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Economic Plantwide Control of the Ethyl Benzene Process

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DOI 10.1002/aic.13964
Published online December 10, 2012 in Wiley Online Library (wileyonlinelibrary.com).

Systematic plantwide control system design for economically optimal operation of the ethyl benzene process over a large throughput range is studied. As throughput is increased, constraints progressively become active with the highest number of active constraints at maximum throughput. An economic plantwide control system (CS1) is designed for operation at this most constrained operating point using a novel ''top-down'' pairing approach with higher prioritization to the economic objectives over regulatory objectives. This structure is adapted for near optimal low throughput operation with constraints that go inactive taking up additional economic variable control. For comparison, a conventional plantwide control structure (CS2) with the throughput manipulator at a fresh feed and ''bottom-up'' pairing for the control objectives is also synthesized. Four overrides are needed in CS2 to handle the hard equipment capacity constraints at maximum throughput. Rigorous dynamic simulations show that CS1 is dynamically and economically significantly superior to CS2. © 2012 American Institute of Chemical Engineers *AIChE J,* 59: 1996–2014, 2013
Keywords: plantwide control, economic operation, bottleneck, capacity constraint control, override control

Introduction

The zero-discharge philosophy, widely practiced in the chemical industry using concepts of material and energy integration, is quite naturally aligned with the requirements of sustainable development. Today's chemical processes are highly integrated for superior energy efficiency and (near) zero discharge. Designing simple yet effective control systems that ensure (near) ''optimal'' steady operation, where optimality is defined in terms of an economic criterion or equivalent energy efficiency and production criteria, is a prerequisite towards fully realizing the sustainability benefits of such highly integrated processes and can be quite a challenge. Typically, multiple constraints are active at the optimum steady state and this active constraint set can change depending on, for example, changes in the desired throughput, raw material composition, equipment characteristics, and of late, volatility in the prevailing economic scenario.

Although significant progress has been made in developing systematic methodologies for sustainable chemical process design,[1,2] it is surprising that plantwide control system design for ''optimal'' steady process operation over a large operating window, where the active constraint set changes, has received very little attention. For example, all reported applications[3–6] of the plantwide control design procedure of Luyben et al.[7] consider process operation around a base-case design where hard process constraints are not active. Similarly, Skogestad's[8] optimization-based approach focuses on identifying self-optimizing controlled variables (CVs) for the unconstrained degrees of freedom (dofs) and leaves the important question of throughput manipulator (TPM) selection,[9] handling any changes in the active constraint set and dynamic pairing issues largely unaddressed.

In today's fragile and fiercely competitive economic environment, operating processes must respond to sudden and potentially large changes in market demand, energy prices, and the desired product mix. For better competitiveness, the plantwide control system implemented on a process must effectively handle likely changes in the active constraint set to these disturbances for ''near'' optimal steady operation over the entire operating space. Our research is motivated toward developing a systematic methodology for devising such a plantwide control system.

In this work, the design of a plantwide control system for economically optimal steady operation of an ethyl benzene (EB) process over a large throughput range is considered. EB is an intermediate in the production of styrene monomer and is conventionally produced by the liquid/vapor-phase alkylation of benzene with ethylene on zeolite catalyst. The EB further alkylates with ethylene to form diethylbenzene (DEB) side product.

In a very recent article, Luyben[10] has developed an economic optimum design of a two-reactor and two-column EB process with a benzene recycle stream and a DEB recycle stream. The DEB is recycled back to the reaction section for transalkylation with benzene to the value added EB product. The DEB inventory in the process is allowed to build to an extent where the DEB consumption by transalkylation exactly balances the DEB formation in the side reaction. The DEB is, thus, ''recycled to extinction'' for a zero-discharge process. Luyben's article[10] develops a near optimum process design explaining the classic engineering tradeoffs as well as a basic regulatory plantwide control system for operating the process around the design steady state. It is shown that effective regulation requires mitigation of snowballing[11] in the DEB recycle loop.

The objective of this article is to take the developed base-case EB process design and devise a simple plantwide

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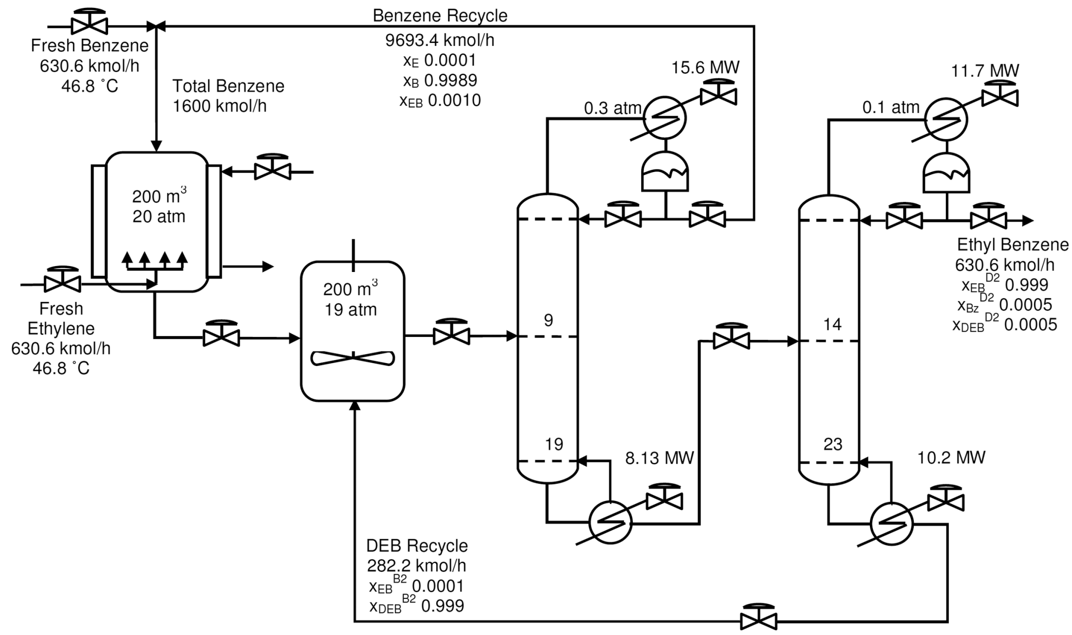


Figure 1. Ethyl benzene process schematic with base design and operating conditions.

control system for economically optimal steady operation over a large throughput range encompassing low to the maximum achievable throughput with hard equipment capacity constraints progressively becoming active. The main contribution of the work is towards resolving the conflicts that arise between the requirements of economic process operation, robust process regulation, and retaining control system simplicity in light of the constraints that become active. In a significant departure from conventional plantwide control system design approaches, the plantwide control structure is first synthesized for the most constrained (maximum throughput) operating point and then adapted for near optimal operation in less constrained operating regions (lower throughputs). Also a novel "top-down" synthesis approach with higher prioritization to economic control objectives (including active hard capacity constraints) over regulatory objectives is applied. A comparison with the conventional plantwide control system using overrides for handling capacity constraints provides compelling evidence of superior economic/dynamic performance as well as overall control system simplicity of the economic plantwide control structure. In particular, the application of the approach naturally gives the location of the TPM at the last equipment capacity constraint to go active, which is inside the plant. This is in contrast to a conventional TPM location at the limiting reactant fresh feed. The work demonstrates that a simple decentralized control system can be synthesized for providing (near) optimum economic operation over a large throughput range, encompassing multiple equipment capacity constraints going active.

In the following, the process is briefly described followed by steady-state optimization results at the design throughput and maximum achievable throughput. A simple economic plantwide control system (CS1) is then synthesized based on the steady-state optimization results. For comparison, a conventional plantwide control structure (CS2) with the TPM at the fresh ethylene feed is also synthesized. The dynamic and economic performance of the two control structures is then compared for process operation at low throughput (least number of active constraints) and higher throughputs (higher number of active constraints). The insights from the work are collected and discussed from the perspective of developing a systematic methodology for economic plantwide control. The conclusions are finally summarized.

Process Description

Figure 1 sketches a schematic of the EB process. Fresh benzene is mixed with recycle benzene and fed to a coil-cooled liquid-phase continuously stirred tank reactor (CSTR). Fresh ethylene is fed directly to this CSTR, where the main alkylation reaction occurs. The reactor effluent is mixed with recycle DEB and fed to an adiabatic liquid-phase CSTR, where transalkylation of DEB to EB occurs. The effluent from the second CSTR is sent to the recycle column which recovers and recycles unreacted benzene as overhead distillate. The EB and DEB flow down the bottoms to the product column recovering 99.9 mol% EB as the distillate and DEB leaving down the bottoms. The DEB bottoms stream is recycled to the adiabatic CSTR.

There are three principal reactions as below:

$$\underset{\text{Benzene}}{C_6H_6} + \underset{\text{Ethylene}}{C_2H_4} \rightarrow \underset{\text{EB}}{C_8H_{10}} \text{ (main reaction)}$$

$$\underset{\text{EB}}{C_8H_{10}} + \underset{\text{Ethylene}}{C_2H_4} \rightarrow \underset{\text{DEB}}{C_{10}H_{14}} \text{ (side reaction)}$$

$$\underset{\text{DEB}}{C_{10}H_{14}} + \underset{\text{Benzene}}{C_6H_6} \rightarrow \underset{\text{EB}}{2\ C_8H_{10}} \text{ (transalkylation)}$$

The two CSTRs in series configuration allows high ethylene conversion via the main alkylation reaction in the first reactor followed by transalkylation in the second reactor to recycle DEB to extinction for a zero-discharge process. The reaction kinetics, thermodynamic property package and base-case process design, and operating conditions have been taken from Luyben.[10] As indicated in Figure 1, the reactors are quite large (200 m^3 each) and the columns are not-too-tall (recycle column: 19 trays; product column: 23 trays) with column operation under vacuum conditions for a water-cooled condenser. Also, both the reactors are operated in excess benzene environment to suppress DEB formation.

Table 1. Steady State Process Optimization Formulation and Results

Objective Function	Mode I: Maximize P (F_{C2} fixed)	Mode II: maximize F_{C2}
Process constraints	$0°C \leq$ CSTR temperature $\leq 200°C$ $0 \leq$ material flows ≤ 2(base-case) kmol/h $0 \leq$ recycle flow ≤ 2(base-case) kmol/h $0 \leq$ Column 1 reboiler duty ≤ 1.2(base-case) kW $0 \leq$ Column 2 reboiler duty ≤ 1.2(base-case) kW $0 \leq$ Reactor Volume ≤ 200 m^3 $x_{EB}^{D2} = 0.999$	
Material cost ($/kmol)	Fresh ethylene: 30; fresh benzene: 85; ethylbenzene: 140	
Energy Cost ($/GJ)	LP Steam (150°C): 7.78; MP steam (180°C): 8.22; Cooling water: 0.16; steam generated in reactor: 6.0	
Throughput (F_{C2})	630.6 kmol/h*	970 kmol/h†,‡
x_{EB}^{D1}	0.087	0.157
x_{Bz}^{B1}/x_{EB}^{B1}	0.00091	0.00039
r_{EB}^{B2}	0.0085	0.02
F_{TotBz}	963.1378 kmol/h	2567.18 kmol/h
T_{Rxr1}	200°C $_{max}$	200°C $_{max}$
U_1	200 m^3 $_{max}$	200 m^3 $_{max}$
U_2	200 m^3 $_{max}$	200 m^3 $_{max}$
x_{EB}^{D2}	0.00092	0.0004
B_2#	122.5 kmol/h	230 kmol/h
Profit per year	$ 1.1246×10^7	$$1.7056 \times 10^7$
Active constraints	x_{EB}^{D2}	V_1^{MAX} V_2^{MAX} L_1^{MAX}, x_{EB}^{D2}
No. of unconstrained dofs	4	2
Unconstrained dof CVs	B_2, x_{EB}^{D2}, L_1/F_{col1}, T_{col2}	B_2, x_{Bz}^{D2}

*F_{C2} is specified.
†F_{C2} also optimized for maximum operating profit.
‡Maximum achievable throughput.
#Calculated value at optimum.

Optimal Steady-State Process Operation

Continuous processes, by their very nature, are operated for sustained periods (many months to a few years) at (or around) a steady state and it is this steady operation that accounts for almost all of the plant operating profit. Accordingly, the steady-state-operating degrees of freedom (dofs) of a process should be optimized for a steady-state economic objective function such as the steady steam consumption per kg product or yield to desired product or yearly operating profit or throughput (production rate), and so forth subject to process constraints (including product quality). Usually, the desired steady throughput (production rate of the value added product or fresh feed processing rate) is decided by the management based on business and economic demand-supply considerations (including effect of supply on prices). Sometimes, the economic scenario can be very favorable, for example, when a high-demand product is the monopoly of a first-to-the-market (and first-to-patent) company and operating the process at maximum achievable steady-state throughput is economically optimal. The steady-state optimization is, thus, performed for two modes: given throughput (Mode I) and maximum throughput (Mode II).

There are nine steady-state operating dofs for the zero-discharge EB process: two for the fresh feeds, two for the main reactor (hold up and temperature), one for the transalkylator (hold up), two for the recycle column, and two for the product column. A reasonable set of specification variables to solve for the steady-state solution, which has been used here, is: fresh ethylene feed rate (F_{C2}), total benzene (fresh + recycle) flow rate (F_{TotBz}), main reactor temperature (F_{Rxr1}), and hold up (U_1), transalkylator hold up (U_2), recycle column distillate EB mol fraction (x_{EB}^{D1}), and bottoms benzene to EB mol ratio (x_{Bz}^{B1}/x_{EB}^{B1}), product column distillate EB mol fraction (x_{EB}^{D2}), and bottoms EB recovery (r_{EB}^{B2}). The minimum EB product purity ($x_{EB}^{D2\cdot MIN}$) is 99.9 mol%.

For Mode I operation (F_{C2} specified), the remaining eight dofs are optimized to maximize the yearly profit, P, defined as

P = [Product sale − raw material cost − energy cost] per year

For Mode II operation (F_{C2} is a decision variable), all nine dofs are adjusted to maximize the EB product rate, F_{EB}. Note that the Mode II objective function is not based on price data as sustained large increases in production typically tend to cause the product price to decrease. Nevertheless, it is important to know the maximum achievable throughput for a process and design a control system that can deliver it, should the economic scenario justify the same.

Table 1 summarizes the constrained optimization problem formulation (including price data used) and results obtained using the Aspen Plus constrained SQP solver for Mode I and Mode II operation. In addition to maximum and minimum material and energy flow constraints, a maximum and minimum limit on the main reactor temperature and reactor levels is imposed. The two column boilups are also constrained to be below a maximum limit (taken as 20% above base-case design boil up) corresponding to the column flooding limit. For Mode I, the initial guess is taken as the base-case steady state (Figure 1) and the optimizer is allowed to search for the optimum. For Mode II, because we expect more constraints to become active as throughput is increased to maximum, the Mode I optimum solution is taken as the input for quicker convergence. For the reported Mode I/II solutions, we have confirmed that the objective function decreases on moving away from the optimum point in a feasible direction. Further the objective function is always lower for randomly chosen suboptimal decision variable values.

In both operation modes, the product quality constraint is optimally active to avoid product give-away. Also, the maximum level constraint on the two reactors (U_1^{MAX} and U_2^{MAX}) is active to minimize the DEB recycle rate which causes a slight reduction in the energy consumption in the two columns. The main reactor maximum temperature constraint (T_{Rxr1}^{MAX}) is also optimally active in both modes for a higher temperature in the adiabatic transalkylator for higher transalkylation conversion giving a lower DEB recycle rate. In Mode II operation, the maximum boilup constraint in both the columns (V_1^{MAX} and V_2^{MAX}) and the maximum reflux constraint in the recycle column (L_1^{MAX}) are additionally active. The Mode I active constraints/specifications, F_{C2}, U_1^{MAX},U_2^{MAX}, T_{Rxr1}^{MAX}, and x_{EB}^{D2}, leave four unconstrained dofs. In Mode II, the three additional active constraints V_2^{MAX}, L_1^{MAX}, and V_1^{MAX} with F_{C2} as an additional dof leaves two unconstrained dofs.

We note that if the prices are assumed stable and the Mode I price data in Table 1 is used to optimize all the nine steady-state dofs as decision variables and obtain the maximum economic throughput solution, the optimum is very close to the maximum throughput (Mode II) solution we have obtained. The profit for the latter is lower than the former only by $<0.05\%$ and the active constraint set is the same with two remaining unconstrained steady-state dofs. This small difference is due to slightly different values for the unconstrained decision variables. For this zero-discharge process, assuming constant prices (this is a major assumption), the maximum profit is, thus, achieved at the maximum throughput.

Top-Down Economic Plantwide Control Structure Synthesis

Optimum steady operation corresponds to operating the process at the optimum steady-state solution, in spite of routine disturbances. This requires process operation at all the optimally active constraints as well as at the optimum values for appropriate CVs corresponding to any remaining unconstrained steady-state dofs. These unconstrained CVs should be chosen (or designed) such that (near) optimal operation is achieved at constant setpoints for the expected routine disturbances. Such CVs are aptly termed as self-optimizing[8] in the plantwide control literature.

Typically, steady deviations away from the active constraint limits are associated with a large economic loss, whereas the loss for steady deviations away from the optimum values of the unconstrained self-optimizing CVs is significantly lower. Economic operation then requires the tightest possible active constraint control with relatively less tight self-optimizing CV control generally being acceptable.

Of the active constraints, many such as maximum product impurity or maximum reactor level are soft constraints, where short-term transient violations are acceptable. As shown in Figure 2a, average process operation at the soft active constraint limit is then usually possible by pairing an appropriate manipulated variable (MV) to tightly regulate the soft constraint variable and fixing the constraint controller setpoint at the constraint limit.

Some of the active constraints represent hard equipment capacity constraints such as a flooded column and short-term transient violations are not acceptable. Given a controller to control the hard active constraint, its setpoint must be sufficiently backed-off from the hard limit to ensure no violation during worst-case transients. As illustrated in Figure 2b, the average process operation would then necessarily be suboptimal due to the need for a back-off from the hard limit(s). The magnitude of the back-off depends on the degree of tightness of control of the constraint variable with loose control requiring higher back-offs with consequently higher steady economic loss.

In addition to control of "economic" variables (active constraints and self-optimizing CVs), the plantwide control system must ensure effective process stabilization in terms of inventory and energy management, that is, consistent material and energy balance control. Conflicts often arise as to whether an MV should be used for robust inventory regulation or tight economic CV control. The challenge is to configure the plantwide control structure to minimize the severity of the transients in the hard active constraints so that the economic loss (from optimum) is as small as possible while ensuring robust stabilization.

The conventional plantwide control system design approach [7,8] is to configure control loops for robust inventory regulation and control of the economic CVs for the design throughput (Mode I), where no hard equipment capacity constraints are active due to equipment overdesign. As throughput is increased, (hard) equipment capacity constraints are encountered and the control of crucial regulatory (e.g., surge level) or economic (e.g., product impurity) CVs is usually lost. To ensure proper process regulation/stabilization on encountering these additional constraints, the conventional approach uses override controllers to appropriately reconfigure the control structure and maintain material/energy balance consistency. The conventional approach, thus, designs the pairings for the design throughput (Mode I) and then adapts it for maximum throughput (Mode II).

In a significant departure from the above conventional approach, in this work, we propose and demonstrate the application of the alternative approach to first design the economic and regulatory loops at the most constrained operating point, that is, the maximum throughput (Mode II) solution, and then adapt it for lower throughput operation with fewer active constraints. Because the Mode II solution is the most constrained one, it has the fewest (potentially zero) unconstrained steady-state dofs, and is, therefore, the most difficult to stabilize. If a consistent control system can be devised for effective regulation of this "difficult" case, it can most certainly be adapted for (near) optimal operation at lower throughputs where additional dofs become available due to constraints becoming (optimally) inactive. The constraint variable that becomes inactive can "take up" control of an appropriate self-optimizing CV ensuring near optimal operation at lower throughputs.

To design a consistent control structure for maximum throughput operation, appropriate pairings for controlling the economic and regulatory CVs must be chosen. The conventional "bottom-up" approach[8] is to first pair the loops for robust regulatory (material/energy balance) control and then implement supervisory controllers that manipulate appropriate regulatory setpoints for controlling the economic CVs. Because the regulatory loops are paired first followed by the economic loops, the supervisory control of the economic objectives is often not as tight. Model predictive control is often necessary for improved economic CV control.

In this work, we apply the alternative "top-down" approach where pairings for the tightest possible control of the economic CVs (including hard equipment capacity constraints) are first chosen followed by the pairings for the regulatory loops. This approach is justified as many of the regulatory loops such as surge drum level loops have only a transient impact and do not affect the process steady state and hence the steady-state process economics. By pairing the

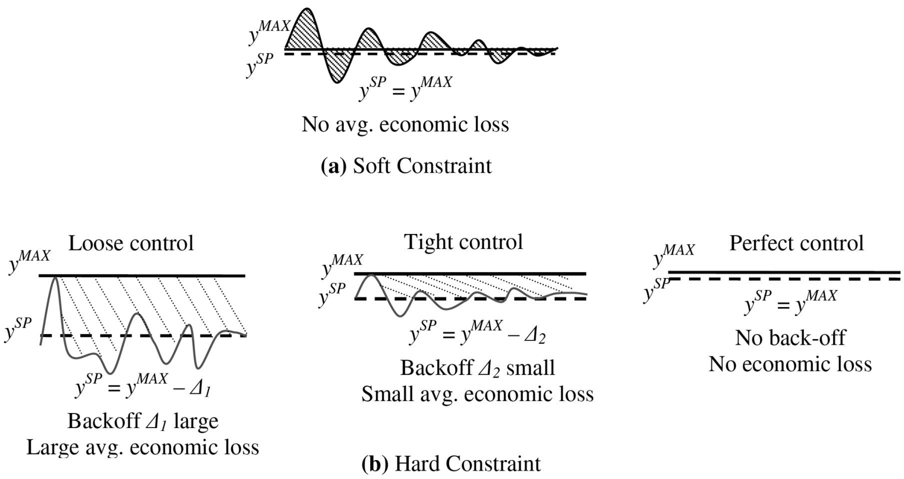


Figure 2. Soft/hard active constraint control and economic operation.

economic CV loops first, the flexibility in the choice of the pairings gets exploited in favor of the tightest possible control of the economic CVs for superior economic performance. Based on the previous discussion on economic CVs, we further prioritize economic CVs with loops for hard active constraint control being paired first for minimum back-off followed by the soft active constraints and the self-optimizing CVs corresponding to any unconstrained Mode II dofs.

After loops for the tightest possible control of economic CVs are paired, it is usually possible to achieve acceptable inventory control/process stabilization because controlling an economic CV usually also regulates an appropriate process inventory (component, phase, material, or energy) and processes are designed with sufficient number of surge drums so that the control dofs (# of control valves) is always greater than the steady-state operating dofs. Thus, even if there are no unconstrained steady-state dofs, control valves would remain available for inventory control. In cases where the inventory control turns out to be fragile, appropriate revision of pairings is done to improve the inventory control at the expense of loose control of the less important economic CVs.

The thinking behind the approach discussed above represents a significant departure from existing plantwide control system design approaches, both in terms of the prioritization of the control objectives (top-down vs. bottom-up) as well as the operating point for which the control system is designed (most constrained or Mode II vs. less constrained or Mode I). In the following, we demonstrate its application to the EB process.

Economic Plantwide Control Structure

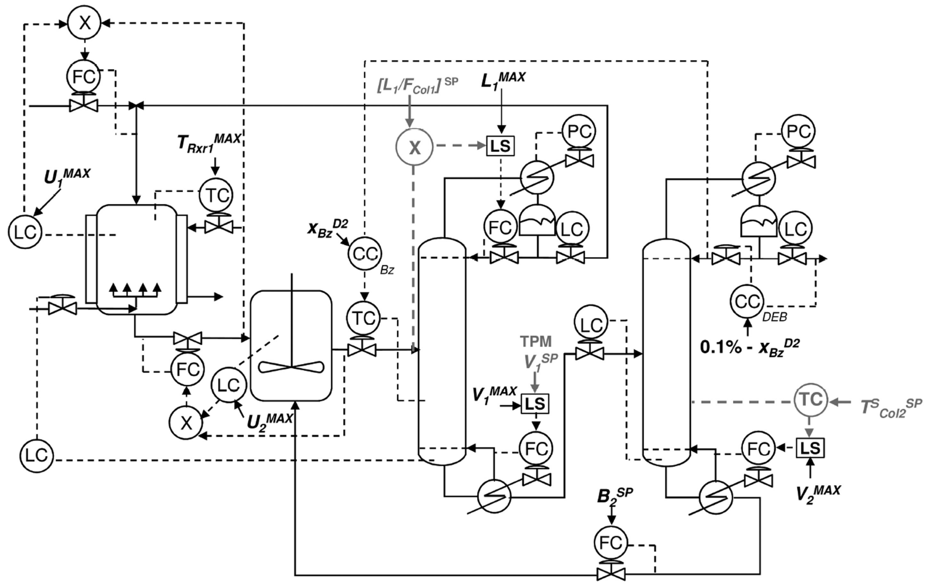
Best structure for maximum throughput operation

The control structure for the tightest possible control of the Mode II (maximum throughput) economic CVs (seven active constraints and two CVs for unconstrained dofs) is shown in Figure 3a. How it has been arrived at using the "top-down" pairing procedure is described below.

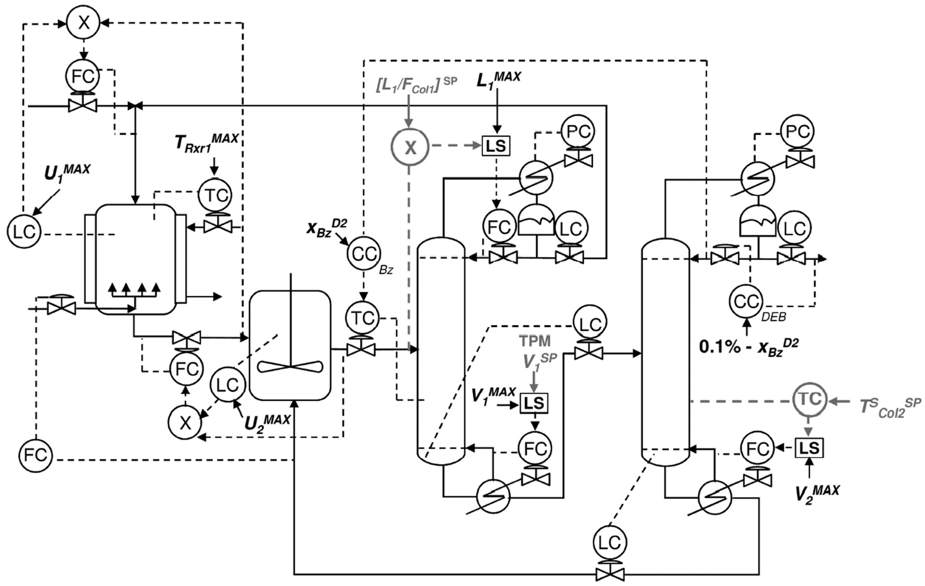
The active constraint set at maximum throughput is $T_{\mathrm{Rxr1}}^{\mathrm{MAX}}$, U_1^{MAX}, U_2^{MAX}, $x_{\mathrm{EB}}^{\mathrm{D2\cdot MIN}}$, V_2^{MAX}, L_1^{MAX}, and V_1^{MAX}. Of these, the first four are soft constraints, whereas the latter three are hard equipment capacity constraints. We, therefore, first pair loops for the tightest possible control of the hard constrained variables for minimum back-off. V_2 and V_1 are controlled by the respective reboiler duty valves (Q_{Reb2} and Q_{Reb1}), whereas L_1 is controlled using the recycle column reflux valve (first to third loops). These are the closest available MVs for the tightest possible control of the hard active constraints. The setpoints for these flow controllers are set at their corresponding maximum limits as tight flow control drives the back-off needed to almost zero.

The next loops to be paired are for the soft active constraints, $T_{\mathrm{Rxr1}}^{\mathrm{MAX}}$, U_1^{MAX}, and U_2^{MAX}, $x_{\mathrm{EB}}^{\mathrm{D2\cdot MIN}}$. Of these, $x_{\mathrm{EB}}^{\mathrm{D2\cdot MIN}}$ is economically the most important corresponding to target product purity. The EB product contains benzene and DEB as impurities and both must be tightly regulated to ensure on-aim product purity. To regulate the benzene leaking down the recycle column, a sensitive stripping tray temperature ($T_{\mathrm{Col1}}^{\mathrm{S}}$) may be controlled. The conventional pairing with V_2 is, however, not possible because V_2^{MAX} is active so that the recycle column feed (F_{Col1}) is used as the MV. The tray temperature location is chosen as corresponding to the 13th tray where the stripping section temperature profile is the steepest. Because this tray is close to the column feed tray (ninth tray), the dynamic lag is small so that the temperature control would be tight. The temperature setpoint is adjusted by a product benzene impurity ($x_{\mathrm{Bz}}^{\mathrm{D2}}$) controller in a cascade arrangement (fourth loop). For tight control of the DEB impurity in the product ($x_{\mathrm{DEB}}^{\mathrm{D2}}$), the product column reflux (L_2) is manipulated (fifth loop). The product DEB and benzene impurities must sum to 0.1% to ensure an on-spec product purity $x_{\mathrm{EB}}^{\mathrm{D2\cdot MIN}}$ of 99.9%. Accordingly, $x_{\mathrm{DEB}}^{\mathrm{D2\cdot SP}} = 0.1\% - x_{\mathrm{Bz}}^{\mathrm{D2\cdot SP}}$ so that only $x_{\mathrm{Bz}}^{\mathrm{D2\cdot SP}}$ is independent.

The remaining soft active constraints are U_1^{MAX}, U_2^{MAX}, and $T_{\mathrm{Rxr1}}^{\mathrm{MAX}}$. These variables must anyway be controlled for stabilizing the two reactors (material and energy inventories). T_{Rxr1} is controlled conventionally using the reactor cooling duty, Q_{Rxr1} (sixth loop). Because the second reactor effluent is already paired for recycle column temperature control, U_2 and U_1 must be controlled in the reverse direction of process flow. To keep the variability in the reactor levels small, a ratio-based level control scheme is used. The feed to the second reactor (F_{Rxr2}) is maintained in ratio with its outflow (F_{Col1}) and the ratio setpoint is adjusted by the U_2 level controller (7th loop). On the first reactor, the total (fresh + recycle) benzene feed (F_{TotBz}) is maintained by manipulating the fresh benzene feed (F_{Bz}) and F_{TotBz} is maintained in ratio with the reactor outflow (F_{Rxr2}). The ratio setpoint is adjusted by the U_1 level controller (8th loop). For optimal operation, the setpoints for these three soft constraint control loops (T_{Rxr1}, U_1, and U_2) are set at maximum.



(a) Original control structure with fragile recycle column sump level controller



(b) Modified control structure with robust level control

Figure 3. Economic plantwide control structure for maximum throughput (Mode II) operation (Grey loops are for low throughput Mode I operation).

This completes the pairings for tight active constraint control. Note that eight loops have been implemented even as there are only seven active constraints. This is because in the two product impurity controllers, setting $x_{EB}^{D2\cdot SP} = 0.1\% - x_{EB}^{D2\cdot SP}$ corresponds to ensuring the minimum product purity constraint ($x_{EB}^{D2\cdot MIN} = 99.9\%$). The $x_{Bz}^{D2\cdot SP}$ is then independently set and its value must be optimally chosen somewhere between 0 and 0.1%. The benzene impurity in the product, x_{Bz}^{D2}, therefore, corresponds to one of the two Mode II unconstrained steady-state dofs.

We need to implement a loop to control a CV corresponding to the second unconstrained Mode II steady-state dof. As the V_2^{MAX} active constraint implies limited capacity to boil off the EB produced in the reaction section, if more EB is being generated in the reaction section than can be boiled-off in the product column, all the extra EB that could not be boiled off would drop down the product column leading to an unmitigated increase in the DEB recycle rate (B_2). This may be prevented by regulating the B_2. A natural CV corresponding to the second Mode II unconstrained dof is then B_2, which can be held tightly at its optimum value by manipulating the recycle column bottoms valve (9th loop).

With pairings chosen for tight control of active constraints and CVs corresponding to the unconstrained steady-state dofs, we consider pairings for regulating the remaining inventories. The inventories that require regulation are the two column pressures, P_{Col1} and P_{Col2}, the two reflux drum levels, U_{RD1} and U_{RD2}, and the two bottom sump levels, U_{Bot1} and U_{Bot2}. The column pressures are conventionally controlled by manipulating the respective condenser duty valves, Q_{Cnd1} and Q_{Cnd2} (10th and 11th loops). The two reflux drum levels are controlled by the respective distillate streams, D_1 and D_2 (12th and 13th loops). As the DEB recycle valve is already paired for holding B_2 (second Mode

II unconstrained CV), the product column bottom sump level is controlled using the feed to the product column, B_1 (14th loop). This leaves no close-by MVs for maintaining U_{Bot1} and the only option is to adjust the fresh ethylene feed rate, F_{C2} (15th loop).

In the synthesized structure in Figure 3a, the recycle sump level controller is a long loop and appears quite unconventional. The loop, however, makes sense with the EB and DEB produced in the reaction section accumulating in the recycle column sump so that its level indirectly reflects the reactor production rate. A reduction in the sump level implies the need to increase production, that is, higher fresh ethylene feed and vice versa. The workability of this unconventional level control scheme depends on how long it takes for a change in the fresh ethylene feed to affect the recycle column sump level. Unfortunately for this process, the total reactor residence time is quite high at $\sim$2 h so that the recycle column sump runs dry or overflows even for small disturbances (e.g., $>$1% throughput change). The "unconventional" level controller, thus, turns out to be quite fragile. It would, however, have been a workable option if the reactors were smaller.

To improve the robustness of recycle column sump level control, the synthesized "optimal" control structure in Figure 3a must be tweaked. We give up on tight B_2 control to free the B_2 valve, which then gets used for maintaining U_{Bot1}-B_1. The reconfiguration of the U_{Bot2} MV frees up the B_1 valve which then gets used to regulate U_{Bot1}. The unconventional $U_{\mathrm{Bot1}}-F_{\mathrm{C2}}$ pairing then gets replaced by the conventional $U_{\mathrm{Bot1}}-B_1$ pairing. The free F_{C2} valve then gets used to loosely regulate B_2. The revised pairings, thus, compromise on the tightness of B_2 control to improve the robustness of U_{Bot1} control. No compromise is, however, made in the tight control of any of the active constraints (soft or hard). The revised control structure for optimal Mode II operation, labeled CS1 for ease of reference, is shown in Figure 3b. Additional loops for near optimum operation at lower throughputs (Mode I) are also shown in figure in grey and explained next.

Throughput reduction and additional Mode I unconstrained CV loops

One would expect sustained periods of operation where the desired throughput is significantly lower than maximum. In CS1, the two setpoints corresponding to the two Mode II unconstrained dofs are $x_{\mathrm{Bz}}^{\mathrm{D2 \cdot SP}}$ and B_2^{SP}. As one reduces throughput, V_1^{MAX}, L_1^{MAX}, and V_2^{MAX} become optimally inactive so that for a given F_{C2} of 630.6 kmol/h (Mode I), we have a total of four unconstrained dofs (two Mode II dofs + three constraints that become inactive $-$ one throughput specification). Of the three input constraints that have become inactive, any one gets used for the desired F_{C2} making it the TPM, whereas the remaining two inputs can take-up control of two self-optimizing CVs for near optimal economic performance in the less constrained low throughput region. We choose V_1 for throughput manipulation as it is the last constraint to optimally become active, that is, the bottleneck constraint. The same TPM then gets used over the entire throughput range. Instead, if L_1 or V_2 is used as the TPM, the TPM will have to be shifted once they hit the maximum limit.

Why V_1^{MAX} is the last constraint to go active is a function of the constraint limits used here as well as the fact that we are free to set the total benzene circulating around the plant, which indirectly fixes V_1. On the other hand, the DEB recycle must be allowed to increase nonlinearly with throughput to recycle DEB to extinction. V_2^{MAX} and L_1^{MAX} limits are then reached before V_1^{MAX} as throughput is increased.

With V_1 as the TPM, what CVs can L_1 and V_2 control on going inactive to mitigate economic inefficiencies in the process operation? Ideally, these CVs should be close-by for tight control. Further, the CVs should be such that maintaining them constant (i.e., constant set-point operation) ensures the process operation is nearly optimal (i.e., self-optimizing CVs). The simplest option of maintaining L_1 and V_2 at their maximum limits even at low throughputs where these should be optimally unconstrained corresponds to over-refluxing in the two columns implying unnecessarily high steam consumption, which is economically not prudent. A simple way of preventing the same is for V_2 to "take up" control of a sensitive product column stripping tray temperature ($T_{\mathrm{Col2}}^{\mathrm{S}}$; 20th tray corresponding to the steepest location in the stripping section temperature profile) and for L_1 to take-up maintaining L_1 in ratio with F_{Col1}. This is accomplished by using a low select on the output of the $T_{\mathrm{Col2}}^{\mathrm{S}}$ and L_1/F_{Col1} controllers, (see Figure 3b). The low select compares the respective controller outputs with the constraint limits (V_2^{MAX} and L_1^{MAX}) and passes the lower of the two for implementation. As-and-when the respective controller outputs reduce below the constraint limits (on sufficient rise in $T_{\mathrm{Col2}}^{\mathrm{S}}$ and sufficient reduction in F_{Col1}), reduction of V_2 and L_1 below their maximum limits is taken up to maintain $T_{\mathrm{Col2}}^{\mathrm{S}}$ and L_1/F_{Col1}, respectively. Similarly, as-and-when the controller outputs increase above their constraint limits, control of the respective CVs ($T_{\mathrm{Col2}}^{\mathrm{S}}$ and L_1/F_{Col1}) is given up and the process is operated at the constraint limits. A good self-optimizing choice for the setpoint of these two CVs is their value at the Mode I optimum.

More on Mode II unconstrained CV setpoints

The CVs corresponding to the two unconstrained Mode II dofs are the product benzene impurity mol fraction ($x_{\mathrm{Bz}}^{\mathrm{D2}}$) and the DEB recycle rate (B_2). To evaluate the effect of these two unconstrained dofs on throughput (Mode II objective function), Figure 4 plots the variation in F_{C2} with B_2 (DEB recycle rate) for different values of product benzene impurity $x_{\mathrm{Bz}}^{\mathrm{D2}}$. Note the maxima in F_{C2} with respect to both the unconstrained dofs. With appropriate choices for the two

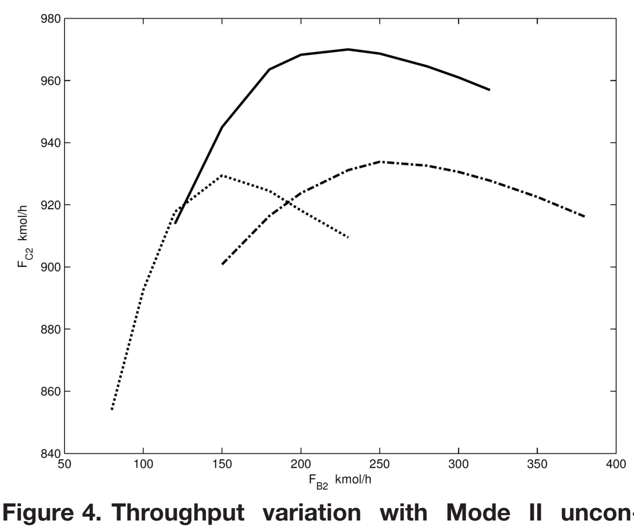


Figure 4. Throughput variation with Mode II unconstrained dofs.

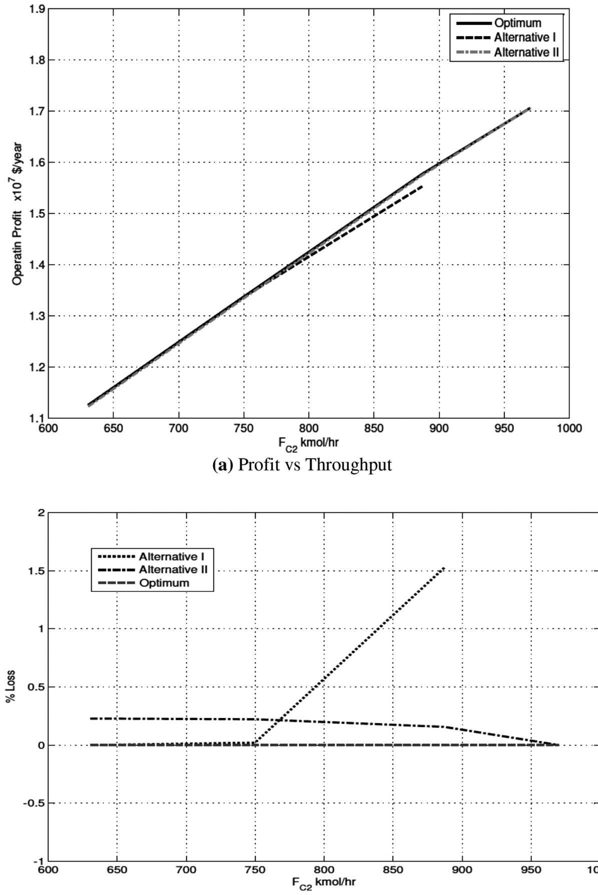
unconstrained setpoints as ${x_{Bz}}^{D2}$ = 0.04% and B_2 = 230 kmol/h (near) maximum production may be achieved. If we change ${x_{Bz}}^{D2}$ to either extreme of DEB or benzene being the principal product impurity, the accompanying throughput decrease is significant at ~4% (see Figure 4).

Towards one extreme of the principal impurity in the EB product being benzene (${x_{Bz}}^{D2}$ ~0.09%), loosening ${x_{Bz}}^{D2}$ requires a sharper split in the product column so that the total (DEB + benzene) product impurity does not exceed 0.1%. The product column reflux must then increase. As V_2^{MAX} is active and B_2 is fixed, the feed to the product column must then decrease so that the throughput decreases. If we go to the other extreme where the principal impurity in the product is DEB, (x_{Bz}^{D2} ~0.01%), the split in the recycle column is sharper. As L_1^{MAX} and V_1^{MAX} are active and, therefore fixed, tightening x_{Bz}^{D2} further causes the feed to the recycle column to decrease implying a reduction in throughput. The Mode II optimum product impurity mix at x_{Bz}^{D2} = 0.04% balances these two opposing effects. This is in contrast to Mode I, where the principal impurity in the EB product is benzene (x_{Bz}^{D2} = 0.09%) as each mol of DEB consumes 1 mol of fresh benzene ($85 per kmol) and 2 mols of fresh EB ($30 per kmol) giving a total raw material price of $145 per kmol DEB lost in EB product. Given that energy is much cheaper than raw material (Douglas' doctrine[12]), it makes economic sense to let the principal impurity at low throughputs (Mode I) be benzene with its lower $85 per kmol price.

The optimum with respect to B_2 is now interpreted. As B_2 is increased sufficiently, EB leaks down the product column bottoms so that a lower reflux is needed to maintain the DEB impurity in the product. As V_1^{MAX} is active and B_2 is fixed, the feed to the product column and hence throughput, must increase. If the B_2 is, however, increased too much, reduction in product column distillate rate due to too much EB leaking down the bottoms dominates implying loss in production. Note that the Mode I optimum B_2 rate (122 kmol/h) is significantly lower than its corresponding value in Mode II (230 kmol/h). If we use the Mode II B_2 value in Mode I, the product column boil-up shoots up. The penalty in the profit is, however, small (~0.1%) as energy is significantly cheaper than the product—raw material price difference (Douglas' doctrine).

In CS1, the setpoints corresponding to the four unconstrained Mode I dofs are: $x_{Bz}^{D2 \cdot SP}$, B_2^{SP}, $L_1/F_1^{\cdot SP}$, and ${T^S}_{Col2}{}^{\cdot SP}$. As reported in Table 1, the optimum value of the former two common unconstrained setpoints between Mode I and Mode II is significantly different. In the interest of simplicity, we would like to implement a constant setpoint policy over the entire throughput range for any unconstrained setpoints while ensuring near optimum operation. Figure 5 plots the variation in operating profit with throughput using the price data in Table 1 for two constant setpoint operation alternatives. In the Alternative 1, the Mode I optimum values for x_{Bz}^{D2} and B_2 are implemented at all throughputs while in the second alternative, the corresponding Mode II optimum values are implemented at lower throughputs. The loss from optimum profit is also shown in figure.

As seen in Figure 5, the maximum achievable throughput in Alternative 1 turns out to be only 887 kmol/h, which is a significant ~8% throughput loss. A further increase in throughput is only possible if $x_{Bz}^{D2 \cdot SP}$ and B_2^{SP} are readjusted to their Mode II optimum values. Also, the steady state profit is ~1.5% lower than the optimum profit at F_{C2} 887 kmol/h, which represents an unacceptable steady economic loss. In contrast, in Alternative 2, the maximum achievable throughput is 970 kmol/h. Also the profit loss (Table 1 price data) compared to the optimum is <0.35% over the entire throughput range. Economically, Alternative 2 is, thus, clearly the better option for the unconstrained CV setpoints. That the steady economic loss is acceptably small using a constant setpoint policy for $x_{Bz}^{D2 \cdot SP}$ and B_2^{SP} is why these CVs are referred to as self-optimizing. Such self-optimizing CVs provide near optimal process operation over the entire throughput range and significantly simplify the control system by eliminating the need for a model based real-time optimizer for obtaining the optimum unconstrained CV setpoints.



(a) Profit vs Throughput

(b) % profit loss (from optimum) vs Throughput

Figure 5. Economic comparison of two alternative constant setpoint operating policies.

Alternative 1: x_{Bz}^{D2} and B_2 fixed at Mode I optimum.
Alternative 2: x_{Bz}^{D2} and B_2 fixed at Mode II optimum.

Using Alternative 2 in CS1, at maximum throughput (Mode II), x_{Bz}^{D2} = 0.04%, B_2 = 230 kmol/h and V_1^{MAX}, L_1^{MAX}, and V_2^{MAX} are active. As throughput is reduced by reducing V_1 (TPM), control of T_{Col2}^S and L_1/F_{Col1} is taken up by V_2 and L_1, respectively. Conversely, as throughput is increased, control of T_{Col2}^S and L_1/F_{Col1} is given up as V_2^{MAX} and L_1^{MAX}, respectively, become active. Finally, maximum throughput is achieved when V_1^{MAX} becomes active.

Conventional Plantwide Control Structure

Structure for robust and near optimal Mode I operation

Conventionally, a process feed is used as the TPM and the overall plantwide control structure is configured around it. First, the material/energy balance loops for the individual

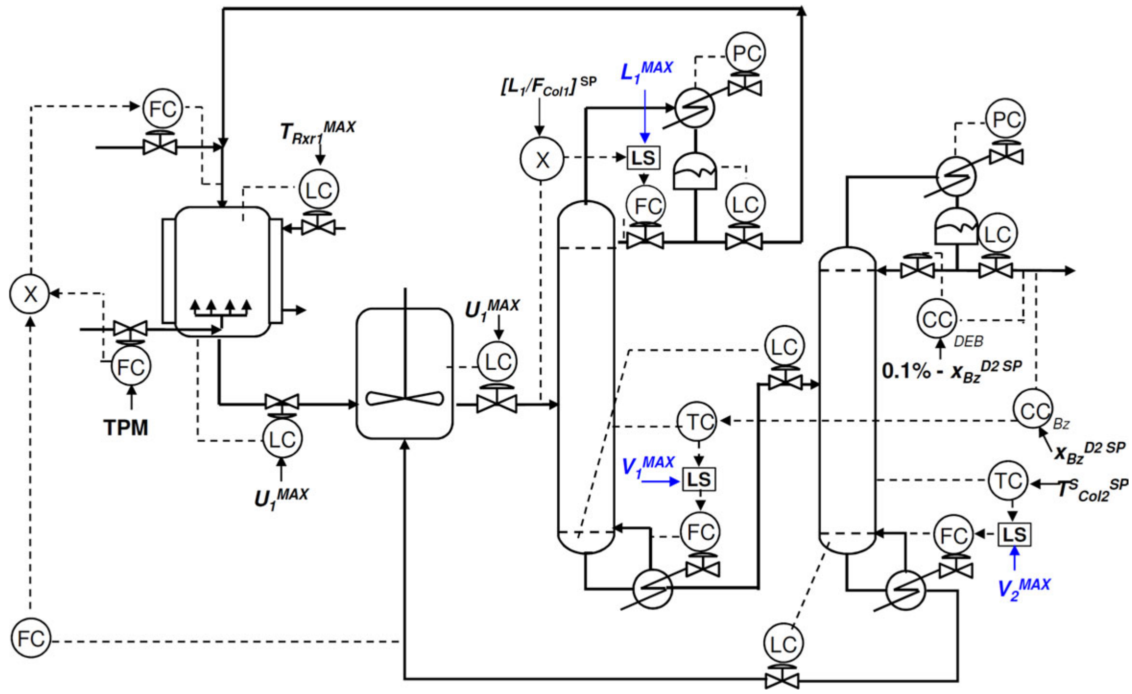


Figure 6. Conventional control structure, CS2, with TPM at ethylene feed.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

units are paired followed by component inventory loops. Luyben[10] has developed such a conventional control structure, labeled CS2, as in Figure 6, for unconstrained process operation around the base-case design (Mode I). To contrast with our ‘‘top-down’’ pairing approach, the pairing sequence followed in the ‘‘bottom-up’’ approach is described briefly.

Fresh ethylene (limiting reactant) is flow controlled and used as the TPM (first loop). Conventional pairings for material and energy balance regulation on the downstream units are then chosen. The reactor levels are controlled using the respective reactor outflows ($U_1 - F_{\mathrm{Rxr2}}$ and $U_2 - F_{\mathrm{Col1}}$), whereas T_{Rxr1} is regulated using Q_{Rxr1} (second to fourth loops). In both the columns, the condenser pressure, reflux drum level, and sump level are controlled using condenser duty, distillate, and bottoms, respectively (5th to 10th loops).

The next step is to pair loops to regulate component inventories using conventional pairings. To regulate the EB leakage up the top and the benzene leakage down the bottoms of the recycle column, respectively, L_1 is maintained in ratio with F_{Col1} and $T^{\mathrm{S}}_{\mathrm{Col1}}$ is maintained using V_1 with $T^{\mathrm{S}}{}_{\mathrm{Col1}}{}^{\cdot\mathrm{SP}}$ being adjusted by the $x^{\mathrm{D2}}_{\mathrm{Bz}}$ (benzene impurity in product) controller in a cascade arrangement (11th and 12th loops). On the product column, the product DEB impurity mol fraction is maintained using the reflux ($x^{\mathrm{D2}}_{\mathrm{DEB}} - L_2$), whereas $T^{\mathrm{S}}_{\mathrm{Col2}}$ is maintained using the reboiler duty to regulate the EB leakage in B_2 (13th and 14th loops). The last loop to be paired is for regulating the benzene inventory circulating around the plant. This is accomplished by manipulating the fresh benzene to hold the total (fresh + recycle) benzene (F_{TotBz}) to the first reactor. F_{TotBz} is maintained in ratio with F_{C2} to mitigate composition transients in the reaction section. For a fast dynamic response for process operation around the base-case design,[10] the $F_{\mathrm{TotBz}}/F_{C2}$ setpoint is adjusted to maintain the DEB recycle rate B_2 (15th loop).

For near optimum Mode I operation ($F_{\mathrm{C2}} = 630.6$ kmol/h) using this conventional structure, we set the reactor level and temperature setpoints at their maximum limits (U_1^{MAX}, U_2^{MAX}, and $T^{\mathrm{MAX}}_{\mathrm{Rxr1}}$). Further, we set $x^{\mathrm{D2\cdot SP}}_{\mathrm{DEB}} = 0.1 - x^{\mathrm{D2\cdot SP}}_{\mathrm{Bz}}$ (on-aim product quality) with $x^{\mathrm{D2\cdot SP}}_{\mathrm{Bz}}$ at its self-optimizing value of 0.04 mol%. Similarly, the setpoint values for the remaining three unconstrained CVs, namely, B_2, L_1/F_{Col1}, and $T^{\mathrm{S}}_{\mathrm{Col2}}$ are chosen to be the same as for CS1 for consistency as well as self-optimizing operation over the wide Mode I to Mode II throughput range using constant setpoints. It is instructive to compare CS1 and CS2 (Figures 3b and 6) for Mode I operation and observe that even as the loop pairings are very different, both structures control the same set of CVs (active constraints and unconstrained CVs).

Handling capacity constraints using override controllers

As throughput is increased by increasing $F^{\mathrm{SP}}_{\mathrm{C2}}$, the constraints V_2^{MAX}, L_1^{MAX}, and V_1^{MAX} become active. L_1^{MAX} implies regulation of EB impurity in the benzene recycle stream is lost, which is acceptable as it is not a product stream. V_1^{MAX} and V_2^{MAX} are more problematic constraints and handling them requires override controllers. The override control scheme is shown in Figure 7 and is briefly explained below.

V_1^{MAX} implies loss of $T^{\mathrm{S}}_{\mathrm{Col1}}$ control and hence regulation of the benzene impurity in the product, which is unacceptable. To ensure $T^{\mathrm{S}}_{\mathrm{Col1}}$ control is not lost, an alternative MV is needed when V_1^{MAX} goes active. The closest MV is F_{Col1} and a $T^{\mathrm{S}}_{\mathrm{Col1}}$ override controller must ‘‘take-up’’ F_{Col1} manipulation from the nominal U_2 (reactor 2 level) controller. To do so, a low select compares the nominal U_2 and override $T^{\mathrm{S}}_{\mathrm{Col1}}$ controller outputs and passes the lower of the two to the F_{Col1} valve. The setpoint of the $T^{\mathrm{S}}_{\mathrm{Col1}}$ override is biased to be below the nominal $T^{\mathrm{S}}_{\mathrm{Col1}}$ setpoint. When V_1^{MAX} is inactive, $T^{\mathrm{S}}_{\mathrm{Col1}}$ is close to the nominal setpoint and the override controller output is high so that F_{Col1} is under nominal U_2 level control. Once V_1^{MAX} is hit, nominal $T^{\mathrm{S}}_{\mathrm{Col1}}$ control is lost and the tray temperature decreases causing the $T^{\mathrm{S}}_{\mathrm{Col1}}$ override output to decrease below the nominal U_2 controller output. F_{Col1} manipulation then passes to the override $T^{\mathrm{S}}_{\mathrm{Col1}}$ controller.

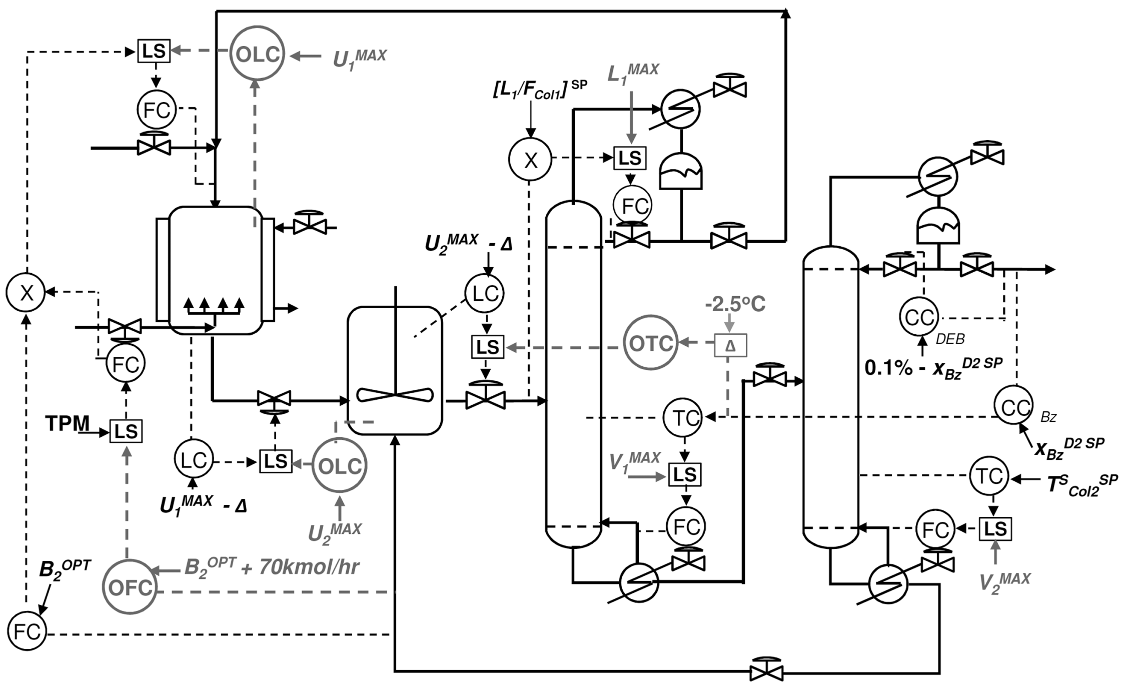


Figure 7. CS2 with overrides for handling equipment capacity constraints.

With F_{Col1} under T^S_{Col1} override control, an alternative MV is needed for regulating U_2 (reactor 2 level), which otherwise would be unregulated. The closest available MV is F_{Rxr2} and an override U_2 controller must take up F_{Rxr2} manipulation from the nominal U_1 (reactor 1 level) controller. Similar to the overrides on the recycle column, a low selector on the nominal U_1 controller and override U_2 controller outputs is used for the purpose. The override U_2 controller setpoint must be higher than the corresponding nominal U_2 controller setpoint for the override scheme to work. With F_{Rxr2} under U_2 override control, an alternative manipulation handle is needed to maintain U_1, which is now unregulated. The closest available MVs are F_{C2} and F_{TotBz}. Of the two, F_{C2} being a gas feed is not appropriate for controlling liquid level. Accordingly, a U_1 override controller is implemented to "take-up" F_{TotBz} manipulation from the nominal F_{TotBz}/F_{C2} ratio controller using a low selector (see Figure 7). The override setpoint must be higher than the nominal setpoint. Handling the V_1^{MAX} constraint requires three override controllers to alter the material balance structure from the recycle column all the way up to the fresh benzene.

The remaining hard constraint, V_2^{MAX}, represents a capacity constraint on the EB that can be boiled off by the product column. Any EB that cannot be boiled off would now necessarily drop down the product column bottoms and accumulate in the DEB recycle loop causing B_2 to increase. In response to this, the slow acting nominal B_2 flow controller would increase the F_{TotBz}/F_{C2} setpoint for a higher F_{TotBz}, which would require the recycle column boilup (V_1) to increase. B_2 and hence V_1 would continue to increase as long as more EB is being produced in the reaction section than can be boiled off in the product column. Thus, V_2^{MAX} presents a stabilization problem due to snowballing in B_2, which is transformed to V_1 by the action of the B_2 controller. The solution to this is to ensure that the EB generated in the reaction section exactly matches that boiled off in the product column at V_2^{MAX} and there is no excess EB generated to prevent accumulation in the DEB recycle loop. A simple way of accomplishing this is to implement an override B_2 controller that cuts the ethylene (limiting reactant) feed to reduce the reactor EB generation rate should B_2 show a large increase. The setpoint of the override B_2 controller setpoint must then be sufficiently higher than the nominal B_2 controller setpoint so that F_{C2} is cut only for large increases in B_2 and not for routine transients. We apply Shinskey's [13] external reset scheme on all proportional-integral (PI) controllers whose output passes through a low/high selector block. This ensures that when inactive, the reset action does not cause output saturation and facilitates a bumpless switching from one controller to the other.

This completes the synthesis of the conventional control structure, CS2, for process operation over a wide throughput range. The CVs controlled and the pairing sequence followed to synthesize CS1 and CS2 is contrasted in Table 2 to illustrate how the application of the "top-down" pairing approach to Mode II (most constrained point) control objectives leads to a structure that is very different from a conventional structure synthesized for using "bottom-up" pairing applied to Mode I (relatively unconstrained point) control objectives.

Before closing this section on control structure synthesis, we highlight that in contrast to the conventional control structure (CS2) with four overrides, the economic plantwide control structure, CS1, has no overrides and is, therefore, much simpler. This difference is primarily because CS2 is designed for unconstrained Mode I operation, whereas CS1 is designed for constrained Mode II operation. Ensuring material/energy balance consistency for the latter necessarily requires accounting for all active constraints which naturally leads to a simple structure with no overrides. It is also worth highlighting that a comparison of the two control structures in Figures 3b and 7 reveals that CS2 with all the override controllers triggered on (i.e., Mode II) is structurally the

Table 2. Pairing Sequence for CS1 (Top-Down) and CS2 (Bottom-Up)

CS1	CS2
Hard constraint control loops	Throughput manipulator
$V_1^{MAX} \leftrightarrow Q_{Reb1}$	F_{C2}
$V_2^{MAX} \leftrightarrow Q_{Reb2}$	Material and energy balance loops
Soft constraint and SOCV control loops	$T_{Rxr1} \leftrightarrow Q_{Rxr1}$
$L_1 \leftrightarrow VLV_{L1}$	$U_1 \leftrightarrow F_{Rxr2}$
$x_{DEB}^{D2{\cdot}MAX} \leftrightarrow L_2$	$U_2 \leftrightarrow F_{Col1}$
$x_{Bz}^{D2} \leftrightarrow T_{Col1}^{S} \leftrightarrow F_{Col1}$	$P_{Col1} \leftrightarrow Q_{Cnd1}$
$T_{Rxr}^{MAX} \leftrightarrow Q_{Rxr1}$	$P_{Col2} \leftrightarrow Q_{Cnd2}$
$U_2^{MAX} \leftrightarrow F_{Col1}/F_{Rxr2} \leftrightarrow F_{Rxr2}$	$U_{RD1} \leftrightarrow D_1$
$U_1^{MAX} \leftrightarrow F_{Rxr2}/F_{TotBz} \leftrightarrow F_{TotBz}$	$U_{RD2} \leftrightarrow D_2$
$B_2 \leftrightarrow F_{C2}$*	$U_{Bot1} \leftrightarrow B_1$
Material and energy balance loops	$U_{Bot2} \leftrightarrow B_2$
$P_{Col1} \leftrightarrow Q_{Cnd1}$	Component inventory loops
$P_{Col2} \leftrightarrow Q_{Cnd2}$	$L_1/F_{Col1} \leftrightarrow L_1$
$U_{RD1} \leftrightarrow D_1$	$x_{Bz}^{D2} \leftrightarrow T_{Col1}^{S} \leftrightarrow Q_{Reb1}$
$U_{RD2} \leftrightarrow D_2$	$x_{DEB}^{D2} \leftrightarrow L_{2z}$
$U_{Bot2} \leftrightarrow B_2$*	$T_{Col2}^{S} \leftrightarrow Q_{Reb2}$
$U_{Bot1} \leftrightarrow B_1$*	$B_2 \leftrightarrow F_{TotBz}/F_{C2} \leftrightarrow F_{TotB}$

*Revised from $B_2 \leftrightarrow VLV_{B2}$, $U_{Bot2} \leftrightarrow B_1$ and $U_{Bot1} \leftrightarrow F_{C2}$ for robust level control.

same as CS1. CS1 is then the most natural control structure for Mode II operation in light of the particular hard capacity constraints. It is appealing in that its basic regulatory control philosophy, as reflected in material/energy balance control structure remains the same regardless of which of the equipment capacity constraints are active, that is, for both Mode I and Mode II operation.

Results

Rigorous dynamic simulations of the synthesized control structures, CS1 and CS2, are performed in Aspen Plus and their closed loop performance evaluated for design throughput and high throughput operation. To illustrate the role of the overrides, variants of CS2 with different overrides for handling V_1^{MAX} and V_2^{MAX} switched on or off are evaluated. We also demonstrate throughput transition from Mode I to Mode II for the two control structures.

Controller tuning

A consistent tuning procedure is followed in the two structures to ensure that any differences in control performance are largely due to structural differences and not due to tuning. All flow controllers (except B_2 flow controller) are PI and use a gain of 0.5 and reset time of 0.5 min for fast setpoint tracking. All level controllers (except reactors) are *P* only with a gain of 2. The nominal reactor level controllers are PI. The override level controllers in CS2 use the same tuning as the nominal level controllers. The maximum level setpoint in the two reactors (U_1^{MAX} and U_2^{MAX}) is 5.06 m. Because the CS2 level override scheme requires the nominal level controller setpoint to be less than the corresponding overrides, the nominal level controller setpoints are chosen as 4.81 m (10% offset) for both the reactors. Override level controller setpoint is then set at 5.06 m (maximum limit).

In CS1, the ratio based reactor level controllers are tuned aggressively for tight level control. The column pressure controllers are PI and tuned for tight pressure control. A 1-min lag is applied to all temperature measurements. Also, to account for cooling/heating circuit dynamics, a 2-min lag is applied to the output of temperature controllers, where appropriate. All temperature controllers (including T_{Col1}^{S} override controller) are PI and tuned using the relay feedback test with Tyreus–Luyben settings. The override T_{Col1}^{S} controller setpoint is offset from the nominal setpoint to be 2.5°C lower. On the product column, as tight product impurity control is more important than stripping tray temperature control, the loops are tuned sequentially in that order so that all the detuning due to multivariable interaction between the two loops gets taken in the stripping loop. The composition controllers use a sampling time and dead time of 5 min each and are tuned using the relay feed back test with Tyreus–Luyben settings.

The slow B_2 flow controller in CS1 is tuned manually for a fast but not-too-oscillatory overall plantwide response. The nominal and override B_2 controllers in CS2 are also similarly tuned. The B_2 override setpoint is offset 70 kmol/h above the nominal setpoint to ensure it does not trigger during routine transients (30–40 kmol/h swings in B_2). Salient controller parameters for CS1 and CS2 (including overrides) are reported in Table 3.

Unconstrained low throughput operation

CS1 and CS2 are tested for a ±10% throughput change at the base-case throughput of 630 kmol/h F_{C2} (Mode I), which is sufficiently away from hard equipment capacity constraints. In CS1, the TPM is V_1^{SP} and large step changes in the setpoint are not permitted to ensure smooth column operation without hydraulic problems such as flooding or weeping. Accordingly, V_1^{SP} is ramped at ±40 kmol/h^2, which corresponds to approximately ±10% boilup change (based on base-case boilup) per hour. To maintain consistency in comparing CS1 and CS2, the CS2 TPM, F_{C2}^{SP}, is ramped at ±60 kmol/h^2, which is nearly ±10% change (based on base-case F_{C2}) per hour.

Figure 8 plots the dynamic response of key process variables to the ramped throughput change. In both structures, the overall plantwide response is smooth taking ~20 h to complete with tight control of the product purity. The product purity control achieved in CS2 is not as tight as in CS1 due to relatively larger deviations in the two reactor levels in the latter. Tighter reactor level control by maintaining reactor outflow in ratio with reactor inflow and the level controller manipulating the ratio setpoint may improve the product purity control. Also note that as the level setpoint for the two reactors in CS2 is lower than in CS1 for proper functioning of the U_1 and U_2 overrides, the steady value of V_1 (initial or final) in CS2 is higher than in CS1. The need for overrides, thus, results in higher steady steam consumption in CS2. Its economic significance is, however, negligible as energy is much cheaper than product/raw material (Douglas' doctrine). The responses in Figure 8 show that for unconstrained operation around the design throughput, where no hard equipment capacity constraints are active, both CS1 and CS2 provide smooth process operation for a throughput change in either direction.

In his article, Luyben[10] also considered the benzene feed being contaminated with DEB as a disturbance purely for illustration purposes. Figure 9 compares the Mode I transient plantwide response to a step increase in the DEB mol fraction in the fresh benzene from 0 to 5%. The CS1 response is observed to be very smooth with B_2 increasing due to the extra DEB in the benzene feed and the B_2 controller cutting F_{C2} appropriately to bring B_2 back to setpoint (230 kmol/h).

Table 3. Controller Parameters*,† for CS1 and CS2

Regulatory Layer									
		CS1				CS2			
CV	CV Span	MV	MV Span	K_C	τ_i (min)	MV	MV Span	K_C	τ_i (min)
U_1	0–100%	F_{Rxr2}/F_{TotBz}	0–2	5	30	F_{Rxr2}	0–2000 kmol/h	2	50
U_2	0–100%	F_{Col1}/F_{Rxr2}	0–1.5	5	30	F_{Col1}	0–2500 kmol/h	2	50
T_{Rxr1}	0–400°C	Q_{Rxr1}	0–22 MW	4.0	25	Q_{Rxr1}	0–22 MW	8	25
T^S_{Col1}	77157°C	F_{Col1}	0–2500 kmol/h	0.8	18.5	V_1	0–1010 kmol/h	4.4	25
T^S_{Col2}	0.0–244.7° C	V_2	0–1113.3 kmol/h	4.4	11	V_2	0–1113.3 kmol/h	4.4	20
x^{D2}_{Bz}	0–0.0016	$T^S_{Col1}{}^{SP}$	77–157°C	0.08	100	$T^S_{Col1}{}^{SP}$	77–157°C	0.045	100
x^{D2}_{DEB}	0 0.002	L_2	0–83251 kg/h	0.32	88.5	L_2	0–83251 kg/h	0.25	66
B_2	0–500 kmol/h	F_{C2}	0–1500 kmol/h	0.4	400	F_{TotBz}/F_{C2}	0–4	0.25	450

Tuning Parameter for CS2 Override Controllers

CV	CV Span	MV	MV Span	K_C	τ_i (min)
U_1	0–100%	F_{TotBz}	0–3000 kmol/h	2	250
U_2	0–100%	F_{Rxr2}	0–2000 kmol/h	5	250
T^S_{Col1}	77–157°C	F_{Col1}	0–2500 kmol/h	1.5	40
B_2	0–500 kmol/h	F_{C2}	0–1500 kmol/h	0.4	400

*All level loops use $K_C = 2$ unless specified otherwise.
†Pressure/flow controllers tuned for tight control.

The product purity control during the transient period is observed to be tight. At the final steady state, the EB production rate is the same as at the initial steady state with each mol of DEB in the fresh feed being recycled to extinction to generate 2 mols of EB. The fresh ethylene then correspondingly reduces by two times the DEB rate in the fresh benzene.

In CS2, a large increase in B_2 occurs initially as F_{C2} is the TPM, which remains fixed till ~4 h with the extra DEB fed during the period accumulating into B_2. The increase in B_2 triggers the B_2 override which takes up F_{C2} reduction to mitigate the increase. Meanwhile, the nominal B_2 controller keeps increasing F_{TotBz}/F_{C2} so that the excess benzene in the reactors increases, suppressing DEB formation. This, coupled with F_{C2} reduction by the B_2 override, causes B_2 to decrease with the override eventually giving-up F_{C2} manipulation. The process finally settles at a steady state with a higher throughput which matches recycle-to-extinction of each mol of DEB in the benzene feed to 2 mols of EB product. Compared to CS1, CS2 exhibits more severe plantwide transients with larger transient deviations in the EB product purity. For the sake of comparison, the plantwide transient response to

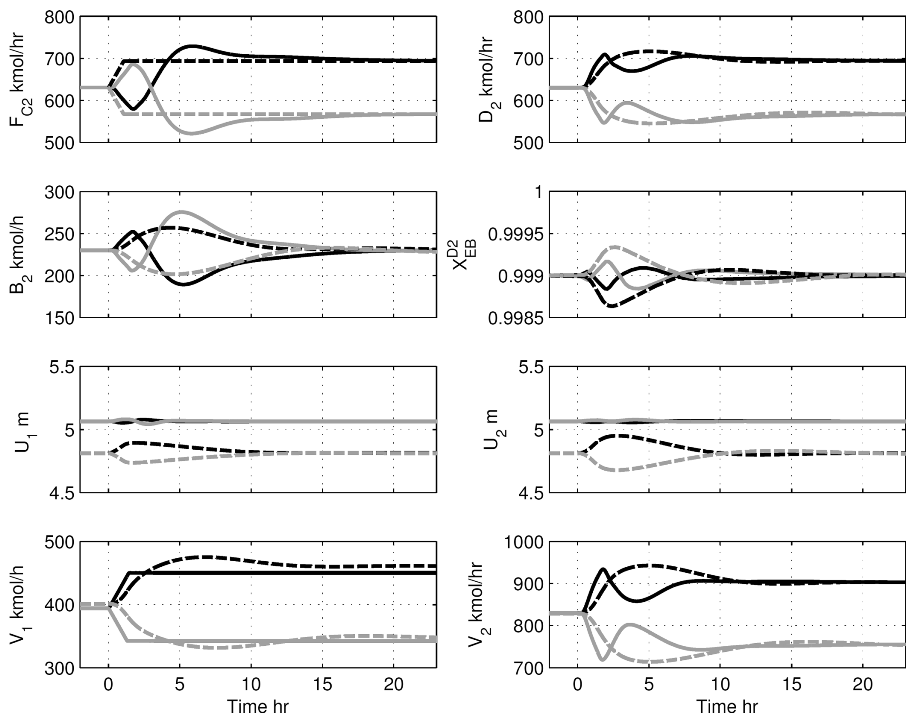


Figure 8. Mode I transient response to ±10% ramped throughput change.

—: CS1 +13% V_1^{SP} ramp change; —: CS1 –13% V_1^{SP} ramp change; – –:CS2 +10% ramp change in F_{C2}^{SP} – –: CS2 –10% ramp change in F_{C2}^{SP}.

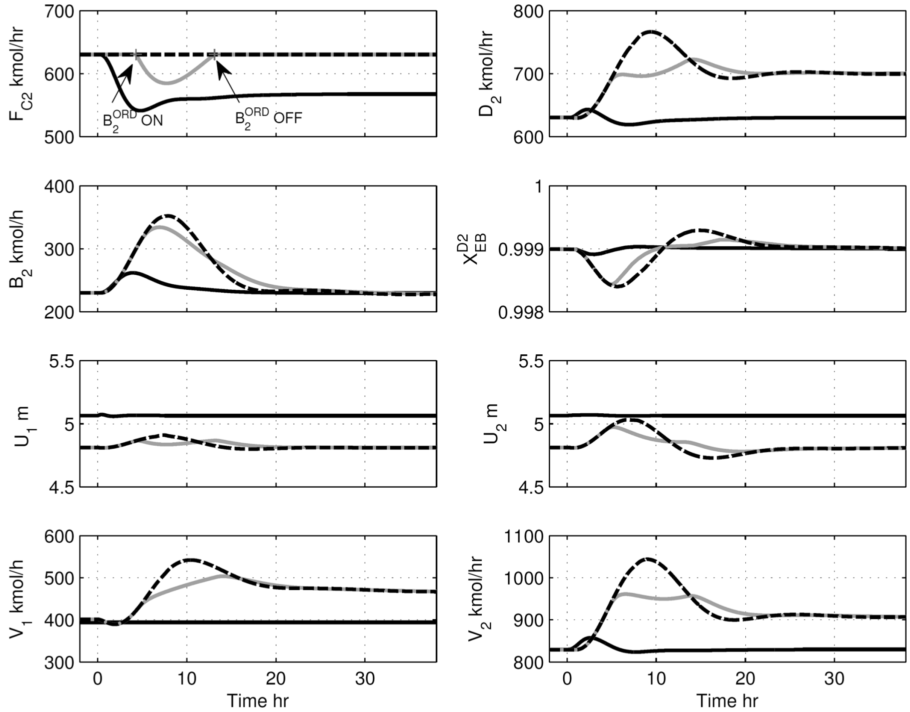


Figure 9. Mode I transient response for +5% DEB composition change in F_{Bz} at base case.

—: CS1 —: CS2 – –: CS2^{B2Off}.

the benzene feed composition disturbance is also obtained with the CS2 B_2 override switched off. A larger transient increase in B_2 and V_1, along with higher product purity deviations is observed. CS2, thus, does not handle the feed composition disturbance as well as CS1 for unconstrained Mode I operation.

High throughput operation

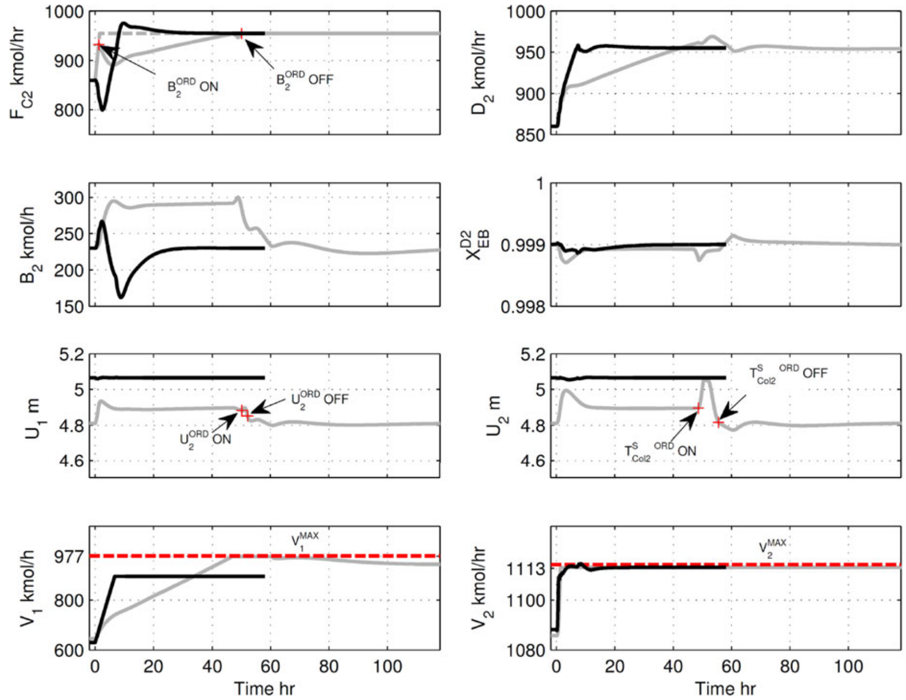
Performance differences between the two basic control structures are further apparent when we try to operate the process at higher throughputs, where V_2^{MAX} (first capacity constraint) is about to go active. For illustration, we consider a ramp increase in the TPM to effect a 95 kmol/h increase in F_{C2} from an initial steady-state F_{C2} of 860 kmol/h. At this F_{C2}, the steady V_2 is close to but below V_2^{MAX}. The ramp rates used are the same as for Mode I.

Figure 10 compares the plantwide transient response of CS1 and CS2 (all overrides on) to the ramped throughput increase. CS1 achieves a smooth increase in throughput with tight product purity control even as V_2^{MAX} goes active with the plantwide response completing in 25 hrs. The plantwide response of CS2, on the other hand, takes about 80 h to complete, which is thrice that of CS1. This is due to additional transients caused by the triggering / untriggering of the different overrides in CS2 (CS1 has no overrides), as explained next.

In CS2, as ${F_{C2}}^{SP}$ is ramped up, V_2 increases to hit V_2^{MAX} and T_{Col2}^{S} control is lost. EB drops down the product column bottoms causing B_2 to increase. In response, the nominal B_2 controller increases F_{TotBz}/F_{C2}^{SP} causing F_{TotBz} and hence V_1 to increase. Meanwhile, as B_2 is increasing, the B_2 override output decreases and takes up ${F_{C2}}^{SP}$ reduction to maintain B_2. Now as B_2 is higher than its nominal value (230 kmol/h), the nominal B_2 controller continues to increase F_{TotBz}/F_{C2}^{SP} causing V_1 to increase till V_1^{MAX} is hit. During this period, as the amount of excess benzene in reactors is higher as F_{TotBz} is increasing, the DEB generation rate reduces and the B_2 override slowly increases the fresh ethylene feed rate to maintain B_2. As V_1^{MAX} goes active, the T_{Col1}^{S} and U_2 override controllers take up, in that sequence, manipulation of their respective unit feed streams (U_1 override does not get triggered). This alteration in the control structure results in additional transients. Now as the override U_2 controller setpoint is higher, the extra reaction capacity of the second reactor consumes additional DEB causing B_2 to decrease with the B_2 override giving up F_{C2} manipulation. B_2 continues to decrease as V_1^{MAX} is active to give a large benzene recycle rate which suppresses DEB formation. The reduction in B_2 causes U_2 to decrease and the U_2 override gives up F_{Rxr2} manipulation. This forces the nominal U_2 controller to take-up F_{Col2} manipulation to maintain the reactor level, which in turn forces the nominal ${T^S}_{Col1}$ controller to take-up the reduction of V_1^{SP} to its final steady-state value, which is slightly below V_1^{MAX}. The overall plantwide transient response, thus, witnesses repeated alteration of the MVs and setpoints for B_2, U_2, and T_{Col1}^{S} causing additional transients for a significantly higher plantwide response settling time with larger product purity deviations. For high throughput operation, CS2 (with overrides) is, thus, dynamically inferior to CS1.

In light of the above results, it is not at all surprising that operators tend to switch-off the overrides and take it on themselves to manually adjust appropriate setpoints. We consider alternative scenarios in CS2 with different overrides switched off. In CS2^{V1Off}, overrides only for handling V_1^{MAX} (T_{Col1}^{S}, U_2, and U_1 overrides) are switched off while in CS2^{B2Off}, only the B_2 override for handling V_2^{MAX} is switched off. In CS2^{AllOff}, all the overrides are switched off.

Let us first consider CS2^{V1Off}. As the U_1 and U_2 overrides are off, no offset is needed in the nominal reactor level controller setpoints and these can be set at their respective maximum limits. The slight increase in reaction capacity would cause the V_1^{MAX} constraint to be hit at a slightly higher



Time (hr)	1.32	48.6	50.06	50.14	52.12
ORD On	B_2	T^S_{Col2}	-	U_2	-
ORD Off	-	-	B_2	-	U_2

Figure 10. Transient response for ramped throughput increase (initial F_{C2} 860 kmol/h).

—: CS1 —: CS2 – –: F_{C2} Ramp. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

throughput. Nevertheless, whenever the V_1^{MAX} constraint is hit, we would lose control of the benzene impurity in the EB product (x_{Bz}^{D2}), which is unacceptable. The maximum achievable throughput in CS2^{V1Off} is then limited by the worst-case disturbance scenario for which the V_1^{MAX} constraint is just approached guaranteeing x_{Bz}^{D2} control is never lost.

For illustration, consider a -30 kmol/h step bias in the F_{C2} sensor as the worst-case disturbance. For the negative bias, the F_{C2} controller "thinks" that the flow is lower than setpoint and opens the valve causing the actual flow to be higher. This is in the worst-case direction of increased throughput causing equipment capacity constraints to be approached.

We did several simulations to obtain the maximum achievable throughput without losing x_{Bz}^{D2} control using CS2^{V1Off}. As shown in the transient plantwide response in Figure 11, for an initial F_{C2} of 920 kmol/h, V_1^{MAX} is approached but not violated. The B_2 override gets triggered to reduce F_{C2} and eventually gives up F_{C2} manipulation. The overall plantwide response does not complete by 60 h. For an initial F_{C2} of 930 kmol/h, however, the V_1^{MAX} constraint is hit and product quality control is lost with the B_2 override remaining triggered. The maximum throughput for the considered worst-case disturbance scenario for CS2^{V1Off} is then 920 kmol/h.

For this same disturbance, Figure 12 shows the dynamic response of CS1^{AllOff} for initial F_{C2} values of 850, 860, and 870 kmol/h. For the higher initial F_{C2} of 870 kmol/h, the transient response is smooth with V_2^{MAX} going active and the response completing in about 50 h. For a lower initial F_{C2} of 860 kmol/h, however, the V_2^{MAX} constraint repeatedly goes active and inactive with the T^S_{Col2} controller taking up and giving up V_2^{SP} manipulation. We have observed this to occur for a final steady value of V_2 very close to V_2^{MAX} (actual $F_{C2} = 890$ kmol/h) and is possibly due to interaction between the two recycle loops. If the initial F_{C2} is reduced to 850 kmol/h, the "on-off" switching of the T^S_{Col2} controller is not as severe. If we take an initial F_{C2} of 870 kmol/h (or 880 kmol/h) and give a lower F_{C2} bias of -20 kmol/h (or -10 kmol/h) so that the actual F_{C2} is again 890 kmol/h, the plant ends up in a limit cycle (data not shown). The limit cycle causes transients, which if deemed unacceptable constrain the maximum throughput for CS2^{B2Off} at 850 kmol/h. If the limit cycle transients are deemed acceptable, CS2^{AllOff} fails for a F_{C2} step bias of -30 kmol/h with the initial F_{C2} at 900 kmol/h. Once V_1^{MAX} goes active, product purity control is lost similar to CS2^{V1Off} (data not shown). The maximum throughput for CS2^{AllOff} is then 890 kmol/h, ignoring the limit cycle.

The maximum achievable throughput in CS2^{B2Off} with only the B_2 override switched off turns out to be 910 kmol/h. We did not observe a limit cycle in CS2^{B2Off}. For the particular worst-case disturbance (-30kmol/h F_{C2} step bias), Figure 13 shows the CS2^{B2Off} transient response. For initial F_{C2} of 920 kmol/h, in response to the step bias, V_1 increases and V_1^{MAX} goes active triggering the T^S_{Col1}, U_2, and U_1 overrides. With T^S_{Col1} regulated by the override, regulation of the benzene impurity in the product is not lost and the product purity remains under control. However, the extra EB that could not be boiled off in the product column due to the V_2^{MAX} constraint, drops down the column and fills up the sump to its maximum limit (overflow) before 40 h (snowballing). For a lower initial throughput of 910 kmol/h, even as the product column sump does not fill up, the plantwide response takes a long time to complete (>60 h) due the additional transients caused by the V_1^{MAX} overrides taking up and then giving up control.

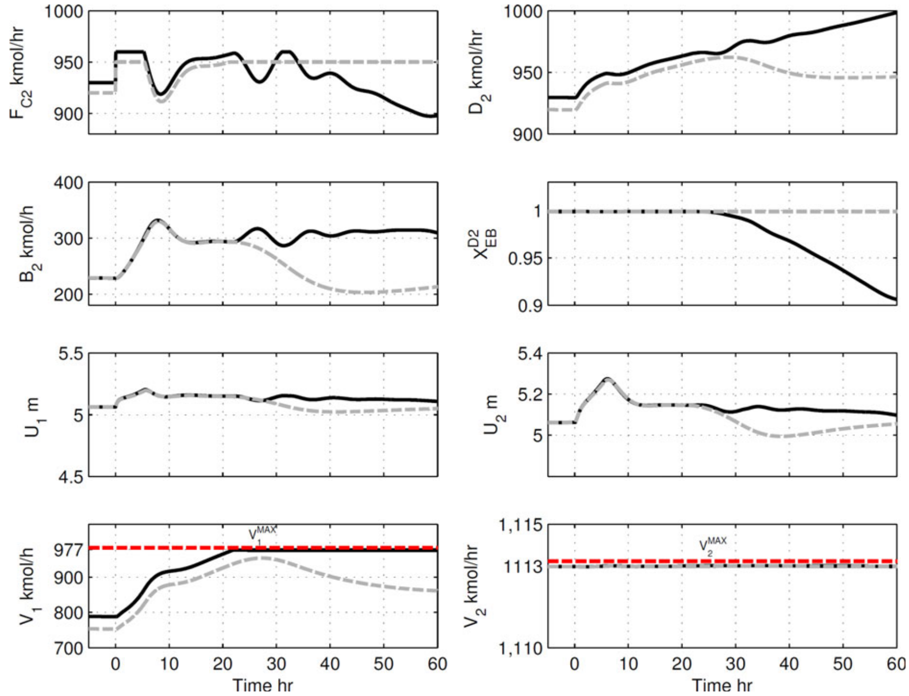


Figure 11. CS2^{V1Off} transient response to −30kmol/hr step bias in F_{C2} sensor.

Initial F_{C2} values (kmol/h) —: 930 – –: 920. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

The lower maximum achievable throughput with B_2 override off (i.e., CS2^{AllOff} and CS2^{B2Off}) is due to V_1^{MAX} going active earlier. This occurs as the control system attempts to maintain B_2 at its nominal value (230 kmol/h), which is significantly lower than the override B_2 value (offset higher to 300 kmol/h). The amount of extra EB not boiled off in the product column (as V_2^{MAX} is active) that can be accommodated in the B_2 stream is then significantly lower compared to when the B_2 override is on. The nominal B_2 controller attempts to transfer most of this extra EB to the benzene recycle stream by increasing the F_{TotBz}/F_{C2} ratio. The rate of increase of V_1 with throughput without the B_2 override is then higher and the V_1^{MAX} constraint is hit earlier giving a significantly lower maximum throughput.

Finally, to close this subsection, we consider maximum throughput operation using CS2 (all overrides on) and CS1

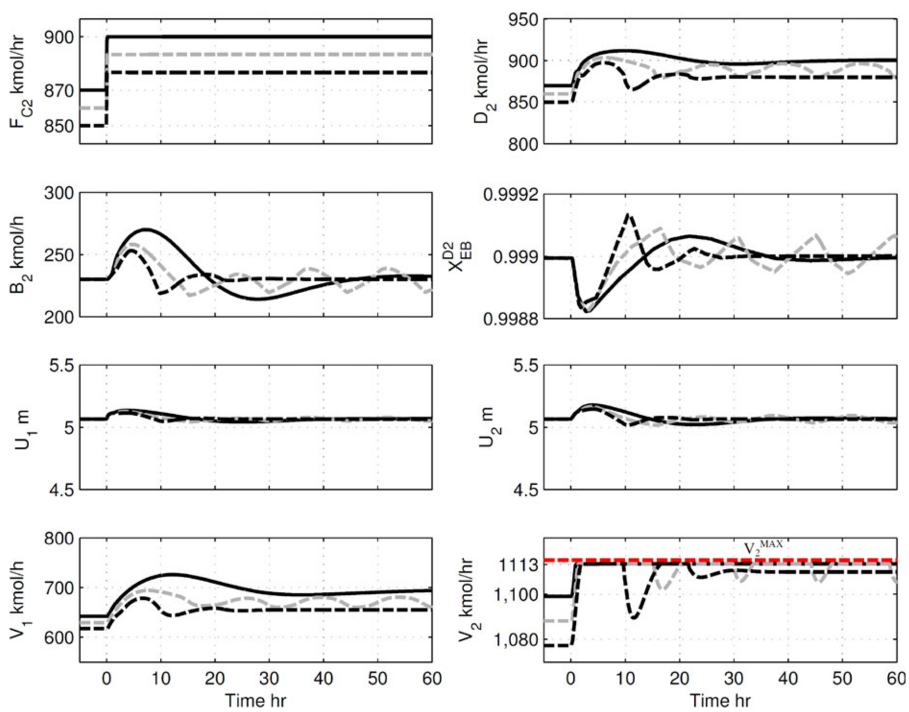


Figure 12. CS2^{AllOff} transient response to −30kmol/hr step bias in F_{C2} sensor.

Initial F_{C2} (kmol/h).—: 870 – –: 860 – –: 850. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

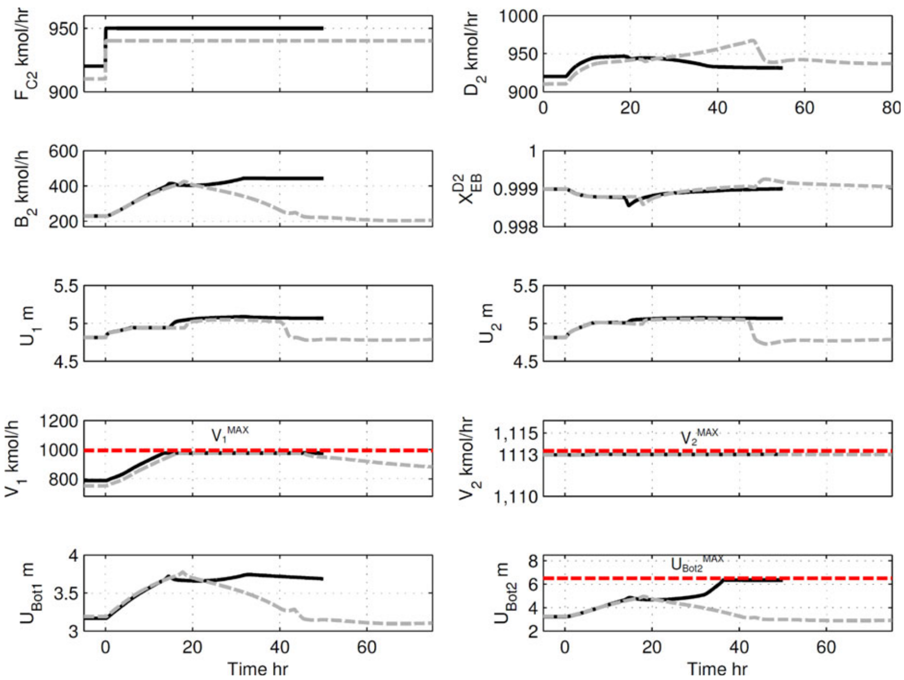


Figure 13. CS2^{B2Off} transient response to −30kmol/hr step bias in F_{C2} sensor.

Initial F_{C2} (kmol/h) —: 920 – –: 910. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

for the worst-case disturbance of −30 kmol/h F_{C2} sensor bias. Because all the overrides are triggered in CS2, it is structurally similar to CS1. Figure 14 compares the plant-wide transient response of CS2 (all overrides on and triggered) and CS1 at maximum achievable throughput. Both the structures effectively handle the F_{C2} step bias disturbance. The negative bias causes the actual ethylene being fed to the process to increase which causes the EB generation rate to increase. This extra EB drops down the product column causing B_2 to increase above its setpoint. The B_2 controller (override B_2 controller in CS2) then reduces F_{C2}^{SP} appropriately to bring B_2 back to setpoint. Note that the maximum achievable throughput in CS2 is 960 kmol/h, 10 kmol/h lower than CS1, which delivers a maximum steady throughput of 970 kmol/h. The ∼1% throughput loss in CS2 is because the B_2 override setpoint must be sufficiently offset from the nominal B_2 so that its value is suboptimal. Thus, once V_2^{MAX} goes active and the B_2 increases to trigger the

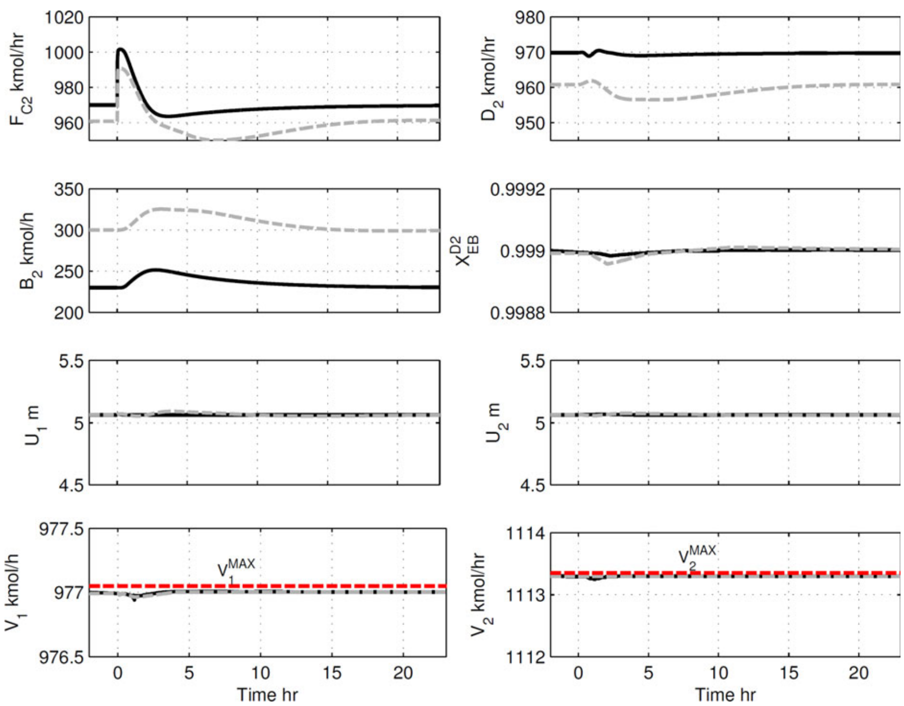


Figure 14. Transient response for −30kmol/hr step bias in F_{C2} flow sensor MAX throughput.

—: CS1 – –: CS2. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

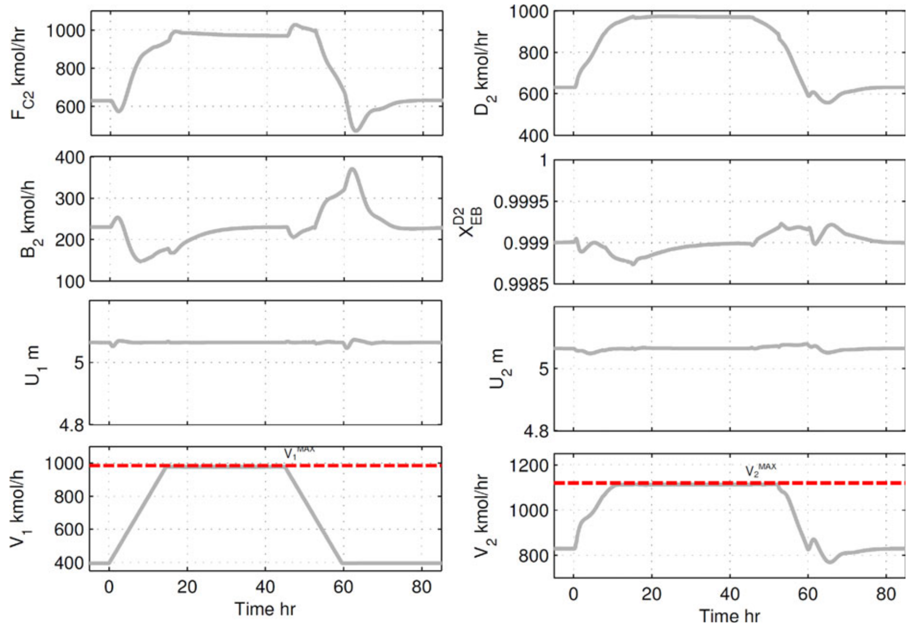


Figure 15. Throughput transition for CS1 with direct B_2 controller and ratioed reactor level control.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

override, the process operates at 300 kmol/h B_2 for which the steady-state throughput is 960 kmol/h (see Figure 4).

Mode I to Mode II throughput transition

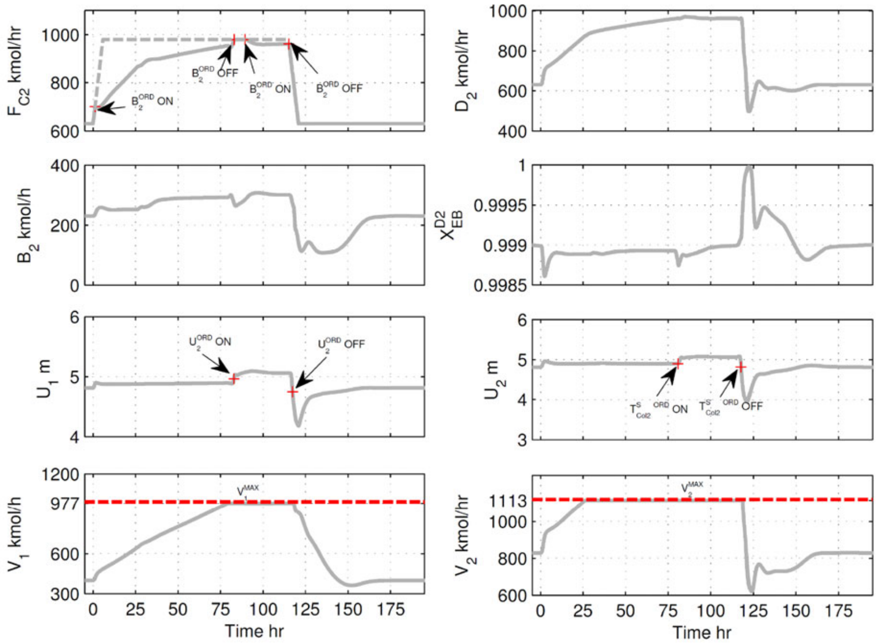
In this final illustration, we consider transitioning the process from a given low throughput (Mode I) to the maximum throughput (Mode II) using CS1 and CS2 (all overrides on). As for a Mode I throughput change, V_1^{SP} (CS1 TPM) is ramped up at a constant rate of 40 kmol/h^2 till V_1^{MAX} becomes active while $F_{\mathrm{C2}}^{\mathrm{SP}}$ (CS2 TPM) is ramped at a rate of 60 kmol/h^2 till 980 kmol/h. After allowing the plantwide transients to die down, the respective TPM setpoints are ramped down to their Mode I values at the same rate.

Figure 15 plots the dynamic response of important process variables to a throughput increase as described above for CS1. The V_1^{SP} ramp completes in about 17 h and then after waiting for $\sim$25 h, V_1^{SP} is ramped down to base-case. During the entire period, the ratio-based reactor level controllers achieve tight level control. Tight EB product purity control is observed with the maximum deviation being within $\pm$0.03%. The maximum achievable steady throughput of 970 kmol/h is reached after the ramp-up completes. Smooth transients are observed in F_{C2}, F_{EB}, and V_2 with B_2 showing a large but smooth positive swing after V_2^{SP} manipulation is taken up by the $T_{\mathrm{Col2}}^{\mathrm{S}}$ controller as V_1^{SP} is ramped down. The economic plantwide control structure CS1, thus, effectively handles the large throughput transition with a fast and smooth transition in either direction along with acceptable product purity control.

The CS2 response to the throughput transition in Figure 16 is more complicated and takes much longer to complete in the direction of increasing throughput. As F_{C2} is ramped up, B_2 increases and the B_2 override gets triggered, which reduces F_{C2} momentarily ($V_2^{\mathrm{MAX}}$is not active yet). As B_2 is higher than nominal, the nominal B_2 controller increases the $F_{\mathrm{TotBz}}/F_{\mathrm{C2}}^{\mathrm{SP}}$ which, coupled with the increased F_{C2}, causes V_1 to increase. F_{TotBz} then increases suppressing DEB generation causing the B_2 override to slowly increase F_{C2} to maintain B_2. V_2^{MAX} goes active at $\sim$25 h, where on B_2 increases toward the override setpoint. Eventually, at $\sim$75 h, V_1^{MAX} goes active triggering the $T_{\mathrm{Col1}}^{\mathrm{S}}$, U_2, and U_1 overrides, in that order. The increase in U_2 due to the higher U_2 override setpoint, leads to a higher DEB consumption rate so that B_2 decreases. The B_2 override then briefly gives up F_{C2} manipulation only to take it up after the U_1 override triggers, which causes the DEB generation and hence B_2 to again increase. F_{C2} finally settles at its maximum achievable value of 960 kmol/h after about 100 h. $F_{\mathrm{C2}}^{\mathrm{SP}}$ is then ramped down at $\sim$120 h and in response, the overrides give-up MV adjustment in the order B_2, U_1, U_2, and finally $T_{\mathrm{Col1}}^{\mathrm{S}}$ with the process finally settling at the base-case throughput after $\sim$170 h.

The EB product purity control is not as tight as for CS1, particularly for the transient period corresponding to a ramp-down of F_{C2}, with significant quality giveaway. The control of the reactor levels is also not as tight and may be improved by implementing ratio-based level control. The overall transition time from Mode I to Mode II and back using CS2 is about twice of CS1 and the maximum throughput is $\sim$1% lower.

To end this section, we briefly summarize the dynamic results. Although CS1 and CS2 are comparable for Mode I throughput change, the dynamic response for a Mode I benzene feed composition disturbance is noticeably superior for CS1, both in terms of the severity of the plantwide transients as well as the tightness of product purity control. The overrides for handling constraints in CS2 make its functioning more complicated. These overrides cause the dynamic performance at high throughputs, where hard constraints go active, to be inferior due to additional transients caused by the taking-up and giving-up of control by the overrides. The need for an offset in the override controller setpoints also leads to an economic disadvantage with a 1% steady throughput loss from maximum achievable (970 kmol/h). No throughput loss occurs in CS1. If the overrides are switched off, the economic penalty is much more severe. The maximum throughput with the V_1^{MAX} overrides switched off is $\sim$5% lower. If only the B_2 override is switched off, the maximum throughput is again $\sim$6% lower. If all overrides are switched



Time (hr)	1.3	80.86	82.84	83.05	84.13	89.95	115.1	115.6	117.3
ORD On	B_2	T^S_{Col2}	U_2	-	U_1	B_2	-	U_1	-
ORD Off	-	-	-	B_2	-	-	B_2	-	U_1

Figure 16. CS2 throughput transition with overrides.

– –: Implemented Ramp Set point for F_{C2}. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

off, a limit cycle is observed for a final steady V_2 very close to V_2^{MAX}. If this limit cycle is not acceptable, the maximum achievable throughput is a significant 12% lower (850 kmol/h F_{C2}). If the limit cycle is deemed acceptable, the maximum achievable throughput is still ~8% lower at 890 kmol/h F_{C2}.

Discussion

The EB process case study on plantwide control system design for economic process operation illustrates several key issues that deserve mention. First and foremost, tight control of hard equipment capacity constraints requiring use of close-by MVs for a negligible back-off and hence economic penalty eliminates several possible regulatory structures. These constraints then cannot be used for process stabilization or economically important control tasks such as product quality control and so forth and may only be used to take-up control of noncritical CVs when inactive. The need for robust material and energy inventory control across a large throughput range (or disturbance space), further screens out unreasonable pairings to give a very small (possibly only one) set of reasonable structures that provide economically optimal operation with robust stabilization. *A priori* knowledge of the full-active constraint set through an offline steady-state optimization or alternatively, through sufficient process experience, is thus the key to synthesizing an effective plantwide control structure for economic process operation. Such a control system with conservatively tuned PI controllers works well over a large operating space encompassing multiple hard equipment capacity constraints suggests that the control system is robust to nonlinear effects, including modeling errors.

In the design of the plantwide control structure, the choice of the TPM plays a crucial role in that it determines an outwardly radiating orientation[14] of the inventory control loops. As in the example studied here, the last hard constraint to become active (the bottleneck constraint) is usually a good choice for use as the TPM as its location remains fixed across the entire throughput range. Overrides to alter the conventional orientation of the material balance structure from "in the direction of process flow" to "in reverse direction of process flow" starting backwards from the bottleneck unit are then avoided. The resulting control structure is much simpler with no overrides for handling the bottleneck constraint and a fixed material balance control structure, which is much appreciated by operators.

There can be cases where the last constraint to become active needs to be maintained constant at lower throughputs for economic reasons. A common example is holding the reactor temperature (or composition) constant at low throughputs for good selectivity (an economic reason) and then after some process constraints become active at higher throughputs, having to increase it to its upper limit for achieving a further increase in throughput. In such cases, a control scheme where the TPM shifts from some location to the reactor temperature (or composition) controller may be economically the most appropriate. We highlight that there is nothing sacrosanct about keeping the TPM fixed at a given location and depending on the full-active constraint set, it may be moved around for economic reasons (see e.g., Jagtap et al.[15]).

This EB case study also highlights that when the hard equipment capacity constraints are inside the plant away from the fresh feeds, which is almost always the case, locating the TPM at a process feed necessitates large back-offs from the hard limits or offsets in the override controller setpoints, with consequent dynamic issues and economic loss. A conventional TPM location at the process feed is, therefore, not a prudent option for economic process operation. As illustrated in recent literature reports,[9,16] the TPM should be chosen at or close to these hard active constraints to minimize the back-off/offset and hence economic loss.

The case study shows that a constraint becoming active can introduce a slow "drifting" (snowballing) mode in the process. Thus, when V_2^{MAX} becomes active, the fresh ethylene being fed to the process cannot be set independently as the limited capacity to boil-off EB implies any extra EB produced in the reactors would necessarily accumulate in the recycle loops introducing a slow drifting mode in the recycle loops. These drifting modes are usually not very obvious and a very careful evaluation of the effect of a constraint becoming active on the process material/energy balances is essential in detecting their presence in a control structure. In cases, where the regulatory control structure has been synthesized using conventional loops for process operation around the base-case design condition with no active capacity constraints, it is very likely that the resulting conventional control structure has "hidden" drifting modes which destabilizes the process when the appropriate constraint(s) becomes active. The slow drifting mode can then result in a severe economic penalty as observed in CS2 with no B_2 override. Conversely, in processes where a conventional control scheme has been implemented, there exists opportunity for improving the process operation by identifying these "hidden" snowballing modes and incorporating appropriate control structure modifications to manage them.

For the EB process, the large difference in the optimum values of the unconstrained CVs common to both Mode I and Mode II suggest that their setpoints be updated to keep the operation at (close) to optimum. In addition to real-time optimization, this may also be achieved by a "hill-climbing" feedback controller[13] or more formally, by tracking necessary conditions for optimality (NCO).[17] For the economic plantwide control problem, we intend to explore the potential benefit and robustness of this approach in future work.

As a final parting thought, we suggest the simplest control structure not requiring any additional loops to be configured when constraints become active, as being the most natural choice for economic plantwide control. Additional loops not being necessary reflects that the structural configuration is such that control of crucial objectives (safety, stability, or economic) is never lost, even when all the constraints in the full-active constraint set are active. Such control systems are much preferred by operators, as its configuration remains the same regardless of where one is operating. Conversely, the need for configuring additional override loops when constraints go active points to structural inconsistencies in the regulatory structure in light of the particular active constraint set. Very often, operators turn-off these additional loops and perform the necessary adjustments themselves. Such structures merit further investigation and possibly, appropriate alteration for consistency with the full-active constraint set so that when the constraints do become active, additional overrides are not needed.

Conclusions

In this work, we have demonstrated the systematic synthesis of a simple decentralized plantwide control structure for (near) optimal operation of the EB process over a large throughput range. The synthesis of such a control structure hinges on *a priori* knowledge of the full-active constraint set, in particular, the hard equipment capacity constraints at maximum throughput, which determine the choice of MVs for tight active constraint control, the TPM, and the material/energy inventory control loops. For the specific EB process example, the conventional control structure (CS2) with the TPM at the fresh ethylene feed and conventional overrides for handling equipment capacity constraints is dynamically and economically inferior. At high throughputs, these overrides cause additional transients due to repeated taking up and giving up of control. When compared to CS1, the throughput and hence operating profit loss is significant, varying from 1 to 12% depending on which overrides are switched off. The work highlights the usefulness of the "top-down" pairing approach applied to the most constrained operating point for economic plantwide control.

Acknowledgments

The corresponding author acknowledges the seminal influence of Prof Charles F Moore from the University of Tennessee, Knoxville, in shaping his perspective on plantwide control. Prof William L Luyben's insights on conventional override controllers for handling capacity constraints are also acknowledged. Last but not least, the financial support from the Department of Science and Technology, Government of India, is gratefully acknowledged.

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Manuscript received Dec. 14, 2011, and revision received Sept. 14, 2012.