 1. Typical control hierarchy in a process plant.

The control layer is subdivided into a supervisory control layer and a regulatory or stabilizing control layer. The main objective of the regulatory layer is to stabilize the process, avoiding drifting away from the desired steady-state, and rejecting disturbances on a fast time scale.[1,2] The supervisory control layer should follow the set points for the controlled variables computed by the optimization layer. Importantly, this involves switching between active constraint changes in these CVs. It also calculates the set points for the regulatory layer and avoids steady-state saturation of the manipulated variables (MVs) used by the regulatory layer. Note that in this paper, the terms "output" (y) and "controlled variable" (CV) are used as synonyms. Similarly, the terms "input" (u) and "manipulated variable" (MV) are also used as synonyms and refer to the physical input variables.

Skogestad[2] proposed a systematic procedure for control structure design for complete process plants. The procedure is separated into two main parts: top-down analysis and bottom-up design. The top-down analysis focuses on identifying the steady-state optimal operation, usually on the basis of economics. The bottom-up part focuses on the design of the control layer structure. The procedure is as follows:

Special Issue: Christos Georgakis Festschrift

Received: August 15, 2019
Revised: September 24, 2019
Accepted: October 12, 2019
Published: October 14, 2019

- Top-down analysis:
  - (S1) Define a cost (J) to be minimized (economics), and identify constraints that must be satisfied during operation.
  - (S2) Identify the degrees of freedom (u, MVs), and determine the optimal operation conditions (including active constraints) for expected disturbances (usually at steady-state).
  - (S3) Identify candidate measurements (y), and from these, select economic controlled variables for the supervisory control layer. Active constraints should always be controlled for optimal operation. For the remaining unconstrained degrees of freedom, the "self-optimizing" variables should be controlled, because when kept constant, they indirectly minimize the cost.[3]
  - (S4) Select the location of the throughput manipulator (TPM),[4] which is where the production rate is set. This is a dynamic decision. For maximizing production, the TPM should be located at the bottleneck.
- Bottom-up design of the control structure:
  - (S5) Select the structure of the regulatory PID control layer. Select "stabilizing" control variables for the supervisory control layer, and because single-loop control is preferred in this layer, choose pairings for these CVs with manipulated variables (MVs).
  - (S6) **Select the structure of the supervisory control layer. It can be model-based (using MPC), but in this paper, we consider the use of classical advanced control elements.**
  - (S7) Select the structure for the online optimization layer (RTO), if required. The RTO layer may be avoided if one can switch between active constraints in the supervisory layer and can identify good self-optimizing variables[3] for the remaining unconstrained degrees of freedom.

This procedure can be followed sequentially, but one decision directly influences the others, such that the procedure may be iterative.[2,5] In this work we focus on step S6, specifically on how to handle switching between active constraints. The decisions taken in the top-down part of the procedure, especially the identified active constraints, directly affect the design of the supervisory control layer, and we assume that these decisions are already taken.

Active constraints are variables that should optimally be kept at their limiting value (step S3). These can be either *manipulated variable* (MV, input) constraints or *controlled variable* (CV, output) constraints. The maximum pressure in a unit is a CV constraint, whereas the maximum opening of a valve is a typical example of an MV constraint. We need to be a bit cautious about what we mean by MV constraint because the term MV generally denotes the degrees of freedom in any layer. For example, when referring to the supervisory layer, it may refer to the set point for the CVs in the regulatory layer. However, in the context of this work, MV constraints mean minimum or maximum values of the *physical* manipulated variable (e.g., valve opening or pump rotational speed).

If there are remaining unconstrained degrees of freedom in step S3, then one should identify associated self-optimizing variables to keep at constant set points.[2] Controlling the self-optimizing variable to its optimal set point keeps the process at or near optimal operation.[3,5] Self-optimizing variables can be a specific measurement, a combination of measurements ($c = Hy$),[6] or a measurement or estimate of the gradient of the cost $\left(J_u = \frac{dJ}{du}\right)$. Note that the self-optimizing variables generally will change when we enter a different active constraint region.

If there were no changes in the operating point and, in particular, no changes in the active constraints, optimal operation would always be achieved by using the same control structure and constant set points in the regulatory control layer. However, all plants are subject to disturbances, which may cause changes in the optimal operation point and the active constraints. Typical disturbances include changes in feed rate, feed composition, product specifications and prices and drifts in process parameters such as efficiencies.

In terms of economics, the most important role of the supervisory control layer is to keep the operation in the right *active constraint region*, which is a region in the disturbance space defined by which constraints are active within it.[7] Stephanopoulos[8] states that an optimizing control strategy in the supervisory layer must identify when the plant must be moved to a new operating point (changing the active constraint region) and then make the appropriate set point changes to bring the plant to the new optimal operating point.

The supervisory control layer is sometimes designed with model predictive control (MPC). The main advantage of MPC in terms of economics is that it can handle many constraints, and it represents a unified systematic procedure to control multivariable processes.[9] The main drawback of MPC is that it requires a dynamic model of the process, which is not always available or is costly to generate and update (e.g., see Georgakis[10]). Furthermore, standard MPC may not handle changes in active constraints effectively, except by the indirect use of weights in the objective function.[11,12]

The supervisory control layer can alternatively be designed using *classical advanced control structures* with PID-controllers and simple blocks, and this is the most common control approach in industry. The main reason is that classical structures can be gradually implemented in the existing "basic" control system using little model information.[13] Some classical advanced control elements (blocks or idioms[14]) used in addition to PID controllers include:[15,16]

- cascade
- feedforward and ratio
- decoupling
- calculation block
- valve position (input resetting)
- selector (max and min)
- split range (input sequencing)

These structures have been used since the 1940s.[17,18] However, there has been limited academic work, and most implementations are ad hoc.

The lack of a systematic procedure to design control structures was pointed out by Foss[19] in his famous paper from 1973, with the title "Critique of Chemical Process Control Theory". He writes that "the central issue to be resolved by the new theories of chemical process control is the determination of control system structure". Following this, some research was initiated to design control structures in a systematic way (e.g., see Vandenbussche,[20] Govind and Powers[21,22] Bristol,[14] and Stephanopoulos[8]). Although some good ideas were introduced, this research has had limited impact. More recently, Hägglund

DOI: 10.1021/acs.iecr.9b04511
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and Guzmán[23] pointed out that little research and development has been presented to the use of the basic control structures, even in the regulatory layer.

To the knowledge of the authors, there is no systematic procedure to design the supervisory control layer structure (step S6) using classical advanced control elements. In this work, we present such a systematic procedure and show its applicability in two industrially relevant case studies.

■ DESIGN PROCEDURE FOR CONSTRAINT SWITCHING USING CLASSICAL ADVANCED CONTROL STRUCTURES

The proposed procedure to design constraint switching strategy for the supervisory layer (step S6) using advanced control structures has five main steps:

Step A1:
: Define the control objectives (CVs), manipulated variables (MVs), and constraints. Distinguish between CV and MV constraints.

Step A2:
: Organize the constraints in a *priority list*. That is, identify which set points or constraints can be given up in order to guarantee feasible operation.

Step A3:
: Identify possible and relevant active constraint switches.

Step A4:
: Design the control structure for normal operation.

Step A5:
: Design the control structures to handle the identified active constraint switches.

We will now detail each step.

Step A1: Define the Control Objectives, MVs, and Constraints. The control objectives in the supervisory layer are specified in terms of controlled variables (CVs) with set points. These follow from step S3 in the top-down analysis. Note that the CVs from step S3 may also include MVs. The main objective of step S6 is to implement this in practice. The main problem is that the variables that we need to control may change during operation because of changes in active constraints.

A detailed analysis in step S3 results in a number of active constraints regions, each with a specific set of controlled variables. However, in practice, such a detailed analysis usually is too time-consuming to perform. Instead we may, on the basis of partial analysis in step S3 and engineering judgment, list the expected controlled variables:

1. Outputs (CVs) with set points (denoted CV equality constraints below): Examples include product specifications and operating pressures and temperatures.
2. Input variables with desired values or set points (denoted MV equality constraints below): An example is a desired value for rotational speed of a compressor.
3. Output (CV) constraints: These may become optimally active at certain steady-state operating points.
4. Input (MV) constraints: These may become optimally active at certain steady-state operating points.
5. Self-optimizing CVs: These are associated with unconstrained degrees of freedom, and keeping them at constant set points should indirectly minimize the economic cost.
6. Desired throughput (production rate): Typically (but not always) this is a flow rate (MV or CV) with a given set point.

Sometimes the throughput is given and may enter as an MV equality constraint. However, in many cases with good market conditions, optimal operation (minimum cost, J) is achieved by maximizing the throughput. In this case, one may set an unachievably high set point for the production rate, and optimal operation (maximum production) is achieved when one reaches the bottleneck, which is when there are no more constraints that can be given up.

The best self-optimizing CV will change when the active constraints change, but for simplicity, we often try to use the same "self-optimizing" CV in several regions. This will imply that its set point may need to vary depending on the disturbance value (e.g., feed rate). To identify self-optimizing variables and their set points, we generally need a process model. Note that otherwise, the procedure proposed in this paper does not need explicit model information.

Step A2: Organize the Constraints in a List of Priorities. At some steady-state operating conditions, it may not be feasible to satisfy all the constraints using the available MVs. In this case, one may use a priority list to decide which constraints can be given up to make operation feasible. This will also help us in making decisions regarding pairing of CVs and MVs.

Physical MV constraints, which of course cannot be violated, are placed at the highest priority. This means that they cannot be given up. Economic objectives such as desired throughput and self-optimizing set points are at the lower end of the priority list. By placing the most important constraints at the top, the priority list typically has the following structure:

(P1) Physical MV inequality constraints: These are physically impossible to give up. Typical examples are maximum or minimum opening of valves or maximum pump speed.

(P2) Critical CV inequality constraints: These may possibly be given up for a short period. These are often safety constraints such as maximum temperature or maximum pressure.

(P3) Nonphysical MV and less critical CV constraints (both equality and inequality constraints): These may be given up and include, for example, a desired pressure (CV equality constraint). By nonphysical MV constraints, we mean a constraint that is not related to a fully open or closed valve (control element). For example, it could be the minimum liquid flow in a distillation column to ensure proper wetting of the packing, or maximum flow to avoid excessive wear.

(P4) Desired throughput: These are MV or CV equality constraints that must be given up when we reach a bottleneck. Typically, this happens when we reach a physical MV inequality constraint, and there are no variables with lower priority that can be given up.

(P5) Self-optimizing variables: These are economic CV equality constraints that can be given up.

It is important to note that the ordering of items P2, P3, and P4 may vary depending on the specific case. Often, the desired throughput has a higher priority than a CV inequality constraint (e.g., a desired set point for a byproduct concentration). Within the constraints in P3, there might be CV of MV equality constraints with a higher priority than others. It should also be noted that the constraints in P3, P4, and P5 may include the same variables that are already used in P1 and P2 but with different bounds.

DOI: 10.1021/acs.iecr.9b04511
Ind. Eng. Chem. Res. 2020, 59, 2229−2241

Usually, few physical MV constraints are active in the base case operating point. When disturbances occur and we operate away from this point, then we may reach physical MV constraints, and we have to give up controlling some other CV or MV constraint. The order in which constraints should be given up as we move away from nominal operation follows the reverse of the priority list. We first give up the constraints at the end of the list (with the lowest priority) and continue satisfying those with higher priority.

Step A3: Identify Active Constraint Switches. Once all expected constraints have been identified and prioritized, we proceed to identify active constraint switches. This will occur (1) when disturbances cause a CV or MV to reach a new inequality constraint, and we have to give up controlling some other variable, or conversely, (2) when an inequality constraint is no longer active, and we can start controlling another variable. Therefore, the priority list from step A2 will be very useful for identifying likely switches.

One may believe that we need to obtain all the active constraint regions as a function of all the disturbances. However, obtaining this information is usually very time-consuming, even for quite simple processes, and fortunately, it is not necessary.[7] We only need to know which active constraint switches are expected. We do not need the actual point (value of the disturbance) at which we change from one active constraint region to the other, as this will be indirectly identified online with the values of the MVs and CVs. It is insightful to know the maximum number of active constraint regions, which is given by[7]

$$n_r^{\max} = 2^{n_c} \tag{1}$$

where n_c is the number of constraints. We should note that, in practice, there are usually much fewer possible and even fewer relevant active constraints regions (n_r), so

$$n_r < n_r^{\max} \tag{2}$$

The following criteria are useful for finding possible active constraint regions so that we can design the control structure considering only the active constraint regions of interest:

- Certain constraints are always active (reduces effective n_c in eq 1).
- Certain constraint combinations are not possible. For example, the maximum and minimum bounds on the same variable cannot be reached at the same time.
- Certain constraints (or regions) cannot be reached by the assumed disturbance set.
- At a given time, the number of active constraints is limited by the number of degrees of freedom (MVs).

Step A4: Design Control Structure for Base Case Operation. The next step is to design a control structure for the base case operating point, which is typically the nominal operating point. This is often a case with relatively few active constraints and in which most if not all constraints in the priority list can be satisfied. In this step, we should follow standard guidelines for designing control structures.[4,13,24,25] For example, we should follow the *pair close rule* for a good dynamic response.[26]

When designing the base case control structure for optimal operation, we should note that a constrained MV does not need to be actively controlled. Thus, if it is optimal to maintain a valve fully open or fully closed, such as in a bypass, then we do not need to implement a controller to achieve this. We simply set it fully open or fully closed. In order to reduce the need of repairing of loops as we go away from the base case, we recommend pairing MVs with CVs according to the *input saturation pairing rule*.[26]

> *A manipulated variable (MV) that is likely to saturate at steady state should be paired with a controlled variable (CV) that can be given up.*

By "can be given up", we mean that it is near the bottom of the priority list. If we do not follow the input pairing rule, then we need to find another MV to take over controlling the CV. An alternative formulation of the rule is "pair an MV that is unlikely to saturate with an important CV".

Step A5: Design Control Structures for Active Constraint Switching. There is a fundamental difference between MV and CV constraints because we need an MV to control a CV, whereas an MV can simply be set at its constraint value. Considering this, the following constraint switches can occur:

Case 1:
CV (output) to CV (output) constraint switching.
Case 2:
MV (input) to MV (input) constraint switching.
Case 3:
MV (input) to CV (output) constraint switching.

Case 1: CV to CV Constraint Switching. This case typically happens when we have one input (MV) that switches between controlling two alternative CVs, meaning that only one CV is controlled at any given time.

To switch between the CVs, we can use two independent controllers and a min/max selector, so that the active CV constraint is always selected. Figure 2 shows the block diagram with two CVs (y_1 and y_2) and one MV (u). It is important to note that antiwindup must be implemented in both controllers (C_1 and C_2).

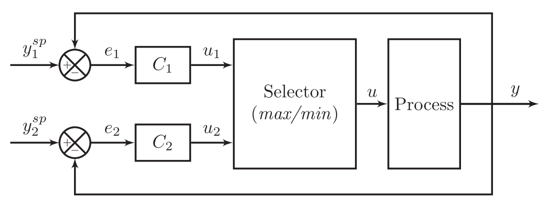

Figure 2. CV to CV switching using a selector for the case with two CVs (y_1 and y_2).

A possible misconception here is that all the CVs (y_1 and y_2 in Figure 2) need to be of the same type (e.g., temperature) as in *auctioneering*, where we have one controller, the selector is on the input of the controller, and we select to control one of several similar outputs.[5] However, in general, the CVs may be of different types if the selector is on the output from the controller,[27] as in Figure 2. As an example, Figure 3 shows a flowsheet in which the coolant flow or actually its set point ($u = \dot{m}_w^{sp}$) is the only available MV to control either the reactor temperature (y_1) or concentration (y_2), both of which can reach their corresponding maximum constraints. A selector on the controller output signals (u_1 and u_2) allows for CV switching between temperature (y_1) and composition (y_2).

Such schemes are sometimes called *override control*.[27−29] However, we prefer to call it CV to CV switching to avoid the connotations of "error" and "emergency" associated with the term "override". On the contrary, CV to CV switching is

DOI: 10.1021/acs.iecr.9b04511
Ind. Eng. Chem. Res. 2020, 59, 2229−2241

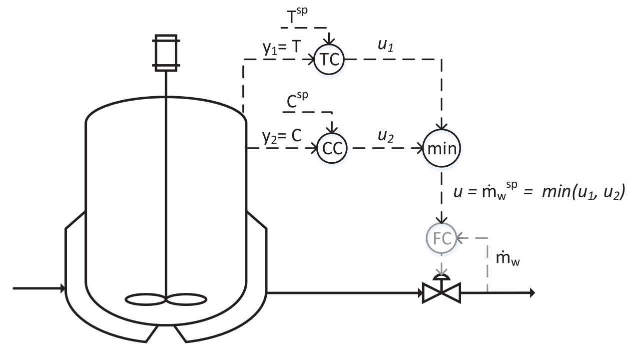

Figure 3. Typical example of CV to CV switching based on controller output signals. The regulatory layer is shown in gray.

desirable and economically optimal. It is also worth mentioning that this is a logical switch. It is not single-input multiple-output (SIMO) control, which usually refers to the use of *one* controller to control two CVs in some weighted or averaged manner (e.g., see Freudenberg and Middleton[30] and Amezquita-Brooks et al.[31]). For a more detailed discussion of CV to CV switching for optimal operation, the reader is referred to Krishnamoorthy and Skogestad.[32]

Case 2: MV to MV Constraint Switching. This case typically happens when the primary MV saturates, and an extra MV is added to cover the whole steady-state range and maintain control of the CV.

Three alternative schemes can be used for input to input constraint switching:

1. Split range control (SRC).
2. More than one controller for the same CV, each with a different set point.
3. Input (valve) position control.

In the first two schemes, only one MV is actively controlling the CV, whereas the other MVs are fixed at a limiting (minimum or maximum) values.

Split range control is the most common scheme. It has been in use for more than 75 years,[17,18] and it is still commonly implemented in industry.[33] Some other names that have been used for split range control are dual control agent,[17] range extending control,[14] and valve sequencing.[34] Figure 4 shows the

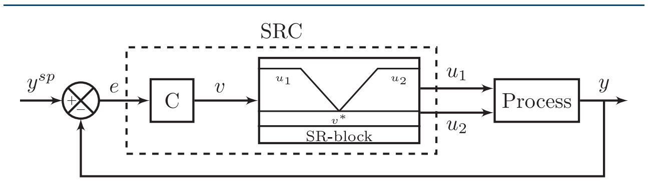

Figure 4. MV to MV constraint switching using split range control (SRC) for a case with two MVs (u_1 and u_2) and one CV (y).

block diagram of a split range controller (SRC) with two MVs (u_1 and u_2) for one CV (y). When the internal control signal (v) is below the split value (v^*), u_1 is used to control y, and u_2 is fixed at a limiting value; when v is above v^*, u_2 is used to control y, and u_1 is fixed at a limiting value.

Split range controllers should be designed considering the different dynamic effects of each MV on the output, as well as steady-state economics. There is a single controller (C) in Figure 4, but independent adjustments of the controller gains are possible by making use of the location of v^* or, equivalently, the slopes in the split range block (SR-block).[35] However, for *standard* split range control, other controller parameters, like the integral time, have to be the same for both inputs (MVs).

The most common alternative to split range control is to use one controller for each MV with different set points (e.g., y^{sp} and $y^{sp} + \Delta y^{sp}$), as shown in Figure 5. Δy^{sp} should be large enough such that only one controller is active at a given time, while the other inputs are at their limits.[36]

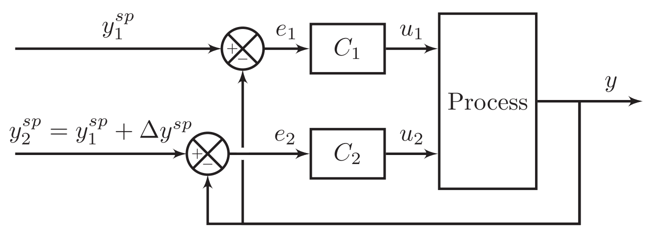

Figure 5. MV to MV constraint switching using two controllers with different set points.

The third option, shown in Figure 6, is input (valve) position control (VPC).[37,38] It is commonly used to improve the

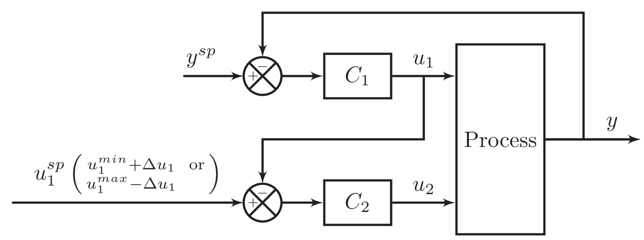

Figure 6. MV to MV constraint switching using input (valve) position control.

dynamic performance via the use of extra dynamic inputs and thus is sometimes referred to as input resetting[5,40] and midranging control.[41] (When used for dynamic reasons, u_1 takes care of the fast control, whereas u_2 takes care of the long-term control by continuously resetting u_1 to its desired setpoint (midrange position)[5,39]).

However, here, we are considering valve position control as an alternative to split range control to extend the steady-state range,[42] as shown in Figure 6. In this case, u_2 is only used to control u_1 when u_1 approaches its constraint. We cannot let u_1 fully saturate because then control of y is lost. If the input (u_1) approaches its limit (u_1^{lim}, upper or lower) given by u_1^{sp} (for example, $u_1^{sp} = u_1^{min} + \Delta u_1$), then input u_2 indirectly takes over the control of y by keeping u_1 close to this value (u_1^{sp}). Δu_1 is the "back-off" (i.e., $\Delta u_1 \neq 0$).

The advantage with the scheme in Figure 6 is that the output (y) is always controlled with the same "primary" input u_1. The disadvantages are that, because of the back-off, one cannot utilize the full steady-state range of this primary input (u_1), and tuning of the outer controller (C_2 in Figure 6) may be challenging.[40]

Case 3: MV to CV Constraint Switching. This happens when we have saturation of the MV (u_1) that we are using to control a CV (y_1). In this case, there are two possibilities:

1. The input saturation pairing rule is followed. This means that the CV (y_1) can be given up, which is shown in Figure 7. Here, the switch is already "built-in". That is, it is not necessary to do anything, except that we must implement antiwindup in C_1 for a good transition performance when

DOI: 10.1021/acs.iecr.9b04511
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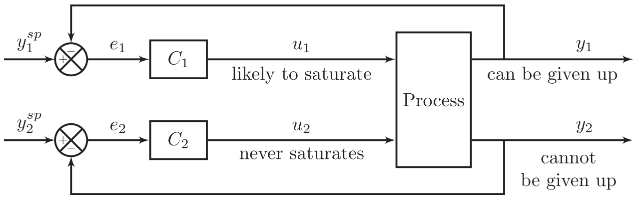

Figure 7. MV to CV switching for the case when the input saturation rule is followed, so control of y_1 can be given up.

control of y_1 is reactivated, that is, when u_1 is no longer saturated.

2. The input saturation pairing rule is *not* followed. This means that we cannot give up controlling the CV (y_1). Thus, when the MV (u_1) reaches its limit (saturates) we need to find another MV (u_2) to take over the task. This will generally invoke changing the pairing, because the new MV (u_2) is already controlling a low-priority CV (y_2). To do this, we may implement an MV to MV switching strategy, such as split range control, in combination with a min/max selector,[42] as shown in Figure 8.

An alternative solution from Shinskey[37] is shown in Figure 9. Here, controllers C_1 and C_2, for y_1 and y_2, are both designed for using u_2 as the input. We then have a selector for u_2, followed by a subtraction block that effectively does the split range control. Controller C_2 is used for controlling y_2 using u_2 as the input. C_2 needs antiwindup because u_2 is reassigned to controlling y_1 when u_1 saturates. Controller C_1, which controls y_1, is always active. It uses u_1 to control y_1 when u_1 is not saturated and switches to using u_2 when u_1 saturates. The "extra" control element for input u_1 (C_1' in Figure 9) can be just a gain, but it can also contain lead−lag dynamics. Note that the subtraction block in Figure 9 provides some built-in decoupling, which may be advantageous dynamically in the unconstrained case when both y_1 and y_2 are controlled.

Use of Antiwindup. When using min/max selectors, as in CV to CV constraint switching (Figure 2), it is necessary to implement tracking of the actual input (antiwindup) for all the controllers, such that the controllers that are *not* selected do not wind up. In MV to MV switching using split range control (Figure 4), there is a single controller (C) that always controls the output, so antiwindup is not needed unless *all* the inputs are saturated, just as for a standard single-input single-output (SISO) controller. In MV to MV switches, when using the selector in combination with input position control, the input (valve) position controller (C_2 in Figure 6) winds up when it is not active, and input tracking is required for this controller.

In MV to CV constraint switching, when the input saturation rule is not followed (Figure 8), antiwindup is necessary for the controller that usually manipulates the MV that is not coming from the split range controller (C_2 in Figure 8). The split range controller (C_1) is always actively controlling the high priority CV (y_1 in Figure 8). If all the inputs (u_1 and u_2 in Figure 8) saturate, antiwindup must also be implemented for C_1 as for a standard SISO controller.

■ CASE STUDY I: MIXING OF AIR AND METHANOL

In a formaldehyde production process, air and methanol (MeOH) are mixed in a vaporizer. Air is fed using a blower with limited capacity. The main controlled variable is the methanol molar fraction at the outlet of the vaporizer ($y_1 = x_{MeOH}$) which should be kept at 0.10 (desired) and with a minimum value of 0.08 (more important), such that the reaction can take place. Additionally, we want to control the total mass flow ($y_2 = \dot{m}_{tot}$) and, in some cases, to maximize it.

Step A1: Control Objectives, MVs, and Constraints. The controlled variables (CVs) are

- $y_1 = x_{MeOH}$: MeOH molar fraction
- $y_2 = \dot{m}_{tot}$: total mass flow

The two manipulated variables (MVs) for the supervisory control layer are

- $u_1 = \dot{m}_{air}^{sp}$: mass flow of air
- $u_2 = \dot{m}_{MeOH}^{sp}$: mass flow of methanol

Note that the physical MVs are the air blower rotational speed ($\dot{\omega}_{air}$) and the MeOH valve opening (z_{MeOH}), but we use a (lower) regulatory control layer with flow controllers for $\dot{m}_{air}$ and $\dot{m}_{MeOH}$, which follow $u_1 = \dot{m}_{air}^{sp}$ and $u_2 = \dot{m}_{MeOH}^{sp}$. Table 1 shows the maximum constraint values and nominal operating conditions. Note that the valve for $u_2 = \dot{m}_{MeOH}$ is not limited, and only $y_1 = x_{MeOH}$ and $u_1 = \dot{m}_{air}$ have relevant constraints. The model for the mixing process can be found in the Supporting Information.

Step A2: Priority List of Constraints. We generate the priority list for the constraints defined in step A1:

(P1) Physical MV inequality constraints:

$$\dot{m}_{air}^{min} \leq \dot{m}_{air} \leq \dot{m}_{air}^{max}, \text{ constraint on } u_1 \tag{3a}$$

$$\dot{m}_{MeOH}^{min} \leq \dot{m}_{MeOH} \leq \dot{m}_{MeOH}^{max}, \text{ constraint on } u_2 \tag{3b}$$

(P2) Critical CV inequality constraint:

$$x_{MeOH}^{min} \leq x_{MeOH} \leq x_{MeOH}^{max}, \text{ constraint on } y_1 \tag{4}$$

(P3) Less critical CV and MV constraint:

$$x_{MeOH} = x_{MeOH}^{sp}, \text{ set point for } y_1 \tag{5}$$

(P4) Desired throughput:

$$\dot{m}_{tot} = \dot{m}_{tot}^{sp}, \text{ set point for } y_2 \tag{6}$$

(P5) In this case, there are no unconstrained degrees of freedom, and thus, there are no self-optimizing variables.

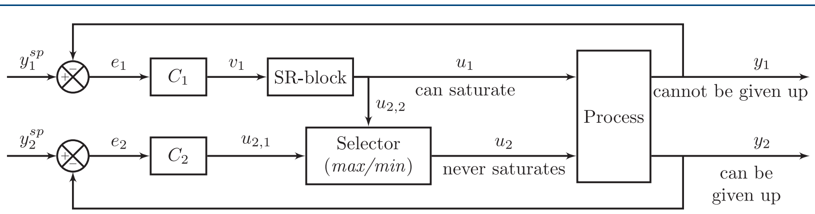

Figure 8. MV to CV switching for the case when the input saturation rule is not followed, so control of y_1 cannot be given up.

DOI: 10.1021/acs.iecr.9b04511
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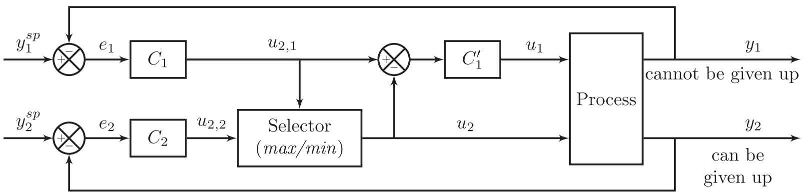

Figure 9. Alternative scheme for MV to CV switching when the input saturation rule is not followed.

Table 1. Maximum and Nominal Values for Case Study I

variable	unit	maximum value	nominal value
$y_1 = x_{MeOH}$	kmol/kmol	0.10	0.10
$y_2 = \dot{m}_{tot}$	kg/h	—	26 860
$u_1 = \dot{m}_{air}$	kg/h	25 800	23 920
$u_2 = \dot{m}_{MeOH}$	kg/h	—	2940

If there is no feasible solution that satisfies constraint 5 or 6 in P3 and P4, then constraints are given up in the order P4, P3, and P2. Constraints in P1 cannot be violated for physical reasons. The maximum set point values correspond to the maximum values given in Table 1.

Step A3: Active Constraint Switches. At the nominal operating point (defined in Table 1), we are able to satisfy all the constraints. It is always possible to control the MeOH concentration, that is, to satisfy constraint 5 in P3. The only relevant constraint switch happens when we reach the maximum bound on constraint 3a in P1, $u_1 = \dot{m}_{air}^{max}$. We then lose a degree of freedom (u_1), and according to the priority list for constraints, we give up controlling the constraint with the lowest priority, $y_2 = \dot{m}_{tot} = \dot{m}_{tot}^{sp}$ (constraint 6 in P4), which is the desired throughput.

Step A4: Base Case Control Structure. We have two available MVs (u_1 and u_2) for two CVs (y_1 and y_2), and we need to design the control structure. We will now consider two cases:

Case A: We follow the input saturation pairing rule; thus, we pair the MV, which may saturate ($u_1 = \dot{m}_{air}$), with the least important CV ($y_2 = \dot{m}_{tot}$). This control structure is shown in Figure 10. Here, there is no need for any additional logic for constraint switching, except that we need antiwindup for the air flow controller.

Case B: There might be some operational situation that prevents us from following the input saturation pairing rule. In this case, we pair $y_1 = x_{MeOH}$ with $u_1 = \dot{m}_{air}$ and $y_2 = \dot{m}_{tot}$ with $u_2 = \dot{m}_{MeOH}$.

Step A5: Control Structures for Active Constraint Switching (Case B). When the input saturation pairing rule is not followed (Case B), we implement an MV to MV switching strategy in combination with a min selector. Figure 11 shows the solution using split range control. We do not need input tracking (antiwindup) for the split range controller because $y_1 = x_{MeOH}$ is always being controlled; that is, the selected signal in the split range controller will always be active. Antiwindup is implemented for the flow controller for $y_2 = \dot{m}_{tot}$, as it will wind up during the period in which it is not selected, and we give up controlling $y_2 = \dot{m}_{tot}$.

Figure 12 shows an alternative implementation for Case B, using input (valve) position control (VPC). With this structure, u_1 is reset to 95% of its maximum capacity ($\omega_{air}^{sp} = 0.95(\omega_{air}^{max} - \omega_{air}^{min}) + \omega_{air}^{min}$) by manipulating $u_2 = \dot{m}_{MeOH}^{sp}$. Antiwindup is required for the input (valve) position controller (VPC) that uses u_2 to control u_1.

Simulations. Figure 13 shows simulation results for:

- Case A: pairing following the input saturation pairing rule, with no need for advanced control structure (see Figure 10).
- Case B: pairing *not* following the input saturation pairing rule, with no advanced control structure.
- Case B−SRC: pairing not following the input saturation pairing rule but using split range control with a min selector (see Figure 11).
- Case B−VPC: pairing not following the input saturation pairing rule but using input (valve) positioning control with a min selector (see Figure 12).

All the structures were tested for a step change in $y_1^{sp} = x_{MeOH}^{sp}$ of −0.005 (from 0.100 to 0.095) at t = 10 s, followed by a 10% increase in $y_2^{sp} = m_{tot}^{sp}$ (from 26 860 to 29 546 kg/h) at t = 30 s. In

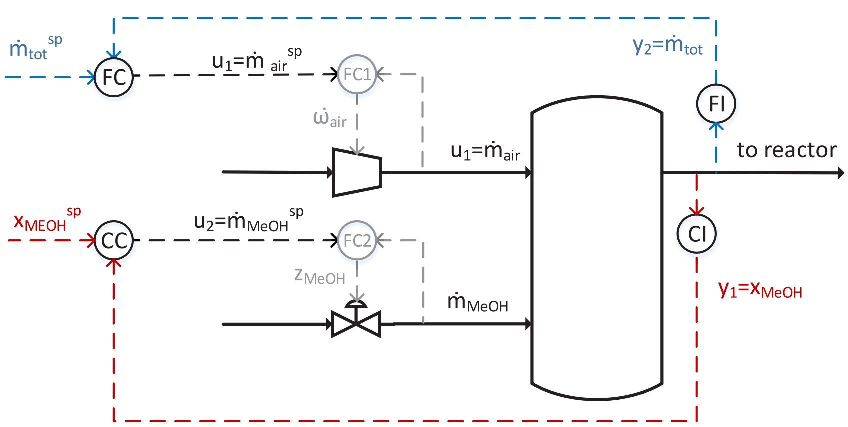

Figure 10. Case A: control structure for mixing of MeOH and air following the input saturation pairing rule. The (lower) regulatory control layer is shown in gray.

DOI: 10.1021/acs.iecr.9b04511
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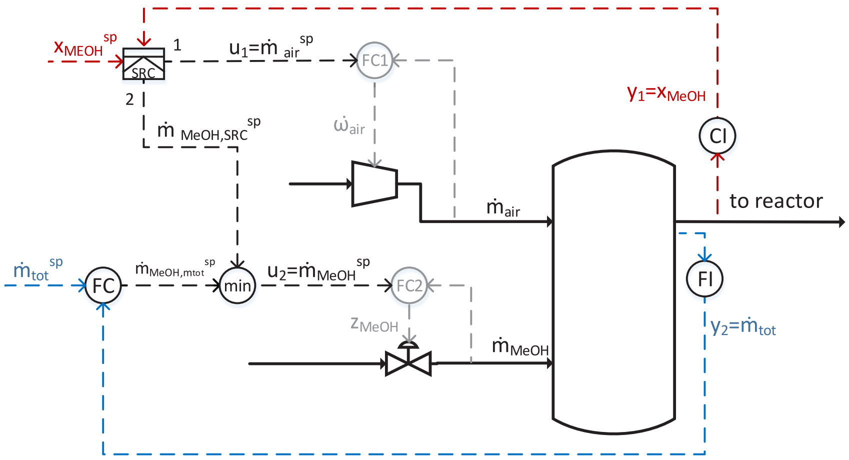

Figure 11. Case B−SRC: control structure for mixing of MeOH and air when not following the input saturation pairing rule, using split range control with a min selector.

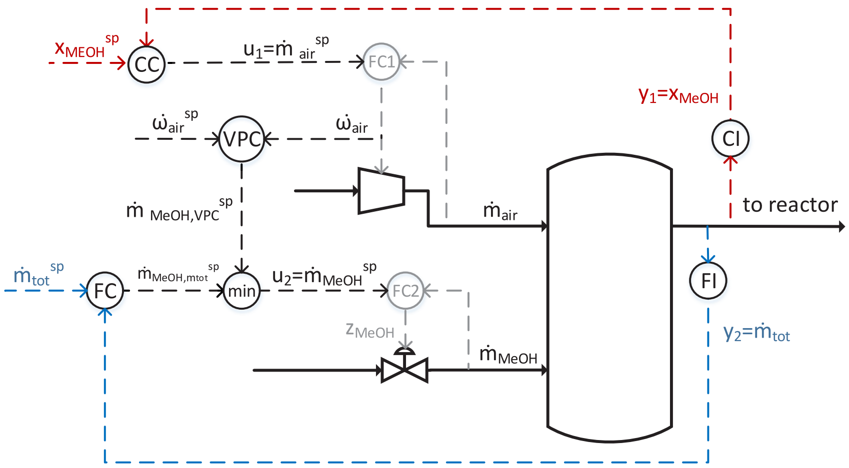

Figure 12. Case B−VPC: alternative control structure for mixing of MeOH and air in Case B, using input (valve) position control (VPC).

this period, $y_2 = m_{tot}^{sp}$ is not achievable, so the system should maximize the throughput ($y_2 = \dot{m}_{tot}$). Finally, we bring m_{tot}^{sp} back to its initial value at $t = 70$ s. All the tunings were found using the SIMC tuning rules.[43] The split range control structure was designed using the systematic procedure proposed by Reyes-Lúa et al.[35]

When we do not follow the input saturation pairing rule and do not implement any advanced control structure (Case B), $y_2 = \dot{m}_{tot}$ is highest, but it comes at the expense of not keeping $y_1 = x_{MeOH}$ at its set point and, thus, violating its maximum constraint (see Table 1).

As expected, the dynamic performance is best for Case A, when we follow the input saturation pairing rule. This is clear by comparing the response for Case A (blue line) with those for Case B with SRC (green line) and VPC (violet dashed line) in the two upper plots in Figure 13. In Case A and in Cases B−SRC and B−VPC, we always keep $y_1 = x_{MeOH}$ at its set point and instead give up controlling y_2 (throughput), which has a lower priority. In Case B−VPC, we are not able to fully maximize the throughput because the air blower (u_1) at steady state is limited to 95% of its capacity.

CASE STUDY II: CONTROL STRUCTURE FOR A DISTILLATION COLUMN

In this case study, we design the control structure for the conventional two-product distillation column in Figure 14. This column is similar to Column A, introduced by Skogestad and Morari,[44] also described by Skogestad and Postlethwaite.[5,45] This column splits a binary mixture with relative volatility α = 1.5 and has 41 equilibrium stages, including the reboiler and a total condenser. The feed (F) enters at stage 21.

The main assumptions for the model used in the simulations are constant relative volatility, constant molar overflow, constant pressure over the entire column, vapor−liquid equilibrium on every stage, and negligible vapor holdups. The product prices are assumed independent of composition, as long as the purity specifications of 95% are satisfied. Column data and prices are given in Table 2. Note that the valuable product is in the bottom.

Dynamically, this distillation column has six available manipulated variables (F, L, V, V_T, D, and B). However, the two levels and pressure must be controlled at all times for stable operation. In general, the set points to the regulatory controllers remain as degrees of freedom, but the two level set points have no steady-state effect and we assume that the pressure set point is constant.[46] We choose to use bottoms flow (B), distillate flow (D), and cooling (V_T) for controlling levels and pressure in the regulatory layer (Figure 14). (Flow controllers for L and V are

DOI: 10.1021/acs.iecr.9b04511
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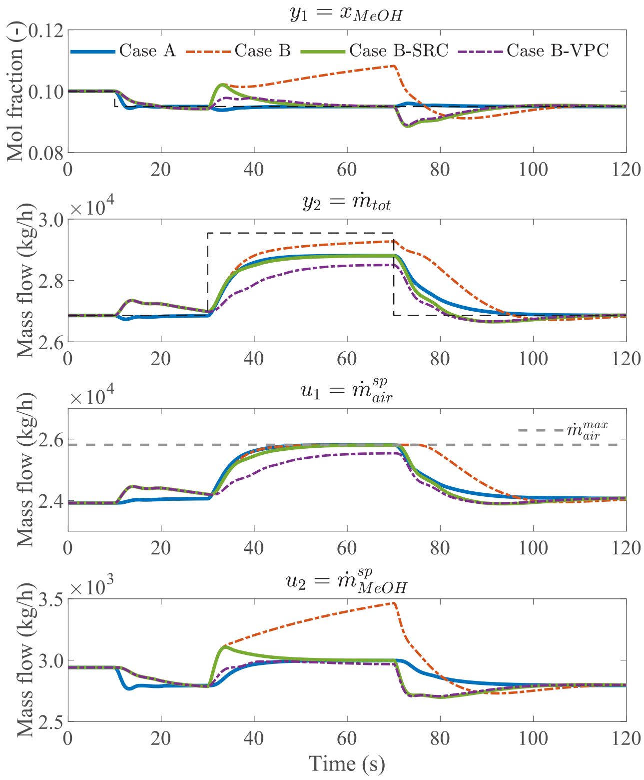

Figure 13. Comparison of control structures for mixing of MeOH and air. The best results are achieved with Case A and Case B−SRC.

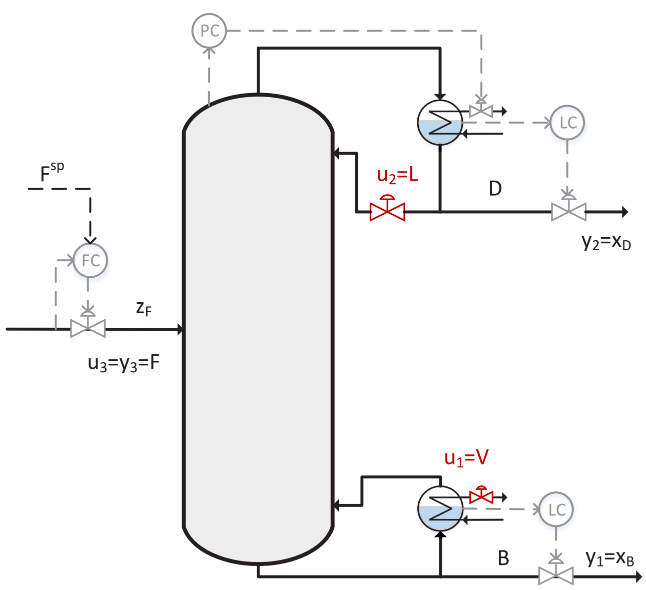

Figure 14. Distillation column with the regulatory control layer in gray. $u_1 = V$ and $u_2 = L$ are MVs for the supervisory control layer.

included in the regulatory layer, but are not shown in Figure 14.) This is the so-called LV configuration,[5] where reflux (L) and boilup (V) are left as manipulated variables for supervisory control. In addition, the feed rate (F) is in principle a manipulated variable, although in most cases it is given, and its set point is regarded as a disturbance.

The main disturbances are the feed set point (F^{sp}) and the energy price (p_V). Then, $d = [F^{sp}, p_V]$, where F^{sp} may vary from 1.0 to 1.68 mol/s, and p_V may vary from \$0.02 to 0.15 per mole. At the nominal point, F^{sp} = 1.0 mol/s and p_V = \$0.07 per mole.

Table 2. Data for Distillation Case Study

variable	unit	value
z_F	mol/mol	0.5
p_F	\$/mol	1.0
p_B	\$/mol	2.0
p_D	\$/mol	1.0
p_V	\$/mol	0.02−0.15
x_B^{min}	mol/mol	0.95
x_D^{min}	mol/mol	0.95
V^{max}	mol/s	4.00

Design of the Supervisory Control Layer. Let us start with the top-down economic analysis (step S1). For this distillation column with one feed stream and two products, the economic optimization problem can be written as[47]

$$\min_u J(u, d) = p_F F + p_V V - p_D D - p_B B$$

s.t.

$$x_B \geq x_B^{min} \quad \text{mole fraction of heavy component in } B \tag{7a}$$

$$x_D \geq x_D^{min} \quad \text{mole fraction of light component in } D \tag{7b}$$

$$V \leq V^{max} \quad \text{boilup} \tag{7c}$$

where F, V, D, and B are the molar flow rates of the feed, boilup, distillate, and bottoms.

Step A1: Control Objectives, MVs, and Constraints. We have three inputs $u = [L, V, F]$. Relevant disturbances are z_F, p_V, F^{sp}, and V^{max}, but for this analysis, we will consider $d = [p_V, F^{sp}]$ because we only need to find which active constraint switches occur, and variations in z_F and V^{max} only affect the value at which the constraints become active but not which constraints become active.

We still have not selected the controlled variables. Because the bottom product is the most valuable, optimal operation always corresponds to having constraint 7a active because this avoids product giveaway,[47,48] such that optimal operation is achieved when

$$y_1 = x_B = x_B^{min} \tag{8}$$

The less valuable distillate product is generally overpurified in order to avoid loss of the heavy component; thus, constraint 7b is normally not active. Under normal operation, the optimal solution is unconstrained, and we will assume that x_D is a good self-optimizing variable, and (close to) optimal operation is achieved when

$$y_2 = x_D = x_D^{opt}(p_V) \tag{9}$$

Note that x_D^{opt} will depend on the energy price (p_V). In addition, we would like to obtain a desired throughput, which is given by the equality constraint

$$y_3 = F = F^{sp} \tag{10}$$

Note that the feed rate (F) is considered both an MV and a CV, and its set point value (F^{sp}) is considered a disturbance (DV). Nominally, the MV and the CV are the same ($y_3 = u_3 = F^{sp}$), but in some cases, we must give up controlling y_3 and its set point, and instead use the MV (u_3) to control a CV with a higher priority, such as y_2 in Figure 18 and y_1 in Figure 21.

DOI: 10.1021/acs.iecr.9b04511
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In addition to these three equality constraints, we should also satisfy inequality constraint 7b on x_D and constraint 7c on V. This may not always be feasible, and the priority list is as follows.

Step A2: Priority List of Constraints.

(P1) Physical MV inequality constraints: maximum boilup, constraint 7c for u_2 ($V \leq V^{max}$).

(P2) Critical CV constraints: none.

(P3) Less critical CV constraints: constraint 7a ($x_B \geq x_B^{min}$) and constraint 8 ($x_B = x_B^{min}$) on bottom product composition (y_1) and constraint 7b ($x_D \geq x_D^{min}$) on top product composition (y_2).

(P4) Desired throughput: constraint 10 for y_3 ($F = F^{sp}$).

(P5) Self-optimizing variable: optimum concentration of less valuable product, constraint 9 for y_2 ($x_D = x_D^{opt}$).

Step A3: Active Constraint Switches. As mentioned, for the valuable bottom product, constraint 7a ($x_B = x_B^{min}$) is always optimally active. Assuming for now that we satisfy the throughput constraint ($F = F^{sp}$), we then have two remaining inequality constraints, one on x_D and one on V. With $n_c = 2$, there are, from eq 1, $2^{n_c} = 4$ possible active constraint regions:

- Region I: Only x_B is active (constraint 7a).
- Region II: x_B and V are active (constraints 7a and 7c).
- Region III: x_B and x_D are active (constraints 7a and 7b).
- Region IV: x_B, x_D, and V are active (constraints 7a, 7b, 7c).

Region IV, with three active constraints, is infeasible if we also want to have a given throughput ($F = F^{sp}$), because then there are only two available degrees of freedom, and we cannot satisfy three active constraints. Therefore, region IV will correspond to operation at maximum throughput, where we give up achieving $F = F^{sp}$.

Figure 15 shows the actual active constraint regions for this system, obtained by numerical optimization of the process (see Supporting Information). We stress that we include this diagram for illustration purposes, and it is not required to design the control structure. The transition between regions I and III, which corresponds to x_D reaching x_D^{min}, is a horizontal line because the column stage efficiency is assumed constant and independent of flow. At $F = 1.68$ mol/s, constraints 7a, 7b, 7c all become active (region IV), and we have to give up controlling $F = F^{sp}$.

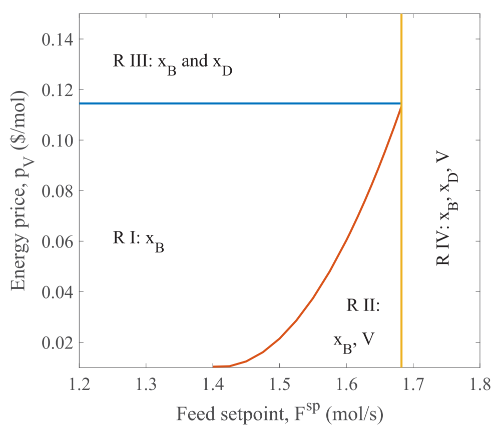

Figure 15. Active constraint regions for binary distillation column with the bottom as the valuable product.

Step A4: Base Case Control Structure. The nominal operating point is in region I, with a low energy price and a low feed rate. The only active inequality constraint is constraint 7a, and we must keep $x_B = x_B^{min}$. We also control the feed rate (constraint 10), and we select x_D as the self-optimizing variable associated with the remaining unconstrained degree of freedom (constraint 9). The optimal concentration, $x_D^{opt}(p_V)$, is given by an equation (see the Supporting Information). We want to use single-loop control, so we have to select pairings. With the standard LV configuration in Figure 14, it is obvious that the best pairing according to the pair-close rule is to use boilup (V) to control the bottom composition (x_B) and reflux (L) to control the top composition (x_D), as shown in Figure 16.

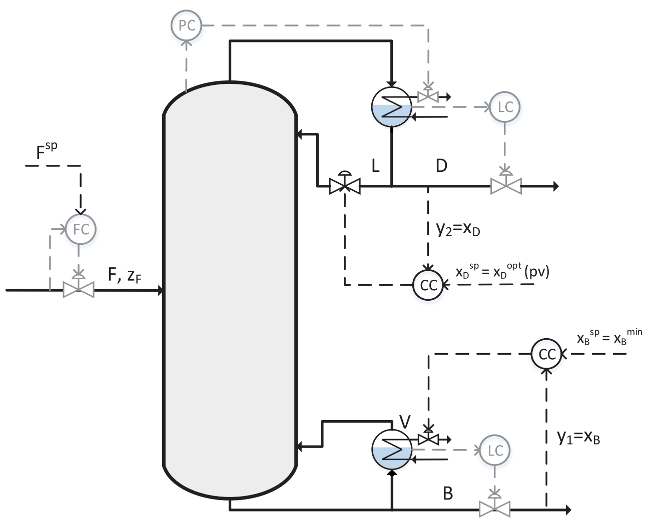

Figure 16. Base case control structure for distillation column (region I).

Step A5: Control Structures for Active Constraint Switching. We used the "obvious" pairing following the pair close rule for the base case structure in Figure 16. However, this implies that we did not follow the input saturation pairing rule because $u_2 = V$, which may saturate, is controlling $y_1 = x_B$, which is a more important CV than $y_2 = x_D$. As we increase the throughput ($d = F^{sp}$ increases), and the required boilup increases, we eventually reach $V = V^{max}$ and enter region II. Following the priority list of constraints, we must then give up controlling the self-optimizing variable $y_2 = x_D$ and start using $u_1 = L$ to control $y_1 = x_B$. We choose to use split range control with a min selector as our MV to CV constraint switching strategy, as shown in Figure 17. Alternatively, we could have implemented an input (valve) position control scheme, using L to prevent V from saturating.

If the energy price for V (p_V) increases, overpurifying the distillate is less favorable, and eventually we enter region III, where the constraint for $x_D(p_V)$ (constraint 7b) becomes active, and $x_D = x_D^{min} = 0.95$. This switch is achieved using a max selector for x_D. The control structure in Figure 17 works for regions I, II, and III. In order to also operate at maximum capacity and also satisfy constraints 7a–7c (region IV), we need to give up controlling $F = F^{sp}$. Thus, we need a CV to CV constraint switching strategy to switch between using $u_3 = F$ from controlling $F = F^{sp}$ to controlling $x_D = x_D^{min}$. One simple modification of the control structure in Figure 17 is the addition of a second controller for x_D (with set point $x_D^{min} + \Delta x_D$) and a min selector to switch between CV constraints on F and x_D. We already have another controller using $u_2 = L$ to control $y_2 = x_D^{min}$ in region III, so we need to introduce a back-off (Δx_D) to make sure that we activate the switch to use $u_3 = F$ only when needed

DOI: 10.1021/acs.iecr.9b04511
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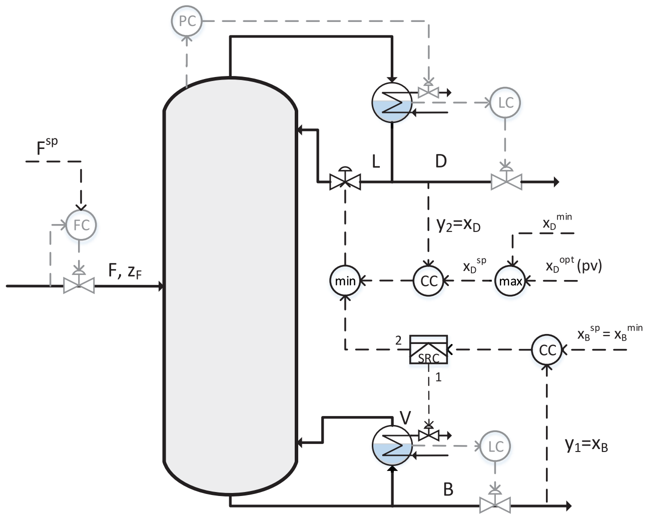

Figure 17. Control structure for distillation column for regions I, II, and III.

(region IV). We have $x_D^{min} = 0.95$ and select $\Delta x_D = -0.01$. Figure 18 shows the suggested control structure valid for all regions.

Table 3 shows how each of the MVs (L, V, and F) is used in each of the active constraint regions when we use the control structure in Figure 18. In region II, $y_2 = x_D$ is "floating"; that is, we are not actively controlling x_D. Note that composition controllers for x_D (CC_2 and CC_3 in Figure 18) will not be active at the same time because of the difference in set points (Δx_D).

Table 3. Pairings in Figure 18 for Each of the Active Constraint Regions

region	L	V	F
R I	$x_D = x_D^{opt}$	$x_B = x_B^{min}$	$F = F^{sp}$
R II	$x_B = x_B^{min}$	$V = V^{max}$	$F = F^{sp}$
R III	$x_D = x_D^{min}$	$x_B = x_B^{min}$	$F = F^{sp}$
R IV	$x_B = x_B^{min}$	$V = V^{max}$	$x_D = x_D^{min} + \Delta x_D$

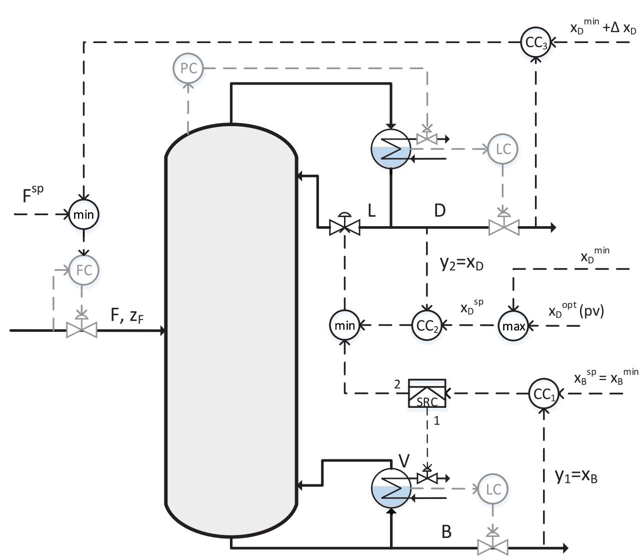

Figure 18. Control structure for distillation column for all regions (I, II, III, and IV).

Simulation. In this section we test the control structure in Figure 18. We first need to find the self-optimizing set point for $x_D^{opt}(p_V)$ to use in region I. Using Figure A3 in the Supporting Information, we observe that in region I, $x_D^{opt} \approx 0.996 - 0.384 p_V$. We use this equation to calculate x_D^{sp}.

For the simulations, we start at $F^{sp} = 1.5$ mol/s and $p_V = \$0.07$ per mole, which is inside region I. Then, at $t = 10$ s, we enter region II by setting $F^{sp} = 1.65$ mol/s. At $t = 50$ min, we enter region III by setting $p_V = \$0.13$ per mole. Finally, at $t = 100$ min, we enter region IV by setting $F^{sp} = 1.75$ mol/s.

Figure 19 shows the simulation results. The changes in active constraint region are marked with vertical dashed lines. As

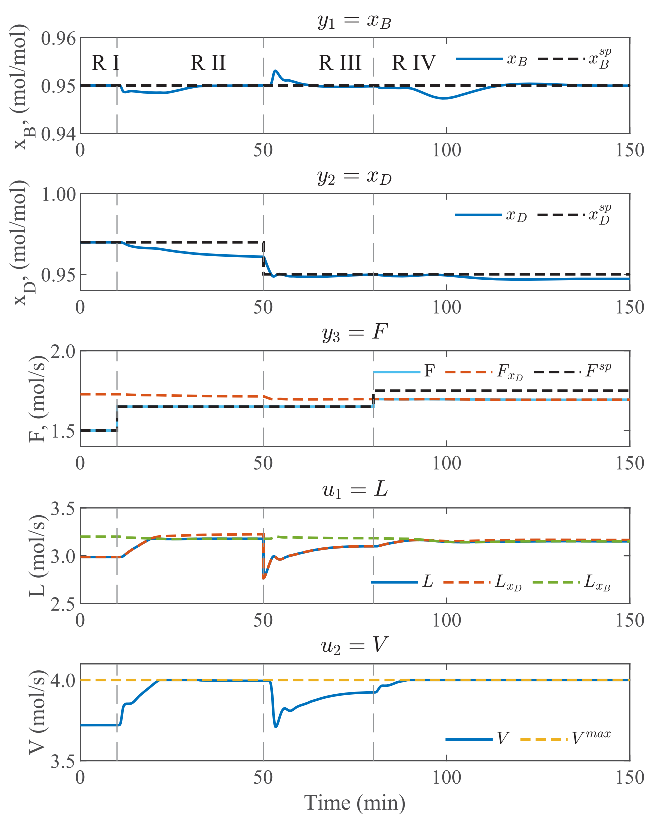

Figure 19. Simulation for structure in Figure 18 for Case Study II.

expected (see Table 3), in region II we give up controlling x_D when $V = V^{max}$, and we switch to using L (L_{x_B}) to control x_B. In region III, with $V < V^{max}$, we use V to control x_B and L (L_{x_D}) to keep $x_D = x_D^{min}$.

Figure 20 shows the value of the cost (J) as a function time.

■ DISCUSSION

Optimal Operation without a Model. In the proposed procedure, we do not need to know the actual value at which each constraint activates, but we need to know which constraints will activate. The switching between active constraints is done online using feedback. In many cases, expected constraint switches can be deduced using engineering insight.[47]

It is common to find cases in which optimal operation is the same as maximum throughput. If we can identify the bottleneck and control it, then we do not need to perform an optimization procedure to maximize throughput.[2,49] In Case Study I, we know that by keeping $\dot{m}_{air}^{max}$ and, thus, maximizing the total outlet flow, we are operating at optimum conditions. In Case Study II,

DOI: 10.1021/acs.iecr.9b04511
Ind. Eng. Chem. Res. 2020, 59, 2229−2241

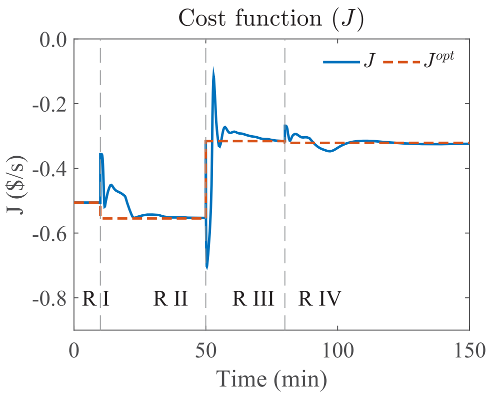

Figure 20. Cost for distillation column case study (which should be minimized).

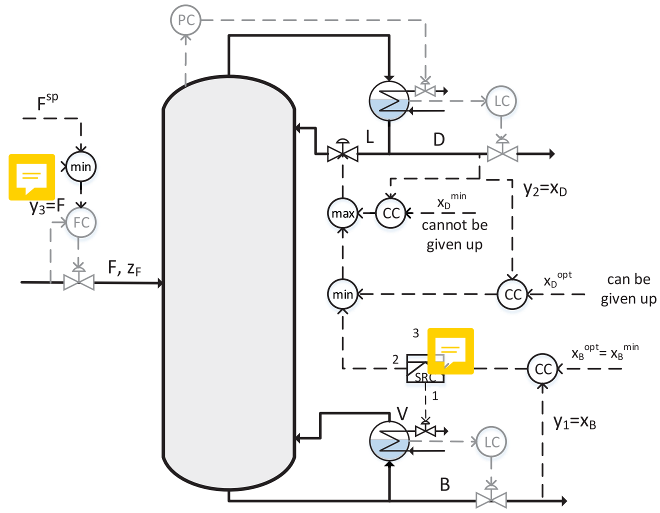

Figure 21. Alternative control structure for distillation column (all regions). This structure behaves differently from that in Figure 18 when maximizing throughput (region IV).

operating with the active constraints in region IV will maximize throughput.

Opposing Pairing Rules. Sometimes there are pairing rules that oppose. In step A4 of Case Study II (distillation column), the pairing suggested by the pair close rule is not the same as the pairing suggested by the input saturation pairing rule. In these cases, we have two options:

1. Follow the pairing rule that leads to the structure that will have better dynamic behavior for most of the time (pair close rule).
2. Follow the pairing rule that will require less loop reconfiguration when we switch among the relevant active constraint regions (input saturation pairing rule).

The decision will depend on each particular case. In Case Study II, we chose to follow the pairings suggested by the pair close rule, because it gave better dynamic behavior, and we considered that the process would normally operate in region I.

Alternative Control Structures. In step A5 of the proposed procedure, there may be alternative options that achieve the required active constraint switches and achieve the same steady state. However, the alternative control structures may differ in dynamic behavior.

For example, in Case Study II, we proposed the control structure in Figure 18. An alternative structure is shown Figure 21, in which we use a split range controller for x_B with three MVs (V, L, and F). The numbers 1, 2, and 3 in the split range block (SRC) refer to the order in which each MV is used.

1. $y_1 = x_B$ is normally controlled using $u_1 = V$ in region I.
2. If V saturates (region II), we switch to using $u_2 = L$.
3. If L has to control $y_2 = x_D^{min}$, then we switch to using $u_3 = F$ to control $y_1 = x_B$.

The structure in Figure 21 is better from a dynamic point of view in region IV because it is better to use F rather than L to control x_B.

CONCLUSION

We introduced a systematic procedure to design constraint switching schemes using classical controllers and logics. We distinguish among three kinds of constraint switches:

- CV to CV constraint switching: Use selectors.
- MV to MV constraint switching: Use split range control or, alternatively, controllers with different set points or input (valve) position control.
- MV to CV constraint switching: Use nothing if the input saturation pairing rule is followed; otherwise, use an MV to MV scheme with a selector to take over control when the main MV saturates.

In the two presented case studies, we achieved steady-state optimal operation, despite changes in active constraint regions, using single-loop PID-based control structures.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.iecr.9b04511.

Appendices containing the model used for Case Study I and the optimization results for Case Study II (PDF)

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Notes

The authors declare no competing financial interest.

ACKNOWLEDGMENTS

The authors thank Cristina Zotică for her valuable input.

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DOI: 10.1021/acs.iecr.9b04511
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