

Systematic design of active constraint switching using classical advanced control structures

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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) due to 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 Fig. 1. The upper layers are related to long-term economic optimization, whereas the two lower layers are control layers, with the objective to keep the controlled variables (CVs) at their desired setpoints.

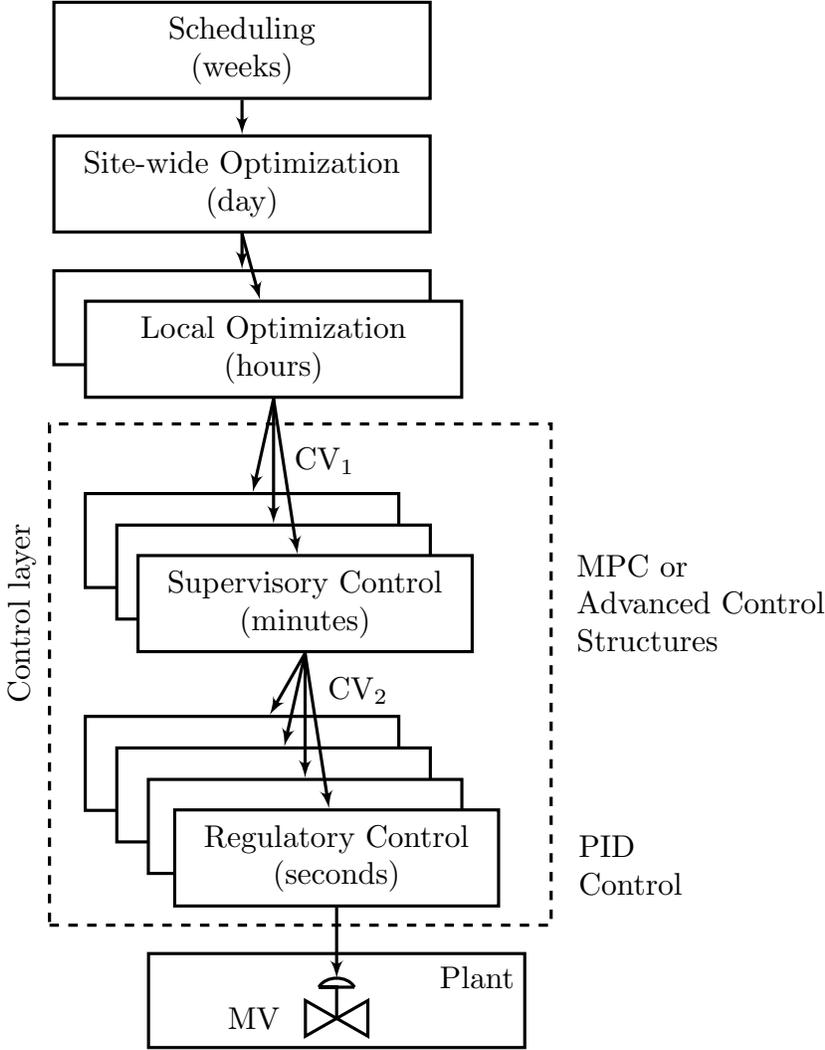


Figure 1: Typical control hierarchy in a process plant.

The control layer is sub-divided into a supervisory control layer and a regulatory or stabilizing control layer. The main objective of the regulatory layer is to stabilize the process and avoid drifting away from the desired steady-state, and to reject disturbances on a fast

time scale^{1,2}. The supervisory control layer should follow the setpoints for the controlled variables computed by the optimization layer (CV₁). Importantly, this involves switching between active constraint changes in CV₁. It also calculates the setpoints for the regulatory layer (CV₂), 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.

Skogestad² proposed a systematic procedure for control structure design for complete process plants. The procedure is separated in two main parts: top-down analysis and bottom-up design. The top-down analysis focuses on identifying the steady-state optimal operation, usually based on economics. The bottom-up part focuses on the design of the control layer structure. The procedure is as follows:

- *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 controlled variables (CV₁). Active constraints should always be controlled for optimal operation. For the remaining unconstrained degrees of freedom we should control "self-optimizing" variables, which, when kept constant, indirectly minimize the cost³.

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 (CV_2) and, since single-loop control is preferred in this layer, choose pairings for CV_2 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 variables³ 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, while 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 setpoint for the CV_2 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 setpoints². Controlling the self-optimizing variable to its optimal setpoint keeps the process at (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 ($J_u = dJ/du$). 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 setpoints 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, prices, and drift 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 it⁷. Stephanopoulos⁸ states that an optimizing control strategy in the supervisory layer must identify when the plant must be moved to a new operating point (changes active constraint region) and then make the appropriate setpoint changes to bring the plant to the new optimum 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 that it represents a unified systematic procedure to control multivariable processes⁹. 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 Georgakis¹⁰). 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 information¹³. Some classical

advanced control elements (blocks, idioms¹⁴) used in addition to PID controllers include^{15,16}:

- cascade
- feedforward and ratio
- decoupling
- calculation block
- valve position (input resetting)
- selector (*max*, *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 Foss¹⁹ 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. Vandebussche²⁰, Govind and Powers^{21, 22}, Bristol¹⁴, Stephanopoulos⁸). Although some good ideas were introduced, this research has had limited impact. More recently Hägglund and Guzmán²³ 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 setpoints 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 objective, MVs and constraints

The control objectives in the supervisory layer are specified in terms of *controlled variables* (CVs) with setpoints. These follow from step S3 in the top-down analysis. These were called CV_1 earlier, but for simplicity we will now just call them CV in the rest of the paper. 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 due to 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, based on a partial analysis in step S3 and engineering judgment, list the expected controlled variables:

1. Outputs (CVs) with setpoints (denoted CV equality constraints in the following). For example, product specifications and operating pressures and temperatures.
2. Input variables with desired values or setpoints (denoted MV equality constraints in the following). For example, 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 setpoints should indirectly minimize the economic cost.
6. Desired throughput (production rate). Typically, but not always, a flowrate (MV or CV) with a given setpoint.

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 unachievable high setpoint 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 setpoint may need to vary depending on the disturbance value; for example, the feed rate. To identify self-optimizing variables and their setpoints, 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 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 setpoints 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.* It is physically impossible to give them 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) *Non-physical MV and less critical CV constraints* (both equality and inequality constraints). These may be given up; for example a desired pressure (CV equality constraint). By non-physical 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, which 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, which 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; for example, a desired setpoint for a byproduct concentration. Within the constraints in P3, there might be CV or MV equality constraints with a higher priority than others. It should also be noted that constraints in P3, P4 and P5 may include the same variables that are already used in P1 and P2, but with different bounds.

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 possible constraints have been identified and prioritized, we proceed to identify active constraint switches. This will occur when disturbances cause a CV or MV to reach a new inequality constraint and we have to give up controlling some other variable or, reversely, that 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 necessary⁷. We only need to know which active constraint switches are relevant. 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 value of the MVs and CVs. It is insightful to know

the maximum number of active constraint regions, which is given by⁷:

$$n_r^{max} = 2^{n_c} \quad (1)$$

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

$$n_r < n_r^{max} \quad (2)$$

The following criteria is useful to find 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, maximum or 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 response²⁶.

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 to pair MVs with CVs according to the following rule²⁶:

Input saturation pairing rule: *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 which 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) which 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 *max/min* selector, so that the active CV constraint is always selected. Fig. 2 shows the block diagram with two CVs (y_1 and y_2) and one MV (u). It is important to note that anti-windup must be implemented in both controllers (C_1 and C_2).

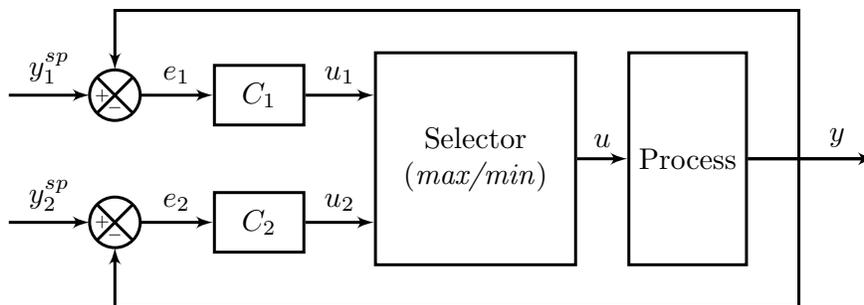


Figure 2: CV to CV switching using a selector for the case with two CVs (y_1 and y_2) .

A possible misconception here is that all the CVs (y_1 and y_2 in Fig. 2) need to be of the same type (e.g. temperature) as in *auctioneering*, where we have one controller and the selector is on the input of the controller and we select to control one of several similar outputs⁵. However, in general the CVs may be of different type if the selector is on the output from the controller²⁷, as in Fig. 2. As an example, Fig. 3 shows a flowsheet in which the coolant flow, actually its setpoint ($u = \dot{m}_w^{sp}$), 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 the CV switching between temperature (y_1) and composition (y_2).

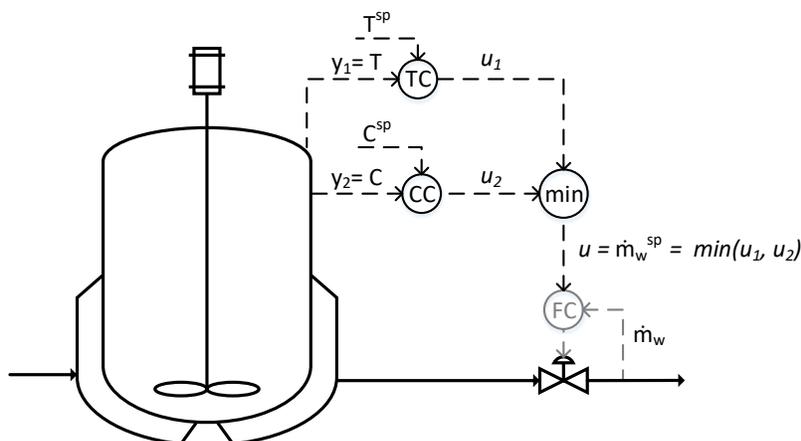


Figure 3: Typical example of CV to CV switching based on controller output signals. The regulatory layer is dimmed in gray.

Such schemes are sometimes called *override control*²⁷⁻²⁹. However, we prefer to call it *CV*

to *CV switching* to avoid the connotation of "error" or "emergency" of the term *override*. On the contrary, the CV to CV switching is 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 average manner (e.g. Freudenberg and Middleton,³⁰ Amezcuita-Brooks et al.³¹). For a more detailed discussion of CV to CV switching for optimal operation, the reader is referred to Krishnamoorthy and Skogestad³².

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 setpoint.
3. Input (valve) position control.

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

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 industry³³. Some other names that have been used for split range control are *dual control agent*¹⁷, *range extending control*¹⁴ and *valve sequencing*³⁴. Fig. 4 shows the 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 , while u_2 is fixed at a limiting value; when v is above v^* , u_2 is used to control y , while 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)

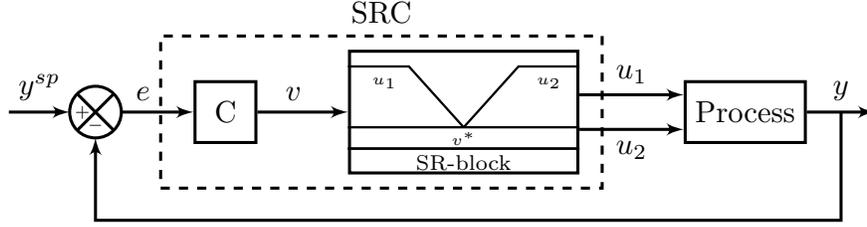


Figure 4: MV to MV constraint switching using split range control (SRC) for a case with two MVs (u_1 and u_2) and one CV (y).

in Fig. 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 setpoints, e.g. y^{sp} and $y^{sp} + \Delta y^{sp}$, as shown in Fig. 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 limits³⁶.

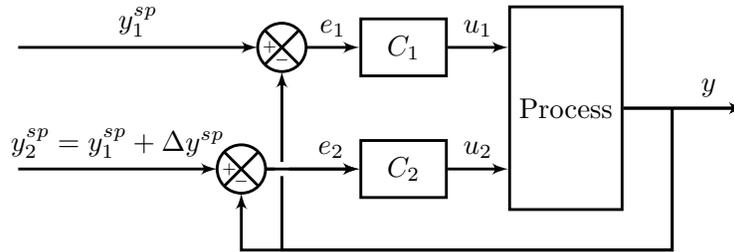


Figure 5: MV to MV constraint switching using two controllers with different setpoints.

The third option, shown in Fig. 6, is *input (valve) position control* (VPC)^{37,38}. It is commonly used to improve the dynamic performance by the use of extra dynamic inputs¹, and then is sometimes referred to as *input resetting*^{5,40} and *mid-ranging control*⁴¹.

However, here we are considering it as an alternative to split range control to extend the steady-state range⁴², as shown in Fig. 6. In this case, u_1 always controls y . We cannot let

¹When used for dynamic reasons, while u_1 takes care of the fast control, u_2 takes care of the long-term control, and u_1 (usually a valve) is slowly *reset* to a desired *mid-range position* (u_1^{sp}) using u_2 ^{5,39}. This way, the MV controlling the CV (u_1) does not saturate.

u_1 fully saturate because otherwise 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 this scheme is that the output (y) is always controlled with the same "primary" input u_1 . The disadvantages are that one cannot utilize the full steady-state range of this "primary" input (u_1), and that tuning of the outer controller (C_2 in Fig. 6) may be challenging⁴⁰.

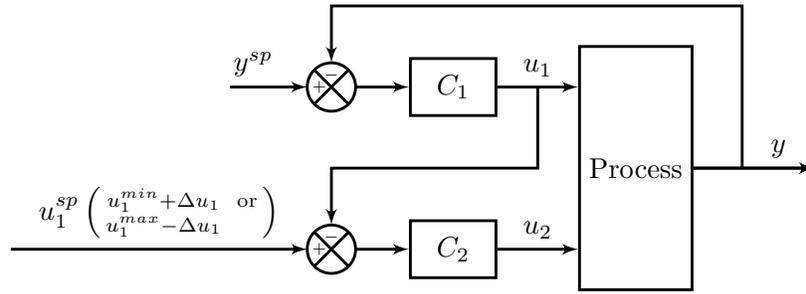


Figure 6: MV to MV constraint switching using input (valve) positioning control.

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* was followed. This means that the CV (y_1) can be given up: This case is shown in Fig. 7. Here, the switch is already "built-in". That is, it is not necessary to do anything, except that we must be implement anti-windup in C_1 for a good transition performance when control of y_1 is reactivated; that is, when u_1 is no longer saturated.
2. The *input saturation pairing rule* was *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 a repairing,

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* selector⁴², as shown in Fig. 8.

An alternative solution³⁷ is shown in Fig. 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 which effectively does the split range control. Controller C_2 is used for controlling y_2 using u_2 as the input. C_2 needs anti-windup 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 Fig. 9) can be just a gain, but it can also contain lead-lag dynamics. Note that the subtraction block in Fig. 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 anti-windup

When using *min/max* selectors, as in *CV to CV constraint switching* (Fig. 2), it is necessary to implement tracking of the actual input (anti-windup) 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 (Fig. 4), there is a single controller (C), which always controls the output, so anti-windup is not needed except if *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 Fig. 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 (Fig. 8), anti-windup is necessary for the controller that usually manipulates the MV that is not coming from the split range controller (C_2 in Fig. 8). The split range controller (C_1) is always actively controlling the high priority CV (y_1 in Fig. 8). If all the inputs (u_1 and u_2

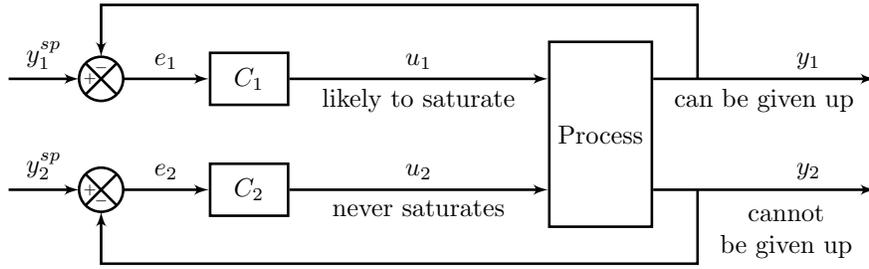


Figure 7: MV to CV switching for the case when the input saturation rule is followed, so control of y_1 can be given up.

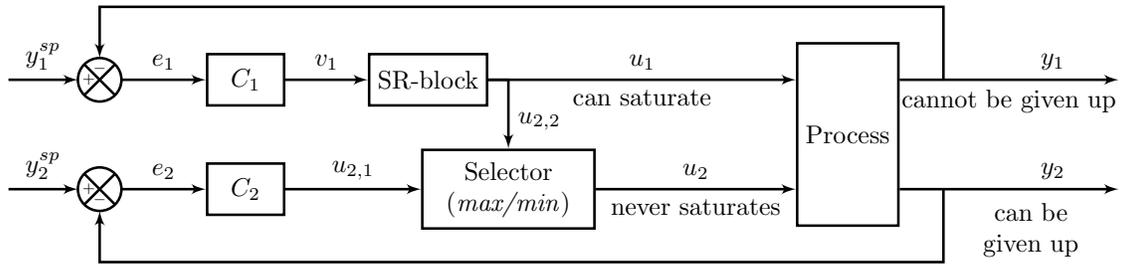


Figure 8: MV to CV switching for the case when the input saturation rule is *not* followed; so control of y_1 cannot be given up.

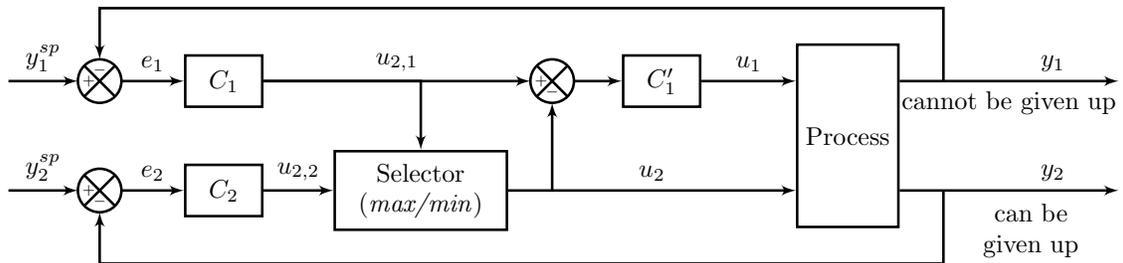


Figure 9: Alternative scheme for MV to CV switching when the input saturation rule is *not* followed.

in Fig. 8) saturate, anti-windup 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 0.1 (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 objective, 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.

Table 1: Maximum and nominal values for case study I.

Variable	Units	Maximum	Nominal
$y_1 = x_{MeOH}$	kmol/kmol	0.10	0.10
$y_2 = \dot{m}_{tot}$	kg/h	-	26860
$u_1 = \dot{m}_{air}$	kg/h	25800	23920
$u_2 = \dot{m}_{MeOH}$	kg/h	-	2940

Step A2: Priority list of constraints

We generate the priority list for the constraints defined in step A1:

(P1) *Physical MV inequality constraints:*

$$\dot{m}_{air}^{min} \leq \dot{m}_{air} \leq \dot{m}_{air}^{max}; \text{ constraint on } u_1 \quad (3a)$$

$$\dot{m}_{MeOH}^{min} \leq \dot{m}_{MeOH} \leq \dot{m}_{MeOH}^{max}; \text{ constraint on } u_2 \quad (3b)$$

(P2) *Critical CV inequality constraints:*

$$x_{MeOH}^{min} \leq x_{MeOH} \leq x_{MeOH}^{max}; \text{ constraint on } y_1 \quad (4)$$

(P3) *Less critical CV and MV constraints:*

$$x_{MeOH} = x_{MeOH}^{sp}; \text{ setpoint for } y_1 \quad (5)$$

(P4) *Desired throughput:*

$$\dot{m}_{tot} = \dot{m}_{tot}^{sp}; \text{ setpoint for } y_2 \quad (6)$$

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

If there is no feasible solution that satisfies Eq. (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 setpoint values are 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 (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, $y_2 = \dot{m}_{tot} = \dot{m}_{tot}^{sp}$ ((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 Fig. 10. Here there is no need for any additional logic for constraint switching, except that we need anti-windup 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 constraints switching (Case B)

When the *input saturation pairing rule* was not followed (case B), we implement an *MV to MV switching strategy* in combination with a *min* selector. Fig. 11 shows the solution

using split range control. We do not need input tracking (anti-windup) 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. Anti-windup 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 $y_2 = \dot{m}_{tot}$.

Fig. 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 $u_2 = \dot{m}_{MeOH}^{sp}$. Anti-windup is required for the input (valve) position controller (VPC) that uses u_2 to control u_1 .

Simulations

Fig. 13 shows simulation results for:

- Case A: pairing following the *input saturation pairing rule*, with no need of advanced control structure, see Fig. 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 Fig. 11.
- Case B-VPC: pairing not following the *input saturation pairing rule*, but using input (valve) positioning control with a *min* selector; see Fig. 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 $y_2^{sp} = \dot{m}_{tot}^{sp}$ (from 26860 kg/h to 29546 kg/h) at $t = 30$ s. In this period, $y_2 = \dot{m}_{tot}^{sp}$ is not achievable, so the system should maximize the throughput ($y_2 = \dot{m}_{tot}$). Finally, we bring \dot{m}_{tot}^{sp} back to its initial value at $t = 70$ s. All the

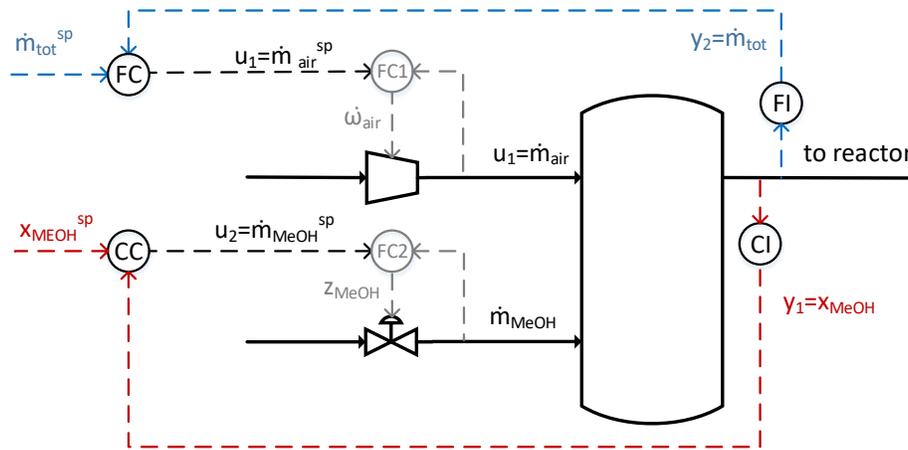


Figure 10: Case A: control structure for mixing of MeOH and air following the *input saturation pairing rule*. The (lower) regulatory control layer is dimmed in gray.

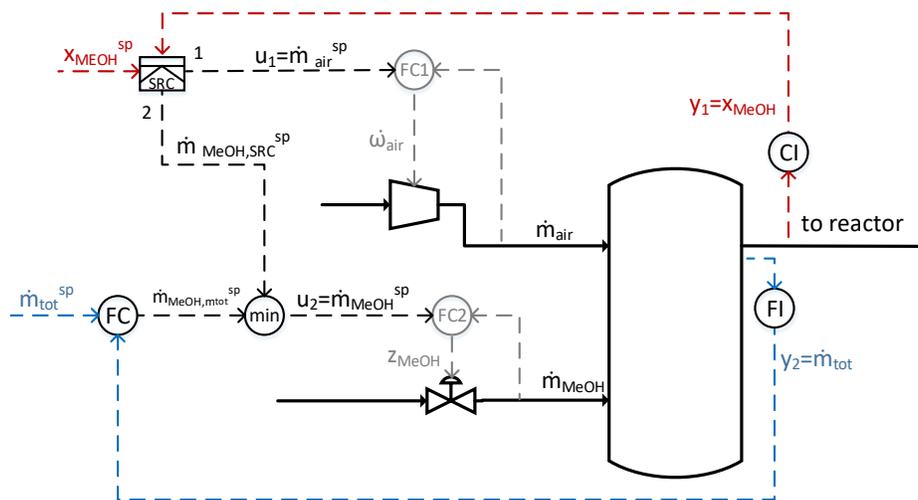


Figure 11: Case B-SRC. Control structure for mixing of MeOH and air when *not* following the *input saturation pairing rule* using split range control with a *min* selector.

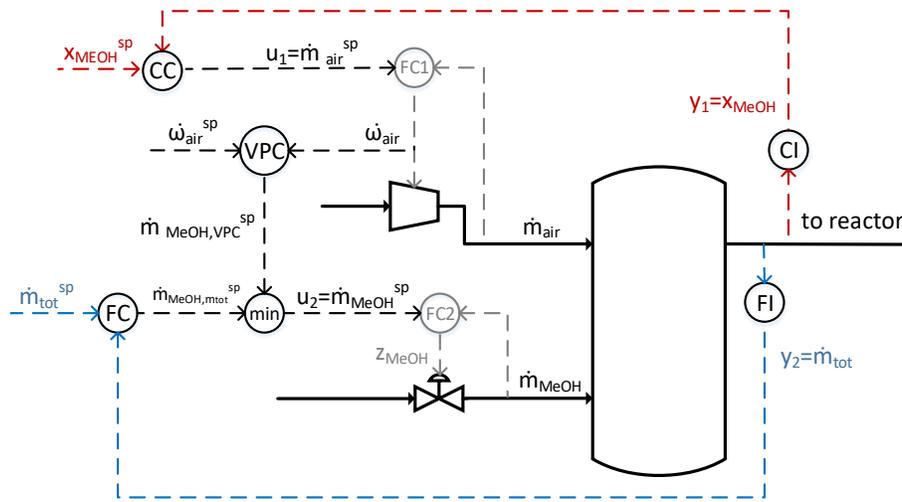


Figure 12: Case B-VPC. Alternative control structure for mixing of MeOH and air in Case B, using input (valve) positioning control (VPC).

tunings were found using the SIMC tuning rules⁴³. 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 setpoint 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 for SRC (green line) or VPC (violet dashed line) in the two upper plots in Fig. 13. In case A and in cases B-SRC and B-VPC, we always keep $y_1 = x_{MeOH}$ at its setpoint 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.

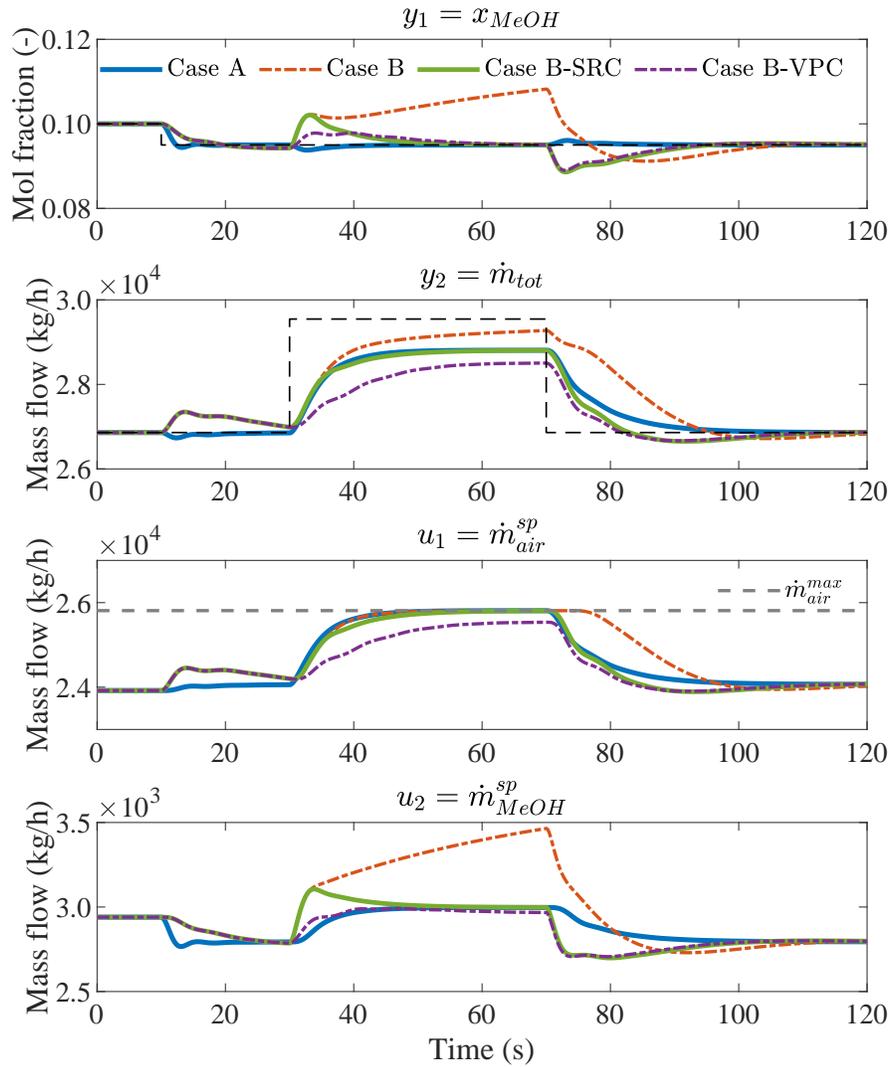


Figure 13: Comparison of control structures for mixing of MeOH and air. The best results are achieved with Case A and case B-SRC.

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 Fig. 14. This column is similar to Column A, introduced by Skogestad and Morari⁴⁴, also described by Skogestad and Postlethwaite^{5,45}. This column splits a binary mixture with relative volatility $\alpha = 1.5$ and has 41 equilibrium stages, including the reboiler and a total condenser. The feed (F) enters at stage 21.

The main assumptions 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 , B). However, the two levels and pressure must be controlled at all times for stable operation. In general, the setpoints to the regulatory controllers remain as degrees of freedom, but the two level setpoints have no steady-state effect and we assume that the pressure setpoint is constant⁴⁶. We choose to use bottoms flow (B), distillate flow (D), and cooling (V_T) for controlling levels and pressure in the regulatory layer (Fig. 14)². This is the so-called LV configuration⁵, where reflux (L) and boilup (V) are left as manipulated variables for supervisory control. In addition, the feedrate (F) is in principle a manipulated variable, although in most cases it is given, and its setpoint is regarded as a disturbance.

The main disturbances are the feed setpoint (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 from 0.02 to 0.15 \$/mol. At the nominal point, $F^{sp} = 1.0$ mol/s and $p_V = 0.07$ \$/mol.

²Flow controllers for L and V are included in the regulatory layer, but are not shown in Fig. 14.

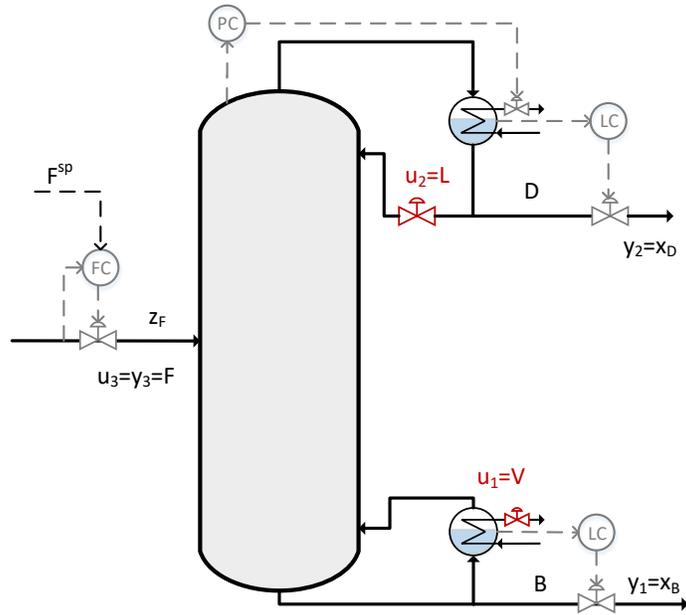


Figure 14: Distillation column with regulatory control layer in gray. $u_1 = V$ and $u_2 = L$ are MVs for the supervisory control layer.

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 as⁴⁷:

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

$$\text{s.t. } x_B \geq x_B^{\min} \quad \text{mol fraction of heavy component in B} \quad (7a)$$

$$x_D \geq x_D^{\min} \quad \text{mol fraction of light component in D} \quad (7b)$$

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

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

Table 2: Data for distillation case study.

Variable	Units	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

Step A1: Control objective, 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. Since 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

$$y_1 = x_B = x_B^{min} \quad (8)$$

The less valuable distillate product is generally overpurified in order to avoid loss of the heavy component; so, 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

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

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

$$y_3 = F = F^{sp} \quad (10)$$

Note that the feedrate (F) is considered both an MV and a CV, and its setpoint value (F^{sp}) is considered a disturbance (DV)³.

In addition to these three equality constraints, we should also satisfy inequality constraints (7b) on x_D and (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 for u_2 (7c) ($V \leq V^{max}$).

(P2) *Critical CV constraints:* none.

(P3) *Less critical CV constraints:* constraint (7a) ($x_B \geq x_B^{min}$) and (8) ($x_B = x_B^{min}$) on bottom product composition (y_1) and (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 ($F = F^{sp}$),

³Nominally, 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 setpoint, and instead use the MV (u_3) to control a CV with higher priority (y_2 in Fig. 18 and y_1 in Fig. 21).

we then have two remaining inequality constraints, on x_D and V . With $n_c = 2$, there are $2^{n_c} = 4$ possible active constraint regions:

- Region I: only x_B active (constraint (7a))
- Region II: x_B and V active (constraints (7a) and (7c))
- Region III: x_B and x_D active (constraints (7a) and (7b))
- Region IV: x_B , x_D and V active (constraints (7a), (7b) and (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 $F = F^{sp}$.

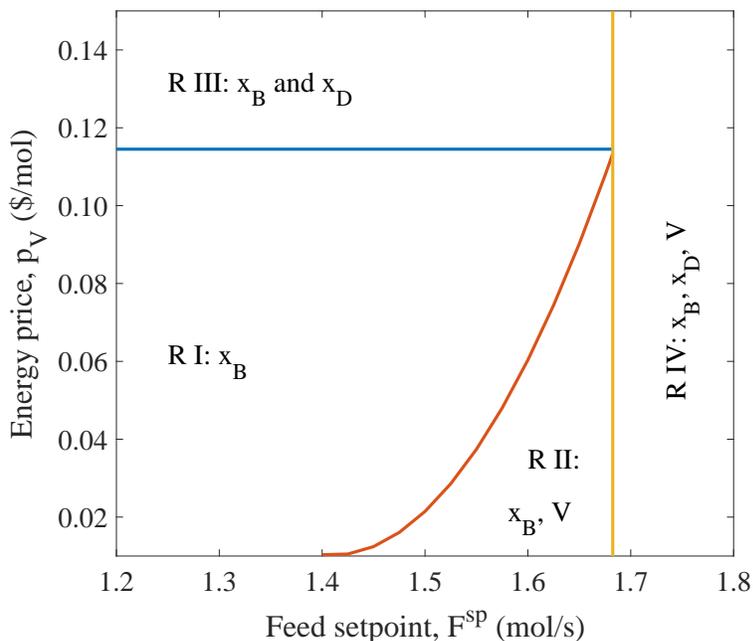


Figure 15: Active constraint regions for binary distillation column with the bottom as valuable product.

Fig. 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, independent of flow. At $F = 1.68$ mol/s, all three inequality constraints in (7) become active (region IV) and we have to give up controlling $F = F^{sp}$.

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 (7a) and we must keep $x_B = x_B^{min}$. We also control the feedrate (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 Supporting Information). We want to use single-loop control so we have to select pairings. With the standard *LV*-configuration in Fig. 14, it is obvious that the best pairing 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 Fig. 16.

Step A5: Control structures for active constraints switching

We used the "obvious" pairing following the *pair close* rule for the base case structure in Fig. 16. However, this implies that we did not follow the *input saturation pairing rule* since $u_2 = V$, 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 Fig. 17. Alternatively, we could have implemented an input (valve) position control scheme, using L to prevent V from saturating.

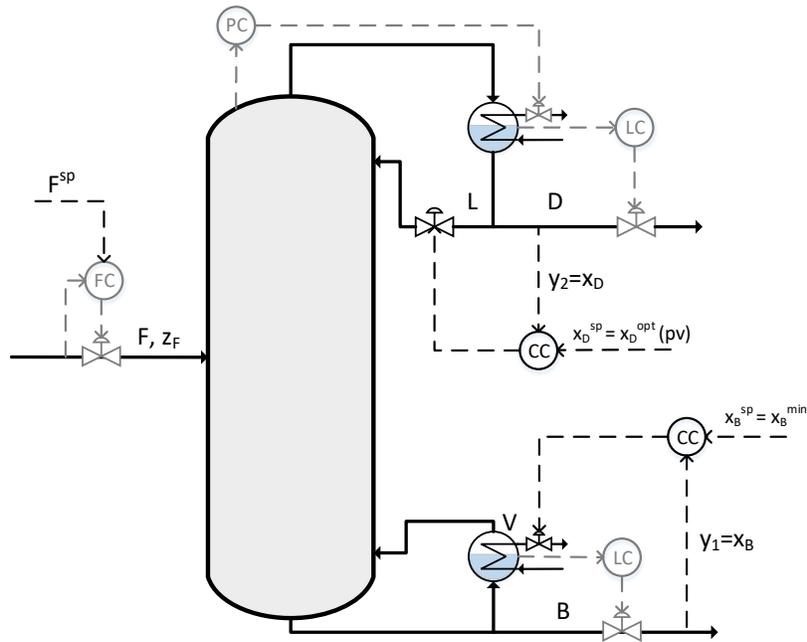


Figure 16: Base case control structure for distillation column (region I)

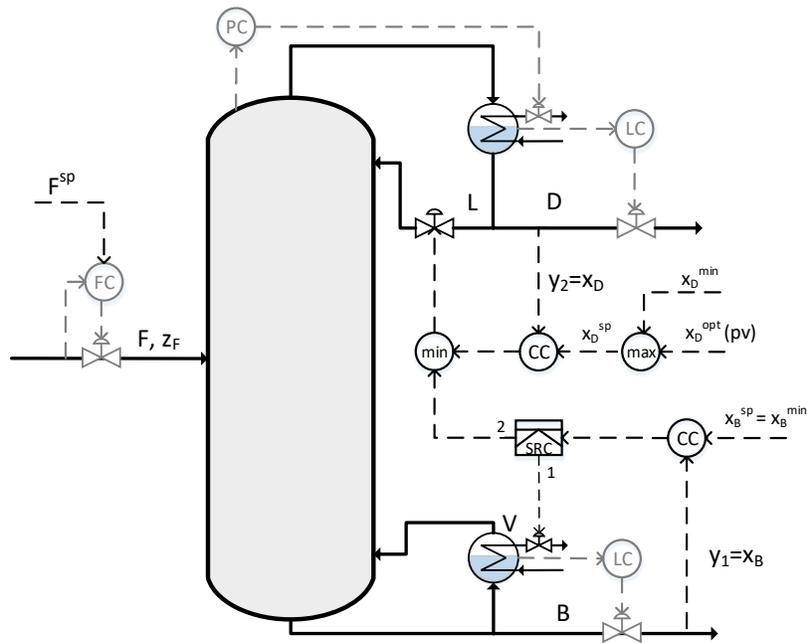


Figure 17: Control structure for distillation column for regions I, II and III.

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 $x_D(p_V)$ (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 Fig. 17 works for regions I, II and III. In order to also operate at maximum capacity and also satisfy all three constraints in (7) (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 Fig. 17 is to add a second controller for x_D (with setpoint $x_D^{min} + \Delta x_D$) 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 (region IV). We have $x_D^{min} = 0.95$, and select $\Delta x_D = -0.01$. Fig. 18 shows the suggested control structure valid for all regions.

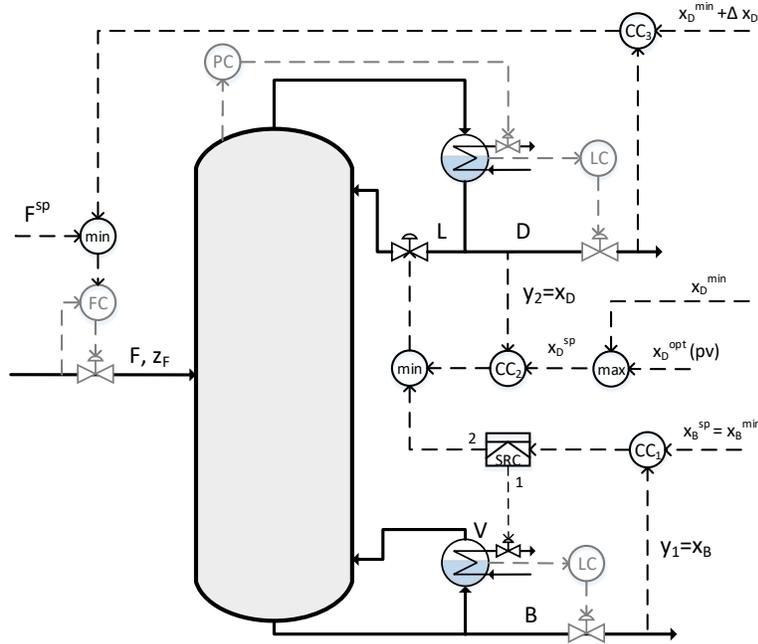


Figure 18: Control structure for distillation column for all regions (I, II, III, IV).

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 Fig. 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 (CC₂ and CC₃ in Fig. 18) will not be active at the same time due to the difference in setpoints (Δx_D).

Table 3: Pairings in Fig. 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	$x_B = x_B^{min}$	$V = V^{max}$	$x_D = x_D^{min} + \Delta x_D$

Simulation

In this section we test the control structure in Fig. 18. We first need to find the self-optimizing setpoint for $x_D^{opt}(p_V)$ to use in region I. Using Fig. A3 in the Supporting Information, we observe that there is an almost linear relation⁴ between x_D^{opt} and p_V in region I.

For the simulations, we start at $F^{sp} = 1.5$ mol/s and $p_V = 0.07$ \$/mol, 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 $p_V = 0.13$ \$/mol. Finally, at $t = 100$ min, we enter region IV by setting $F^{sp} = 1.75$ mol/s.

Fig. 19 shows the simulation results. The changes in active constraint region are marked with vertical gray dashed lines. As 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 $x_D = x_D^{min}$.

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

⁴The linear approximation of x_D^{opt} as function of p_V in region I is $x_D^{opt} \approx 0.996 - 0.384p_V$. We use this equation to calculate x_D^{sp} .

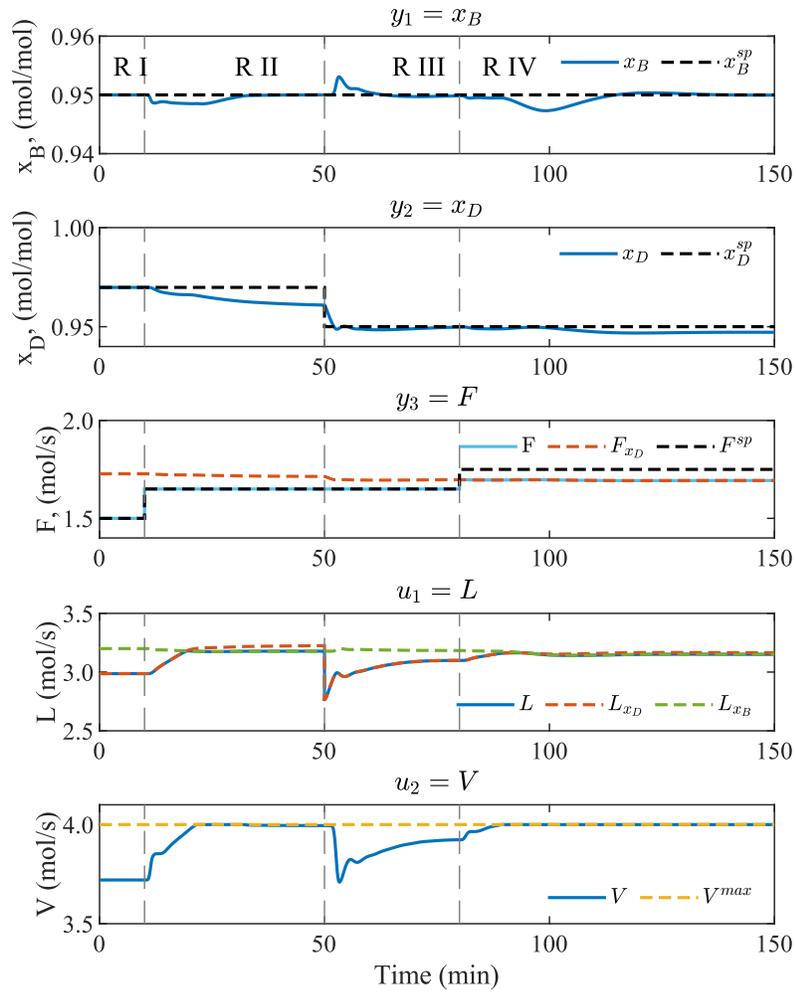


Figure 19: Simulation for structure in Fig. 18 for case study II.

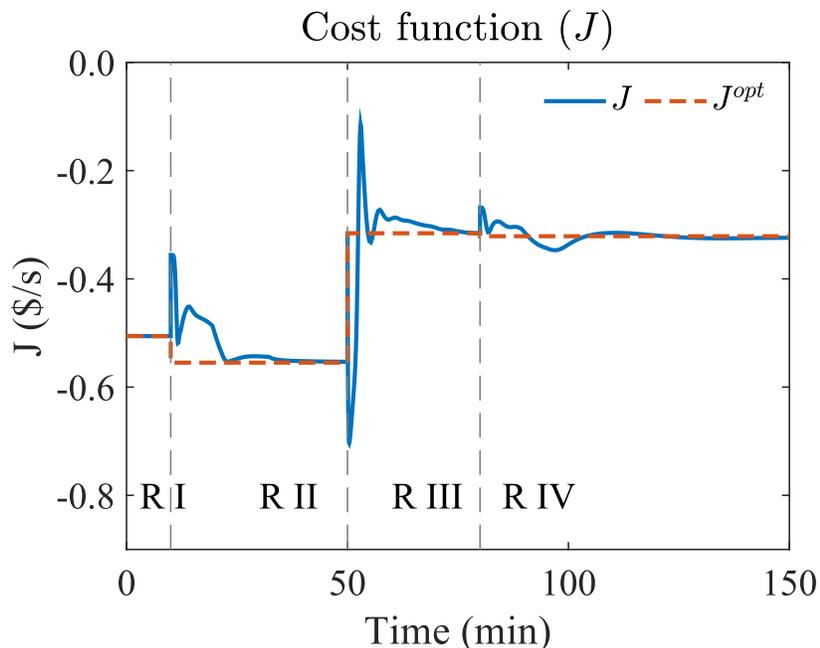


Figure 20: Cost for distillation column case study (which should be minimized).

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 insight⁴⁷.

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, 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 the better dynamic behavior or 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 *pair close rule*, because it gives a better dynamic behavior and we consider that the process will 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 Fig. 18. An alternative structure is shown Fig. 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 $u_2 = L$, and
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 Fig. 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 .

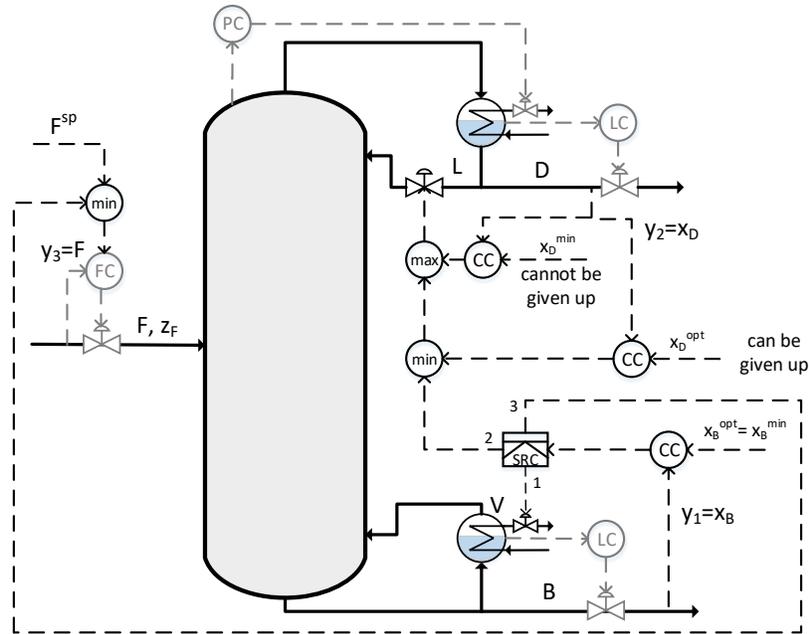


Figure 21: Alternative control structure for distillation column, all regions. This structure behaves differently from Fig. 18 when maximizing throughput (region IV).

Conclusion

We introduced a systematic procedure to design constraint switching schemes using classical controllers and logics. We distinguish between 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 setpoints 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, used single-loop PID-based control structures.

Acknowledgement

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Supporting Information Available

Supporting Information:

- SystematicDesign_Supporting_Information.pdf: Appendix containing the model used for Case Study I and Optimization Results for Case Study II.

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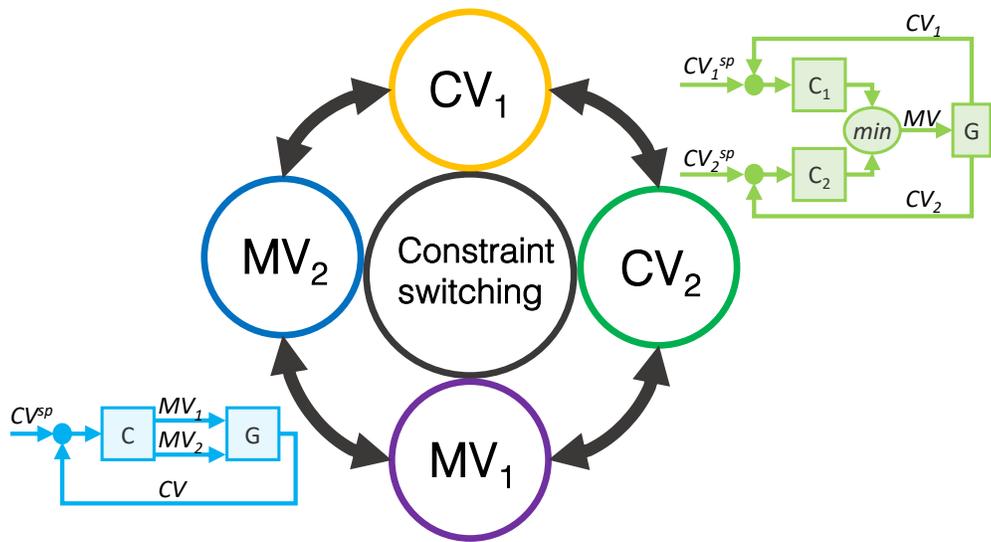


Figure 22: For Table of Contents Only.