

Supplementary information for the article:
Systematic design of active constraint switching using
selectors

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A. Example 3: Distillation column

A.1. Simulator Model

We consider a two-product distillation column with N_T stages as shown in Fig. 1 . The following assumptions are made about the model:

- Binary mixture
- constant pressure, relative volatility and molar flows
- no vapor holdup
- linear liquid dynamics
- equilibrium on all stages

The total mass balance and the mass balance for the light component on stage i , except in the condenser ($i = N_T$), feed stage ($i = N_f$) and reboiler ($i = 1$) is given by:

$$\frac{dM_i}{dt} = L_{i+1} - L_i + V_{i-1} - V_i \quad (1)$$

$$\frac{dM_i x_i}{dt} = L_{i+1} x_{i+1} + V_{i-1} y_{i-1} - L_i x_i - V_i y_i \quad (2)$$

$$\forall i \in \{2, \dots, N_T - 1\} \setminus \{N_f\}$$

where L_i and V_i are the liquid and vapor flows from the i^{th} stage (in kmol/min), respectively, and M_i is the liquid holdup in the i^{th} stage (in kmol). x_i and y_i

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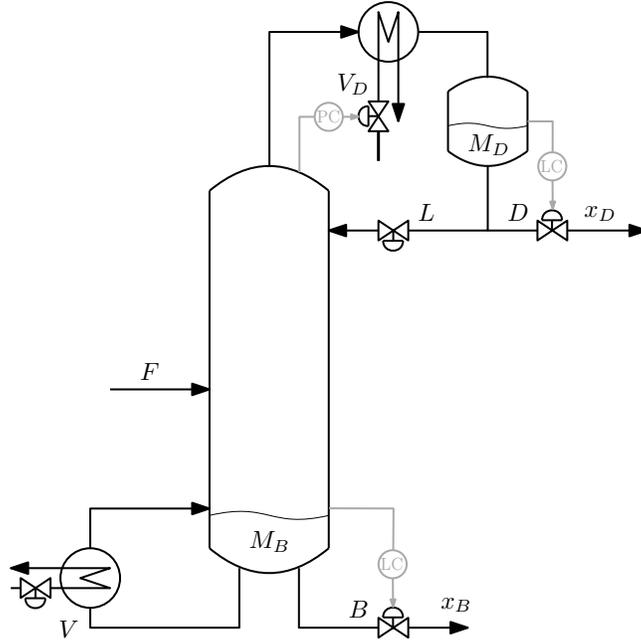


Figure 1: Schematic representation of the distillation column

are the liquid and vapor mole fractions of light component on the i^{th} stage, respectively.

The mass balance on the feed stage ($i = N_f$) is given by,

$$\frac{dM_{N_f}}{dt} = L_{N_f+1} - L_{N_f} + V_{N_f-1} - V_{N_f} + F \quad (3)$$

$$\frac{dM_{N_f}x_{N_f}}{dt} = L_{N_f+1}x_{N_f+1} + V_{N_f-1}y_{N_f-1} - L_{N_f}x_{N_f} - V_{N_f}y_{N_f} + Fz_F \quad (4)$$

The mass balance on the reboiler ($i = 1$) is given by,

$$\frac{dM_B}{dt} = L_2 - V - B \quad (5)$$

$$\frac{dM_Bx_1}{dt} = L_2x_2 - Vy_1 - Bx_1 \quad (6)$$

where B is the bottom flow rate and V is the boilup as shown in Fig. 1.

The mass balance on the condenser ($i = N_T$) is given by,

$$\frac{dM_D}{dt} = V_{N_T-1} - L - D \quad (7)$$

$$\frac{dM_Dx_{N_T}}{dt} = V_{N_T-1}y_{N_T-1} - Lx_{N_T} - Dx_{N_T} \quad (8)$$

where D is the distillate flow rate and L is the reflux as shown in Fig. 1.

From this, we get the expression for the rate of change of liquid mole fraction

$$\frac{dx_i}{dt} = \frac{1}{M_i} \left(\frac{dM_i x_i}{dt} - x_i \frac{dM_i}{dt} \right) \quad \forall i \in \{1, \dots, N_T\} \quad (9)$$

The model therefore has $2N_T$ differential states denoted by $[\{x_i\}_{i=1}^{N_T}, \{M_i\}_{i=1}^{N_T}]^T$.

The liquid flows depend on the liquid holdup on the stage above and the vapor flow as follows

$$L_i = L0_i + \frac{1}{\tau_i} (M_i - M0_i) + (V - V0)_{i-1} \lambda \quad (10)$$

where $L0_i$ (in kmol/min) and $M0_i$ (in kmol) are the nominal values for the liquid flow and holdup on stage i . The effect of vapor flow on the liquid flow is captured by λ .

The vapor composition can then be computed from the vapor-liquid equilibrium

$$y_i = \frac{\alpha x_i}{1 + (\alpha - 1)x_i} \quad (11)$$

where α is the constant relative volatility.

A.2. Controller design

We assume that the overhead vapour V_D is used to maintain a constant pressure. Stable operation of the column requires the levels M_B and M_D to be controlled. In this model, the column is stabilized using the LV-configuration where we use D to control M_D , and B to control M_B as shown in Fig. 1. We use a P-controllers for each level control loop, with the controller gain $K_P = 10$ for both the loops.

As mentioned in the manuscript, the purity constraint on x_D will always be active, since this is the most valuable product. The x_D composition is controlled using the reflux L using a PI controller that is tuned using the SIMC tuning rules. For a desired closed loop time constant of $\tau_c = 10$, this results in the proportional gain $K_P = 7.8947$ and $K_I = 0.2193$.

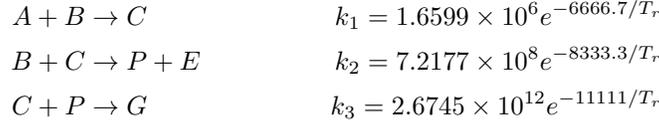
The composition control for the bottom product x_B is also achieved using a PI controller that is tuned using the SIMC rules. For a desired closed loop time constant of $\tau_c = 10$, this results in the proportional gain $K_P = 2.2140$ and $K_I = 0.123$.

The MATLAB scripts for the distillation column example is given below or can be found in <https://github.com/dinesh-krishnamoorthy/Feedback-based-RT0/tree/master>Selectors/Cola>.

B. Example 4: Williams-Otto reactor

B.1. Simulator model

The benchmark Williams-Otto reactor converts the raw materials A and B into useful products P and E along with a byproduct G via a series of reactions,



The reactor is modeled as,

$$\begin{aligned} \frac{dx_A}{dt} &= \frac{1}{W}(F_A - Fx_A) - k_1 x_A x_B \\ \frac{dx_B}{dt} &= \frac{1}{W}(F_B - Fx_B) - k_1 x_A x_B - k_2 x_B x_C \\ \frac{dx_C}{dt} &= \frac{-Fx_C}{W} + 2k_1 x_A x_B - 2k_2 x_B x_C - k_3 x_C x_P \\ \frac{dx_P}{dt} &= \frac{-Fx_P}{W} + k_2 x_B x_C - 0.5k_3 x_C x_P \\ \frac{dx_E}{dt} &= \frac{-Fx_E}{W} + 2k_2 x_B x_C \\ \frac{dx_G}{dt} &= \frac{-Fx_G}{W} + 1.5k_3 x_C x_P \end{aligned}$$

where the mass holdup $W = 2105$ kg. The reactor is controlled using the reactor temperature $MV_1 := T_r$ and the feed rate $MV_2 := F_B$ with pure B component. Feed rate F_A with pure A component is a disturbance and we assume that it is expected to vary between 1kg/s and 2kg/s . We assume perfect level control such that the outflow $F = F_A + F_B$.

B.2. Controller design

The objective is to maximize the production of useful products P and E . In addition, there are purity constraints on G and A on the product stream, and a minimum outflow rate F_{out} . The steady-state optimization problem is formulated as,

$$\begin{aligned} \min_{T_r, F_B} & -1043.38x_P F - 20.92x_E F \\ & + 79.23F_A + 118.34F_B \\ \text{s.t.} & \\ & x_G \leq x_{G_{max}} \\ & x_A \leq x_{A_{max}} \\ & F \geq F_{min} \end{aligned} \tag{12}$$

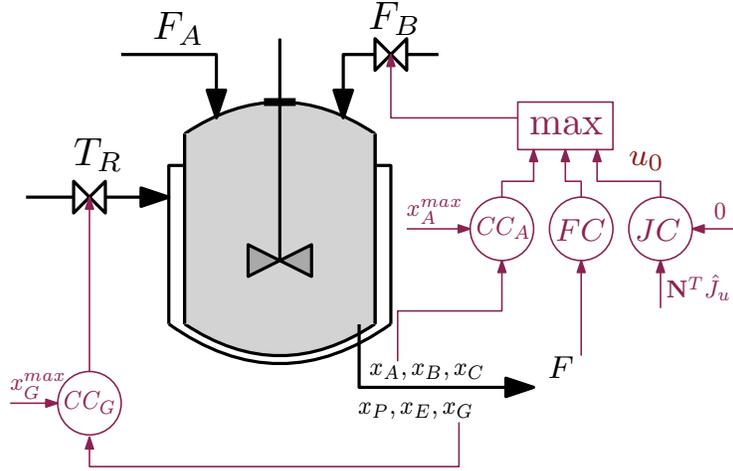


Figure 2: Example 4: Proposed control structure design for optimal operation of a Williams-Otto reactor over regions R-I and R-II.

where $x_{G,max} = 0.08$, $x_{A,max} = 0.12$, and $F_{min} = 4.4 \text{ kg/s}$.

Since the purity constraint on x_G is very low, it will always be active for the assumed disturbance range of $F_A \in [1, 2] \text{ kg/s}$. Therefore the relevant active constraint combinations are

- only x_G active (R-I)
- x_G and x_A active (R-II)
- x_G and F active (R-III)

Since we have two MVs, we first pair the reactor temperature $u_1 = T_r$ to tightly control x_G to its limit of $x_{G,max} = 0.08$ using a PI control. This leaves us with one degree of freedom, namely $u_2 = F_B$, which will be used to control either the self-optimizing CV y_0 to a desired setpoint in region R-I, or control x_A to its limit of $x_{A,max} = 0.12$ in region R-II, or control F to its minimum limit of $F_{min} = 4.4 \text{ kg/s}$ in region R-III. In this case,

$$\mathbb{Y}^- = \{x_{A,max}, F_{min}\}$$

and since we have only \mathbb{Y}^- , a single maximum selector block can be used to switch between the different active constraint regions (cf. Remark ??).

Therefore, we use four SISO controllers to control the CVs in each active constraint region, namely,

1. Composition controller denoted by CC_G that uses T_r to control x_G to $x_{G,max}$ (in regions R-I, R-II, and R-III).
2. Composition controller denoted by CC_A that uses F_B to control x_A to $x_{A,max}$ (in region R-II).

Table 1: Example 4: Controller gains.

	CC_G	CC_A	JC	FC
K_P	193.4236	-66.2252	0.1251	0
K_I	1.2895	-0.1104	1.5640×10^{-4}	1
K_{aw}	-	0.0017	0.0013	0.005

3. Flow controller denoted by FC that uses F_B to control F to F_{min} (in region R-III).
4. Self-optimizing controller denoted by JC that uses F_B to control the self-optimizing CV y_0 to $y_{0,sp}$ (in region R-I).

In region R-I, we have used a linear gradient combination as the self-optimizing CV $y_0 = \mathbf{N}^T \nabla_u J$ controlled to a constant setpoint of $y_{0,sp} = 0$. In this example, the linear gradient combination is given by $y_0 = 0.9959 \nabla_{F_B} J + 0.0906 \nabla_{T_r} J$.

The control structure design is shown in Fig. 2. The controller tuning parameters are shown in Table 1.

Fig. 3 shows the simulation results using the proposed control structure design. It can be clearly seen that as the disturbance changes, the max selector block is able to automatically handle the CV-CV switching between R-I, R-II and R-III. The MATLAB scripts for the distillation column example is given below or can be found in <https://github.com/dinesh-krishnamoorthy/Feedback-based-RTO/tree/master/Selectors/WilliamsOtto>.

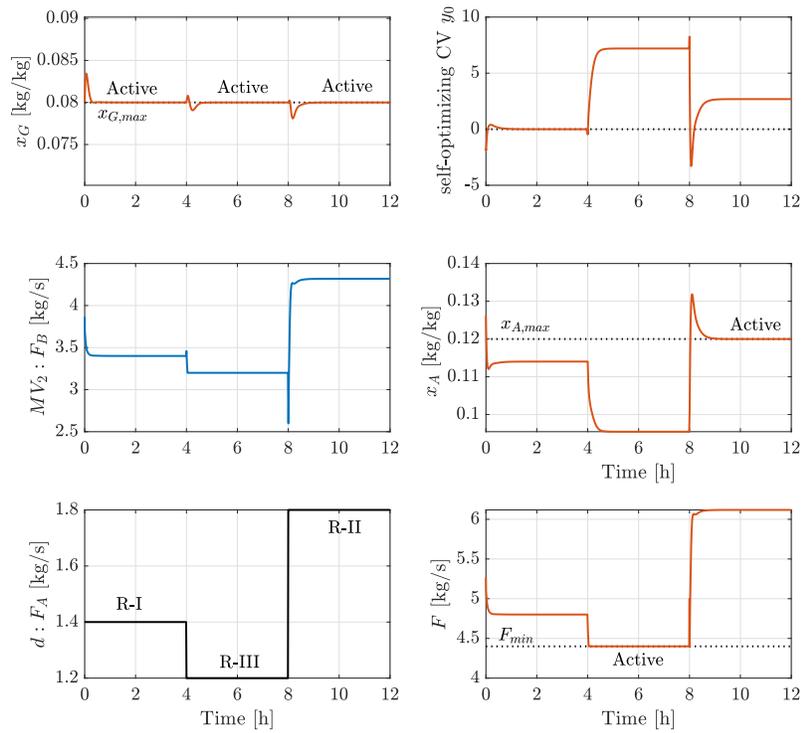


Figure 3: Example 4: Simulation results showing the automatic switching between the active constraint regions as the disturbance changes using selectors designed according to Theorem 1.