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Application of Plantwide Control to the HDA Process. II—Regulatory Control

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This paper describes the design of a control structure for a large-scale process known as the HDA plant. A steady-state "top-down" analysis and optimization of the process (described in Part I of this series of papers) was used to select 16 sets of candidate "self-optimizing" primary (economic) variables. In this paper, we focus on the remaining "bottom-up" steps, which involve the following: selecting where in the plant the production rate should be set; design of the regulatory control layer; design of the configuration of the supervisory control layer; and nonlinear dynamic simulations to validate the proposed control structure. Emphasis is given to the systematic design of the regulatory control layer which constitutes the backbone for the optimal operation in the higher layers. To perform the analysis, steady-state and dynamic models are necessary and Aspen Plus and Aspen Dynamics are used extensively. The final control structure is robust and yields good dynamic performance.

1. Introduction

In Part I of this series of papers,[1] the "top-down" portion of the plantwide design procedure of Skogestad[2] was applied to the HDA process. The result was 10 candidate sets of self-optimizing primary controlled variables (y_1). The present paper involves the bottom-up portion, where the following steps are considered (see Table 1, presented later in this paper):

Step 4: Selection of the production rate manipulator

Step 5: Structure of the regulatory control layer, including selection of secondary controlled variables (y_2)

Step 6: Structure of the supervisory control layer

Step 7: Decision on use and possibly structure of the optimization layer (RTO)

Step 8: Validation of the proposed control structure

One of the main issues in the design of the regulatory control layer is to ensure "stable" and smooth operation. By "stable", we mean not only the mathematical stabilization of unstable modes (e.g., related to control of level loops) but also that the regulatory layer should prevent the plant from drifting too far away from its nominal operating point and that it should be designed such that the supervisory layer (or the operators) can handle the effect of disturbances on the primary outputs ($y_1 = c$).

We base the design of the regulatory control layer on steady-state as well as dynamic considerations and use more-detailed measures for evaluating the controllability of the linearized model of the process, such as the existence of right-half-plane (RHP) transmission zeroes and the relative gain array (RGA).

In step 6, we choose a decentralized supervisory control layer, because, as observed later, this layer seems to be non-interacting and also suitable for the HDA process, where the active constraints remain constant, despite the set of disturbances considered.[1]

The resulting control structure of the HDA plant is then tested by conducting nonlinear dynamic simulation in Aspen Dynamics for various disturbances, to evaluate the final performance.

Previous work on the regulatory control structure for the HDA process includes the work by Luyben,[3] as well as the original work by Brognaux,[4] and, more recently, Qiu and Krishnaswamy[5] and Konda et al.[6] However, to the authors' knowledge, no systematic design procedure has been applied to this process until now.

In this paper, we use a slightly modified version of the steady-state and dynamic models given by Luyben[3] to design the entire control structure of the HDA process. Luyben's structure[3] is then compared with the one proposed in this paper, using our nominal optimal steady-state operating point.

2. Plantwide Control Structure Design Procedure

In practice, a control system is usually divided into several layers, separated by a time scale (see Figure 1). The layers are linked by the controlled variables, whereby the setpoints are computed by the upper layer and implemented by the lower layer.

Control structure design is also known as plantwide control and involves the structural decisions that must be made to design a control structure for, in our case, a complete chemical plant. Table 1 summarizes the procedure of Skogestad,[2] which has two main points:

(I) *Top-down analysis*, including definitions of operational objectives, degrees of freedom, and selection of primary controlled variables (y_1) (steps 1−4 in Table 1).

(II) *Bottom-up design* of the control system, starting with the stabilizing control layer (steps 5−8 in Table 1).

Steps 1−3 are thoroughly discussed in Part I of the series[1] and are applied to the primary variable selection of the HDA process.

2.1. Production Rate Manipulator. The decision in regard to where to place the production rate manipulator is closely related to where in the process there are bottlenecks that limit the flow of mass and energy. In addition, the decision directly affects the way inventory (liquid or gas) in individual units is controlled, because a self-consistent inventory control (see Figure 2) requires the following:[7,8]

(1) The use of outflow for inventory control downstream of the location where the production rate is set, and

(2) The use of inflow for inventory control upstream of this location.

We distinguish between two main modes of operation:

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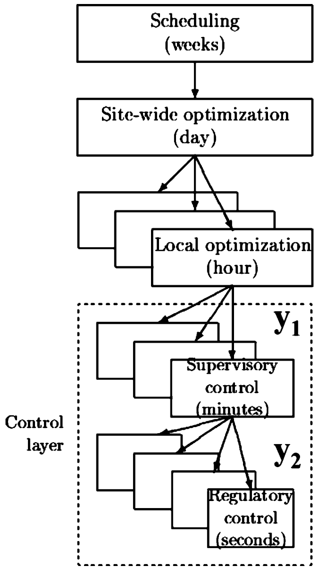

Figure 1. Typical control hierarchy in a chemical plant.

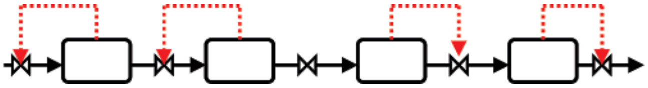

Figure 2. General representation of inventory control (with the production rate set inside the plant).

Mode I: Given throughput. This mode of operation occurs when (a) the feed rate is given (or limited) or (b) the production rate is given (or limited, e.g., by market conditions).

Mode II: Maximum throughput. This mode of operation occurs when the product prices and market conditions are such that it is optimal to maximize throughput.

The production rate is commonly assumed to be set at the inlet to the plant, with outflows used for level control. This is reasonable for mode I with a given feed rate. However, during operation, the feed rate is usually a degree of freedom, and, very often, the economic conditions are such that it is optimal to maximize production (mode II). As the feed rate is increased, one eventually reaches a constraint (a bottleneck) where further increases are not feasible. To maximize production, we must have maximum flow through the bottleneck unit at all times. This gives the following rule for mode II: *Determine the main bottleneck in the plant by identifying the maximum achievable feed rate for various disturbances; to maximize the flow through the bottleneck, the production rate should preferably be set at this location.* To avoid reconfiguration, the same production rate manipulator also should be used in mode I.

However, one should be careful when applying this rule. First, other considerations may be important, such as the control of the individual units (e.g., distillation column) that may be affected by whether inflow or outflow is used for level control.[9] Second, stabilization of the unit may require the "active" use of some flow variable, thus preventing one from maximizing the flow at the bottleneck (this turns out to be the case for the HDA plant). Third, the bottleneck may move, depending on the disturbances. In any case, the control systems should be such that close to optimal operation (that is, almost-maximum bottleneck flow) can be achieved.

2.2. Regulatory Control Layer. We define the regulatory control system as the layer in the control hierarchy that has operation as its main purpose and normally contains the control loops that must be in service for the supervisory layer (operators) to be able to operate the plant in an efficient manner. The main objective of this layer is generally to facilitate smooth operation and not to optimize objectives related to profit, which is done at higher layers. Usually, this is a decentralized control system that keeps a set of measurements y_2 at given setpoints. This is a cascaded control system where the values of these setpoints are determined by the higher layers in the control hierarchy (see Figure 1). In addition, this layer should allow for "fast" control, such that acceptable control is achieved using "slow" control in the layer above. Also, it should avoid "drift", so the system stays within its linear region, which allows the use of linear controllers.[10]

2.2.1. Selection of Measurements y_2 and Pairing with Inputs u_2. Typically, the variables y_2 to be controlled in this layer are pressures, levels, and selected temperatures. A major structural issue in the design of the regulatory control layer is the selection of controlled variables y_2 and corresponding manipulations u_2. The following guidelines may be useful:

In regard to the selection of secondary measurements y_2 for regulatory control:

(1) y_2 should be easy to measure.

(2) Avoid "unreliable" measurements, because the regulatory control layer should not fail.

(3) y_2 should have good controllability; that is, favorable dynamics for control. Avoid variables y_2 with large (effective) delay.

(4) y_2 should be located "close" to the manipulated variable u_2 (as a consequence of rule 3, because, for good controllability, we want a small effective delay).

(5) The (scaled) gain from u_2 to y_2 should be large.

Note: Items 2 and 3 normally exclude compositions as secondary controlled variables y_2.

In regard to the selection of input u_2 (to be paired with y_2):

(6) Select u_2 so that controllability for y_2 is good; that is, u_2 has a "large" and "direct" effect on y_2. Here, "large" means that the gain is large, and "direct" means good dynamics with no inverse response and a small effective delay.

(7) Avoid using variables u_2 that may saturate.

(8) Avoid variables u_2 where (frequent) changes are undesirable, for example, because they disturb other parts of the process.

2.2.2. Indirect Control of Primary Variables—Possible Intermediate Layer. Often, the self-optimizing controlled variables y_1 (both those related to active constraints and the unconstrained degrees of freedom) are compositions that are often unreliable and delayed. Therefore, in addition to the regulatory control layer, we sometimes must include an intermediate layer between the supervisory and regulatory control layers for "indirect control" of the primary variables y_1. This is to ensure that the (near) optimal operation of the process can be "maintained" in case of the failure of any of the primary (composition) loops. Because the time scale for the composition control layer is long, the variables y_1' for this intermediate layer can be selected using the "maximum (scaled) gain rule", based on steady-state considerations.[10] For simplicity, we want to avoid the intermediate layer, so the preferred situation is that indirect composition control is achieved with constant y_2 and u_1 (where u_1 are the remaining unused inputs after closing the regulatory layer).

2.3. Supervisory Control Layer. The purpose of the supervisory control layer is to keep the (primary) controlled outputs y_1 at their optimal setpoints y_{1s}, using, as degrees of freedom, the setpoints $y'_{1,sp}$ or $y_{2,sp}$ in the composition control or regulatory layer, plus any unused manipulated inputs. The main issue about this layer is to decide on whether to use a decentralized or a multivariable control configuration (e.g.,

Table 1. Plantwide Control Structure Design Procedure

step
(I) Top-Down Analysis
1. Definition of operational objectives
Identify operational constraints, and preferably identify a scalar cost function J to be minimized.
2. Manipulated variables u and degrees of freedom
Identify dynamic and steady-state degrees of freedom (DOF).
3. Primary controlled variables
Which (primary) variables $y_1 = c$ should we control?
Control active constraints
Remaining DOFs: control variables for which costant set points give small (economic) loss when disturbances occur (self-optimizing control)
4. Production rate
Where should the production rate be set? This is a very important choice as it determines the structure of remaining inventory control system.
(II) Bottom-Up Design (with Given Primary Controlled c and Manipulated u Variables)
5. Regulatory control layer
Purpose
“Stabilize” the plant using low-complexity controllers (single-loop PID controllers) such that (a) the plant does not drift too far away from its nominal operating point and (b) the supervisory layer (or the operators) can handle the effect of disturbances on the primary outputs ($y_1 = c$).
Main structural issue
Selection of secondary controlled variables (measurements) y_2.
Pairing of these y_2 with manipulated variables u_2.
6. Supervisory control layer
Purpose
Keep (primary) controlled outputs $y_1 = c$ at optimal set points c_s, using as degrees of freedom (inputs) the set points $y_{2,sp}$ for the regulatory layer and any unused manipulated variables u_1.
Main structural issue
Decentralized (single-loop) control: (a) may use simple PI or PID controllers; (b) structural issue: choose input-output pairing.
Multivariable control (usually with explicit handling of constraints (MPC)). Structural issue: Size of each multivariable application.
7. Optimization layer
Purpose
Identify active constraints and compute optimal set points c_s for controlled variables.
Main structural issue
Do we need real-time optimization (RTO)?
8. Validation
Nonlinear dynamic simulation of the plant.

MPC). The decentralized single-loop configuration is the simplest and it is preferred for non-interacting processes and cases where active constraints remain constant. Advantages with decentralized control include the facts that (i) tuning may be done on-line, no (or minimal) model requirements are required, and (iii) it is easy to fix and change. On the other hand, the disadvantages include the facts that (i) one must determine the pairing, (ii) the performance loss is compared to multivariable control, and (iii) complicated logic is required for reconfiguration when the active constraints move.

The decision on how to pair inputs ($y_{2,sp}$ and u_1) and outputs y_1 is often done based on process insight. In more difficult cases, an RGA analysis may be useful, and the rule is pair such that the resulting transfer matrix is close to an identity matrix at the cross-over expected frequency, provided the element is not negative at steady state.[10]

2.4. Optimization Layer (RTO). The purpose of the optimization is to identify the active constraints and recompute the optimal setpoints y_{1s} for the controlled variables. The main structural issue is to decide if it is necessary to use real-time optimization (RTO). RTO is costly in the sense that it requires a detailed steady-state model to be obtained and continuously updated. If the active constraints do not change, and we are able to find good self-optimizing controlled variables, then RTO gives little benefit and should not be used.

2.5. Validation. Finally, after having determined a plantwide control structure, it is recommended to validate the structure, for example, using nonlinear dynamic simulation of the plant.

3. Control Structure Design of the HDA Process

3.1. HDA Process Description. In the HDA process, fresh toluene (pure) and hydrogen (97% hydrogen and 3% methane) are mixed with recycled toluene and hydrogen (see Figure 3). This reactant mixture is first preheated in a feed-effluent heat exchanger (FEHE), using the reactor effluent stream, and then is heated in a furnace before being fed to an adiabatic plug-flow reactor.

A main reaction and a side reaction occur in the reactor:

$$\text{toluene} + H_2 \rightarrow \text{benzene} + \text{methane} \qquad (1)$$

$$2\text{benzene} \rightleftharpoons \text{diphenyl} + H_2 \qquad (2)$$

The reactor effluent is quenched by a portion of the recycle separator liquid flow to prevent coking, and further cooled in the FEHE and cooler before being fed to the vapor−liquid separator. Part of the flow from the compressor discharge that contains unconverted hydrogen and methane is purged to avoid the accumulation of methane within the process, while the remainder is recycled back to the process. The liquid from the separator is processed in the separation section, which consists of three distillation columns. The stabilizer column removes hydrogen and methane as overhead (distillate) product, and the benzene column gives the desired product benzene as overhead. Finally, in the toluene column, toluene is separated from diphenyl and recycled back to the process.

The dynamic model of the HDA process used in this paper is based on (but is not the same as) Luyben’s HDA model with small recycle flow.[3] In this paper, we have used essentially the same parameters as in Luyben’s work[3] (e.g., the same number of stages in the distillation columns, as well as the same PFR configuration, area for heat exchanger HX, pumping characteristics, valve characteristics, and so on). The main difference between the two models is in the steady-state operating point, where ours is optimized according to our definition of optimal operation, as given in the previous work in this series,[1] whereas in the work by Luyben,[3] the steady state is defined differently. A schematic flowsheet of the process without the control loops

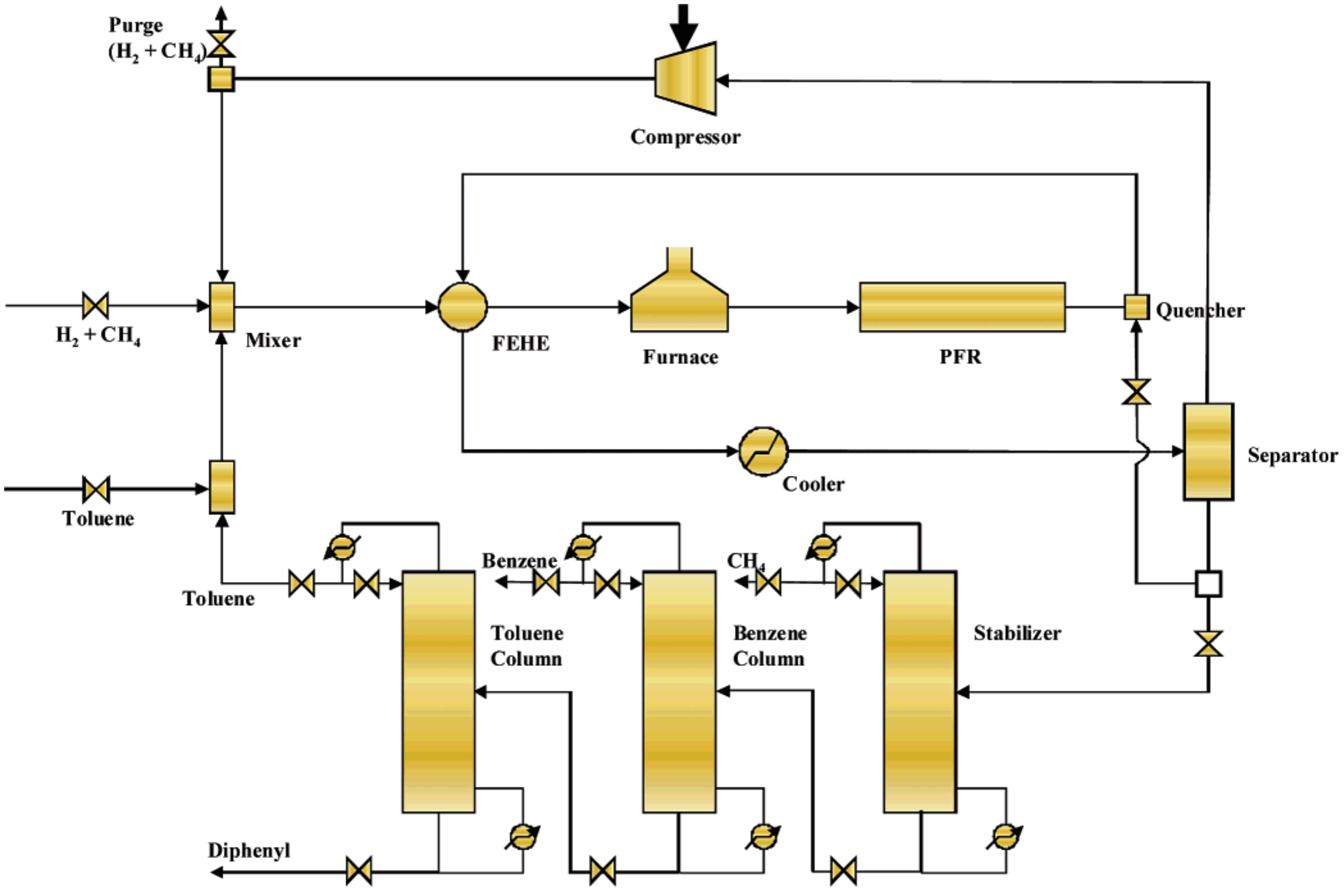

Figure 3. HDA process flowsheet.

is depicted in Figure 3. The stream table for the nominally optimal operating point can be found in Part I of this series of papers.[1] [The entire set of Aspen files can be found on Sigurd Skogestad's home page at http://www.nt.ntnu.no/users/skoge/.]

Note that the conversion of toluene in the reactor is high (∼95%). The result is that the liquid recycle is small and the reactor−recycle section and the distillation section are almost decoupled, from an operational point of view. Therefore, the design of the control structure for each of the two sections is performed separately.

3.2. Selection of Primary Controlled Variables (Mode I). We reported in Part I of this series of papers[1] that there are 20 manipulated variables available for control, 7 of which have only a dynamic effect, because there are 7 liquid levels with no steady-state effect that need to be controlled. This leaves 13 degrees of freedom at steady state. Moreover, in mode I (with given feed rate), 5 constraints are optimally active for all operating points (defined by 12 different disturbances), namely (1) the quencher outlet temperature, $T_{\text{quencher}} = 1150$ °F (upper bound); (2) the separator temperature, $T_{\text{sep}} = 95$ °F (lower bound); (3) the fresh toluene feed rate, $F_{\text{tol}} = 300$ lb-mol/h (upper bound); (4) the reactor inlet pressure, $P_{\text{r,in}} = 500$ psi (upper bound); and (5) the hydrogen-to-aromatic ratio in the reactor inlet, $rH_2 = 5$ (lower bound).

In addition, for the distillation columns, it was decided to control the compositions.[1] However, for the overhead in the stabilizer, this is not a good choice. The small value of $x_{\text{D,ben}}^{\text{stab}}$ used in Part I of this series of papers[1] leads to cryogenic conditions that are very costly. In practice, one would use cooling water or air and maximize the cooling to minimize the benzene loss. Therefore, in this paper, we control the condenser temperature T_1^{stab} at its lowest possible level ($T_1^{\text{stab}} = 77$ °F). Note that the flow rate of this distillate stream is very small, so this does not change the economics of the process. We then end up with the following controlled variables: (6) the condenser temperature at the stabilizer column, $T_1^{\text{stab}} = 77$ °F (lower bound); (7) the methane mole fraction in the stabilizer bottoms, $x_{\text{B,met}}^{\text{stab}} = 10^{-6}$ ("optimal" value); (8) the benzene mole fraction in the benzene column distillate, $x_{\text{D,ben}}^{\text{bc}} = 0.9997$ (lower bound); (9) the benzene mole fraction in the benzene column bottoms, $x_{\text{B,ben}}^{\text{bc}} = 0.0013$ ("optimal" value); (10) the diphenyl mole fraction in the toluene column distillate, $x_{\text{D,dip}}^{\text{tc}} = 0.0005$ ("optimal" value); and (11) the toluene mole fraction in the toluene column bottoms, $x_{\text{B,tol}}^{\text{tc}} = 0.0004$ ("optimal" value).

The "optimal" values for the distillation columns were determined as a tradeoff between maximizing the recovery of valuable component and minimizing energy consumption.[1]

Because of the fact that the benzene column distillate is essentially composed of benzene and toluene only, we control, in practice, the toluene mole fraction in the benzene column distillate ($x_{\text{D,tol}}^{\text{bc}}$), instead of $x_{\text{D,ben}}^{\text{bc}}$, because of measurement accuracy. We also add that, except for this active constraint (lower bound), tight control of the compositions is not important, because the tradeoff makes the optimum flat.[1] Therefore, in practice, temperature control will be acceptable for the other products.

The remaining number of unconstrained steady-state degrees of freedom is 2 (13 − 11 = 2). The 10 best sets of self-optimizing control variables with the minimum loss are given in Table 2.[1] Note that all the best candidates involve compositions and that they all involve controlling the inerts in the reactor inlet (mixer T2 outlet). The approach is to select

Table 2. Candidate Sets of Controlled Variables with Small Losses (Mode I)

set	variables	average loss[a] [× 10^3 \$/yr]
I	mixer outlet inert (methane) mole fraction, $x_{mix,met}$ quencher outlet toluene mole fraction, $x_{quen,tol}$	15.39
II	mixer outlet inert (methane) mole fraction, $x_{mix,met}$ toluene conversion at reactor outlet, $c_{rout,tol}$	26.55
III	mixer outlet inert (methane) mole fraction, $x_{mix,met}$ separator liquid benzene mole fraction, $x_{sepliq,ben}$	31.39
IV	mixer outlet inert (methane) mole fraction, $x_{mix,met}$ separator liquid toluene mole fraction, $x_{sepliq,tol}$	40.40
V	mixer outlet inert (methane) mole fraction, $x_{mix,met}$ separator overhead vapor benzene mole fraction, $x_{sepvap,ben}$	51.75
VI	mixer outlet inert (methane) mole fraction, $x_{mix,,met}$ gas recycle benzene mole fraction, $x_{gasrec,ben}$	58.18
VII	mixer outlet inert (methane) mole fraction, $x_{mix,met}$ quencher outlet benzene mole fraction, $x_{quen,ben}$	63.46
VIII	mixer outlet inert (methane) mole fraction, $x_{mix,met}$ separator liquid diphenyl mole fraction, $x_{sepliq,dip}$	66.97
IX	mixer outlet inert (methane) mole fraction, $x_{mix,met}$ mixer outlet benzene mole fraction, $x_{mix,ben}$	72.59
X	mixer outlet inert (methane) mole fraction, $x_{mix,met}$ quencher outlet diphenyl mole fraction, $x_{quen,dip}$	77.54

[a] The average loss is calculated with each variable in the set kept at its nominal optimal setpoint and also taking into account its implementation error.

Table 3. Re-optimizing with Variable Toluene Feed Rate (F_{tol})

variable	nominal	maximum	maximum reached at F_{tol} (lb-mol/h)	comments
compressor power (hp)	454.39	545.27 (+20%)	380 (+27%)	
furnace heat duty (MBtu)	16.26	24.39 (+50%)	393 (+31%)[a]	bottleneck
cooler heat duty (MBtu)	21.57	32.36 (+50%)	410 (+37%)[a,b]	bottleneck[b]
reactor outlet temperature (°F)	1277	1300	420 (+40%)[a,b,c]	bottleneck[b,c]
distillation heat duties		(+50%)	up to 450 (+50%)	maximum not reached[d]

[a] With compression power at maximum. [b] Disregarding maximum furnace heat duty. [c] Disregarding maximum cooler heat duty. [d] The constraints on the heat duties of the distillation columns (reboiler and condenser) were not reached for F_{tol} values up to 450 lb-mol/h.

the set with the best steady-state cost (here, Set I), unless there turns out to be other factors related to implementation that clashes with this choice.

3.3. Maximum Throughput (Mode II). As previously mentioned, we consider two modes of operation: mode I (the given feed rate) and mode II (the maximum input). With regard to mode I, the given feed rate (F_{tol}), the optimal operation for this case is described in Part I of this series of papers[1] and the main results have been given in the previous section. With regard to mode II, the maximum throughput, with the given prices, it is optimal, from an economic point of view, to increase the production rate F_{ben} as much as possible, because the prices are such that the profit J increases almost linearly with F_{ben}. However, as discussed in detail below, other process constraints result in bottlenecks that prevent increasing F_{ben} above a certain maximum.

In addition to the process constraints already considered in Part I of this series of papers,[1] we also introduce maximum capacities for the compressor power (+20%, compared to nominal), furnace heat duty (+50%), and distillation columns heat duties (+50%). To determine the maximum throughput (mode II), we use the available (maximum) toluene feed rate as a degree of freedom and reoptimize the process (using the profit J from mode I). The results are summarized in Table 3, and the profit J as a function of F_{tol} is shown graphically in Figure 4.

Note that the four active constraints for the nominal case ($T_{quencher}$, T_{sep}, $P_{reactor}$, and rH_2) were determined to be also active, when increasing F_{tol}.

From Table 3, we see that the optimal compressor power hits its maximum constraint (+20%) when the feed rate is increased by 27%. This does not constitute a bottleneck for the process, because the toluene feed rate can be further increased by increasing the reactor temperature to counteract for the loss in toluene conversion (reduced gas recycle flow rate) caused by the constraint on compression power. However, as the toluene feed rate is further increased from 27% to 31%, the maximum constraint on the furnace heat duty Q_{fur} is reached. This is the real bottleneck, because a further increase in F_{tol} with Q_{fur} at its maximum causes infeasible operation. This may be explained because an increase in the feed rate with a fixed furnace heat duty results in a decrease in the reactor temperature, reducing the conversion of toluene, which leads to a buildup of toluene. There is a possibility of counteracting the reduced overall conversion in the reactor by using the remaining unconstrained degree of freedom or “backing off” from one of the economically optimum constraints. However, because of the fact that maximum conversion is already favored by the economics (and

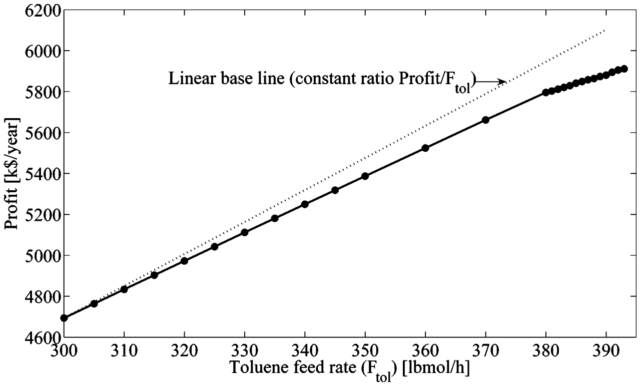

Figure 4. Optimization of the HDA process with variable toluene feed rate. The compressor power reaches its maximum at $F_{tol} = 380$ lb-mol/h, and the furnace heat duty becomes a bottleneck at $F_{tol} = 393$ lb-mol/h.

Table 4. Mode II−Maximum Production Rate: Loss by Selecting $x_{\mathrm{mix,met}}$ as the Unconstrained "Self-Optimizing" Controlled Variables

case	description	Optimal $x_{\mathrm{mix,met}}$	Optimal profit [× 10^3\$/yr]	loss[a] [× 10^3\$/yr]
nominal	$F_{\mathrm{tol}} = 393$ lb-mol/h	0.5555	5931.2	0
D1	fresh gas feed rate methane mole fraction = 0.03−0.08	0.5254	6316.4	175.8
D2	hydrogen-to-aromatics ratio in reactor inlet = 5.0−5.5	0.4943	6249.6	329.0
D3	reactor inlet pressure = 500 −507 psi	0.5643	6198.7	181.0
D4	quencher outlet temperature = 1150−1170 °F	0.5381	6371.5	190.4
D5	product purity in the benzene column distillate = 0.9997−0.9980	0.5202	6531.1	277.3
n_y	implementation error of 0.0001 in $x_{\mathrm{mix,met}}$	0.5556	5977.5	46.3

[a] Loss with fixed $x_{\mathrm{mix,met}} = 0.5555$ (nominal optimum).

the system is already optimal), none of these options can be used. Therefore, the reactor−recycle system becomes a bottleneck when the constraint on the furnace heat duty is reached. If the maximum furnace heat duty was higher, then other potential bottlenecks would be a cooler heat duty or reactor outlet temperature, which, according to Table 3, are reached at a production increase of 37% and 40%, respectively.

However, the focus here is on the case where the furnace heat duty is the bottleneck. For optimum operation, we must then have $Q_{\mathrm{fur}} = Q_{\mathrm{fur,max}}$ for optimal operation and the production rate should be set at this location.

We are then left with one unconstrained degree of freedom, and we must find a self-optimizing controlled variable for it. With given feed rate (mode I), we observed that the mixer outlet inert (methane) mole fraction $x_{\mathrm{mix,met}}$ is present in all candidate sets (see Table 2) and, to minimize the reconfiguration of loops when switching from one mode of operation to another (from mode I to mode II and vice versa), it would be desirable to select $x_{\mathrm{mix,met}}$ as the self-optimizing controlled variable. Fortunately, the loss by keeping $x_{\mathrm{mix,met}}$ at its nominally optimal setpoint in mode II is reasonable, as shown in Table 4. The main exception is the implementation error of $x_{\mathrm{mix,met}}$, where the loss is quite large, even with a small error of 10^{-4} mole fraction units. Nevertheless, we decide to select $x_{\mathrm{mix,met}}$ as the unconstrained "self-optimizing" controlled variables also in mode II.

Remark: *Actual implementation errors are usually larger than the assumed value of 0.0001. A 10-fold increase in this value would probably increase the economic loss, causing the proposed configuration in mode II to seem economically unattractive. We then have assumed here that the measurement device (an on-line chromatograph) has a high resolution, so that the measurement error is small.*

3.4. Selection of Throughput Manipulator. In mode II, the bottleneck is the furnace heat duty, and, optimally the production rate should be set here, so that $Q_{\mathrm{fur}} = Q_{\mathrm{fur,max}}$. However, the reactor is unstable and the furnace heat duty is the most favorable input for closing a stabilizing temperature loop. We must accept some "backoff" from the maximum furnace heat duty to avoid saturation in this stabilizing loop. Therefore, we decide to locate the throughput manipulator at the main feed rate (toluene) both in modes I and II. In mode II, we use a duty controller that keeps the furnace heat duty at a given value (backoff) below its maximum.

3.5. Structure of the Regulatory Control Layer. The main objective of this layer is to provide sufficient quality of control to enable a trained operator to keep the plant running safely without the use of the higher layers in the control system. The regulatory control layer should be designed such that it is independent of the mode of operation.

3.5.1. Stabilization of Unstable Modes (Including Liquid Levels). In the reaction section, a temperature must be controlled to stabilize the reactor operation. As previously mentioned, the input with the most direct effect on the reactor temperature is the furnace heat duty (Q_{fur}). We choose to control the reactor inlet temperature ($T_{\mathrm{r,in}}$), because Q_{fur} has a direct effect on $T_{\mathrm{r,in}}$ (with a small effective delay). In addition, there is a lower limit of 1150 °F for this temperature, which may become an active constraint in other cases.

The levels in the separator and the reboiler sumps and reflux drums of the distillation columns must be stabilized. Because of the fact that the throughput manipulator is located at the feed, the inventory control for the columns are set up assuming a

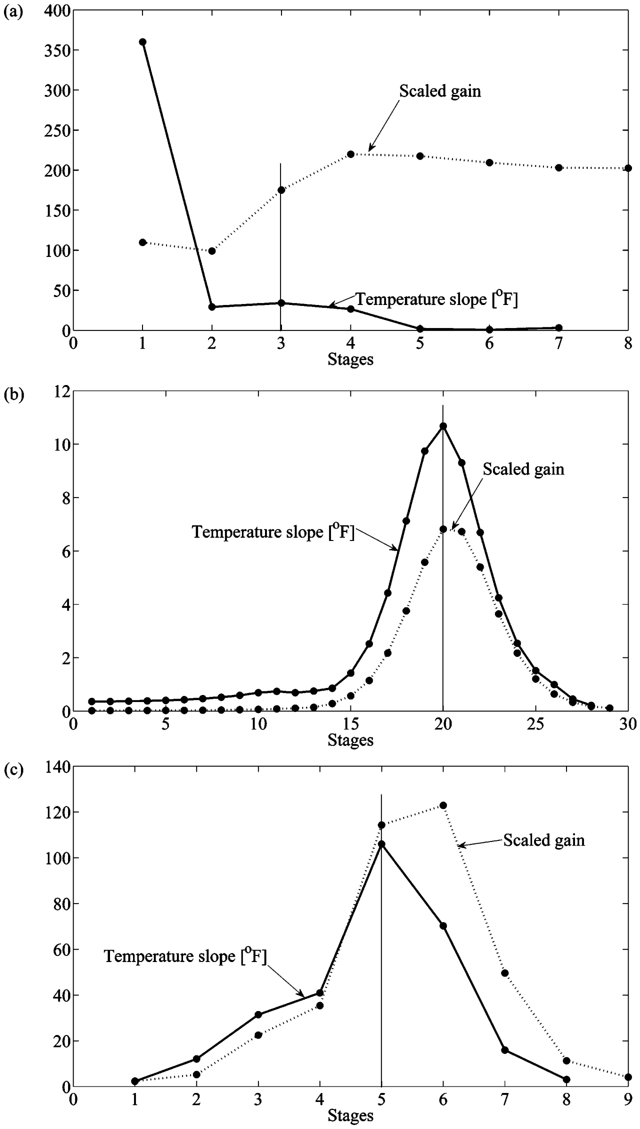

Figure 5. Temperature slope (solid line) and scaled gain (dotted line) for distillation columns. Temperature should be controlled at a location where both are sufficiently large: (a) results for stabilizer, (b) results for the benzene column, and (c) results for the toluene column.

Table 5. Local Analysis for Possible "Intermediate" Regulatory Control: Maximum (Scaled) Singular Rule of Best Sets of Candidate Controlled Variables (W_s is Assumed to be Constant)

set	controlled variables	$\underline{\sigma}(S_1 G J_{uu}^{-1/2}) \times 1000$
I	FEHE hot side outlet temperature, $T_{fehe,hs}$ fresh gas feed rate, F_{hyd}	0.4939
II	FEHE hot side outlet temperature, $T_{fehe,hs}$ mixer outlet flow rate, F_{mix}	0.4937
III	FEHE hot side outlet temperature, $T_{fehe,hs}$ separator vapor outlet flow rate, $F_{sep,vap}$	0.4929
IV	FEHE hot side outlet temperature, $T_{fehe,hs}$ quencher outlet flow rate, F_{quen}	0.4923
V	reactor outlet temperature, $T_{r,out}$ fresh gas feed rate, F_{hyd}	0.4911
VI	reactor outlet temperature, $T_{r,out}$ mixer outlet flow rate, F_{mix}	0.4909
VII	furnace outlet temperature, $T_{r,in}$ fresh gas feed rate, F_{hyd}	0.4907
VIII	furnace outlet temperature, $T_{r,in}$ mixer outlet flow rate, F_{mix}	0.4906
IX	reactor outlet temperature, $T_{r,out}$ separator vapor outlet flow rate, $F_{sep,vap}$	0.4900
X	furnace outlet temperature, $t_{r,in}$ separator vapor outlet flow rate, $F_{sep,vap}$	0.4895

Table 6. Tuning Parameters for the Reactor−Recycle Section (Modes I and II)

				PI-Controller Parameters	
No.	input	loop output	tag[a]	K_c (%/%)	τ_I (min)
RR1	V_1	F_{hyd}	FC02	3.08	0.65
RR2	F_{purge}	$P_{r,in}$	PC01	144.7	0.80
RR3	V_3	F_{tol}	FC01	3.13	0.57
RR4	$F_{sep,liq}$	$T_{quencher}$	TC01	34.98	0.47
RR5	Q_{fur}	$T_{r,in}$	TC03	9.83	0.67
RR6	Q_{cool}	T_{sep}	TC02	1.36	0.80
RR7	V_4	M_{sep}	LC01	2	
SR1[b]	$T_{r,in,sp}$	$x_{quen,tol}$	CC02	0.69	2.93
SR2	$F_{hyd,sp}$	$x_{mix,met}$	CC01	0.54	12.48
SR3	W_s	rH_2	RC01	0.27	2.86
SR2[c]	$T_{r,in,sp}$	$x_{mix,met}$	CC01	0.54	12.48
SR3[c]	$F_{hyd,sp}$	rH_2	RC01	0.07	49.55
SR4[c]	$F_{tol,sp}$	Q_{fur}	QC01	1	100

[a] See tags in Figures 7 and 8. [b] This loop is only activated in mode I. [c] This loop is only activated in mode II.

Table 7. Tuning Parameters for the Distillation Section (Modes I and II)

				PI-Controller Parameters	
No.	input	loop output	tag[a]	K_c (%/%)	τ_I (min)
RD1	V_{11}	P_{stab}	PC11	122.02	0.80
RD2		$Q^{tc}_{cond} P_{tc}$	PC33	56.30	0.80
RD3		$Q^{bc}_{cond} P_{bc}$	PC22	21.047	0.80
RD4			$Q^{stab}_{reb}\, T^{stab}_{3}$ TC11	1.23	0.80
RD5	L_{tc}	T^{tc}_5	TC33	110.44	1.12
RD6			$Q^{bc}_{reb}\, T^{bc}_{20}$ TC22	5.82	4.8
RD7			$Q^{stab}_{cond}\, M^{stab}_{D}$ LC11	2	
RD8	B_{stab}		M^{stab}_{B} LC12	2	
RD9	D_{bc}		M^{bc}_{D} LC21	20	
RD10	B_{bc}		M^{bc}_{B} LC22	2	
RD11	D_{tc}		M^{tc}_{D} LC31	2	
RD12	B_{tc}		M^{tc}_{B} LC32	20	
SD1			$Q^{tc}_{reb}\, x^{tc}_{B,tol}$ CC31	40.96	16.19
SD2			$T^{bc}_{20,sp}\, x^{bc}_{B,ben}$ CC21	6.69	4.56
SD3	L_{bc}		$x^{bc}_{D,tol}$ CC22	432.64	25.60
SD4			$T^{stab}_{3,sp}\, x^{stab}_{B,met}$ CC11	5611.33	1.74
SD5			$T^{tc}_{5,sp}\, x^{tc}_{D,dip}$ CC32	56.95	52.61
SD6	L_{stab}		T^{stab}_{1} TC12	4243.41	0.8

[a] See tags in Figures 7 and 8.

given feed. For the distillation columns, we use the standard LV configuration, which means that the reboiler sump and reflux drum levels are controlled by the outflows. The exception is the reflux drum level of the stabilizer, which is controlled by the condenser heat duty.

3.5.2. Avoiding Drift I: Pressure Control. In addition to stabilizing truly unstable modes, a primary objective at the regulatory control layer is to prevent the plant from drifting away from its desired operating point on the short time scale. Pressure dynamics are generally very fast, so pressure drift is avoided by controlling pressure at selected locations in the plant. First, pressure should be controlled somewhere in the reactor recycle loop. The obvious choice is the reactor inlet pressure ($P_{r,in}$), which is an active constraint and must be controlled at its nominal optimal setpoint for optimal operation. There are three manipulated variables that can effectively be used to controlled $P_{r,in}$, namely, fresh gas feed (F_{hyd}), compressor power (W_s), and purge flow rate (F_{purge}). One could also consider cooler heat duty (Q_{cool}); however, because the separator temperature T_{sep} must be also controlled (active constraint) and Q_{cool} has a direct effect on T_{sep}, we decided not to consider Q_{cool} as an alternative. Furthermore, because pressure control should be fast, F_{hyd} and W_s are not good choices. First, excessive movement of F_{hyd} will likely upset the plant too much, because F_{hyd} directly affects the mass balance of the process. Second, the compressor is an expensive and delicate piece of equipment, so the compressor power W_s is usually avoided as a manipulated variable, at least on a fast time scale. This leaves F_{purge} as the preferred choice for controlling reactor inlet pressure $P_{r,in}$.

The pressures in the distillation columns also must be controlled, and we use condenser heat duty as the manipulated variable. An exception is made for the stabilizer, where the distillate rate (vapor) is used instead.

3.5.3. Avoiding Drift II: Temperature Loops. Temperature measurements are fast and reliable, so temperature loops are frequently closed, to avoid drift.

Because the operation of the separator has a large impact on both the gas recycle loop and the separation section, its temperature should be controlled. Moreover, this temperature has been identified as an active constraint. Therefore, a temperature loop is placed in the separator. The choice for the manipulated variable, in this case, is the cooler heat duty.

In addition, the quencher outlet temperature $T_{quencher}$ (also an active constraint) must be controlled to prevent coke formation upstream from the quencher. We use the flow rate of the cold liquid stream from the separator as the manipulated variable.

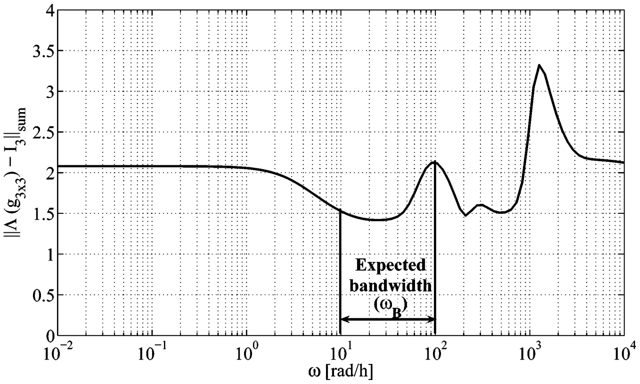

Figure 6. RGA number, as a function of frequency, for $\hat{g}_{3\times3}$ with pairing given by $T_{r,in,sp}-x_{quen,tol}$, W_s-rH_2, and $F_{hyd,sp}-x_{mix,met}$.

The composition control in the distillation columns is usually slow, because of measurement delays and interactions. Thus, temperatures should also be controlled in the distillation columns to avoid drift on the fast time scale. However, it is not clear which stages to select for temperature control, and this calls for a more-detailed analysis based on self-optimizing control considerations. The idea is to select a temperature location at a given stage in the distillation column (T_j), so to minimize the offset in the composition of important products when disturbances occur. To find the best location, we use the maximum gain rule that maximizes the gain of the linearized model G from $u = Q_{reb}$ to $y = T_j$.[10] For dynamic reasons, we should also avoid locations where the temperature slope is small.[11] The results are shown in Figure 5.

For the stabilizer, Figure 5a shows that the best choice from a steady-state point of view would be to control temperature around stage 5 since the scaled gain is higher at this location. However, because the temperature slope at this stage is very small, this may give difficult control problems dynamically, so we decided to use stage 3 (T_3^{stab}) instead.

The benzene and toluene columns are essentially binary columns, and we expect the scaled gain and temperature slope to have their peaks at the same section. This is confirmed by Figure 5b and c. Therefore, for the benzene column, we control the temperature at stage 20 (T_{20}^{bc}), and for the toluene column at stage 5 (T_5^{tc}).

3.5.4. Avoiding Drift III: Flow Control. To reduce drift caused by pressure changes, but also to avoid nonlinearity in control valves, we use flow controllers for the toluene feed rate F_{tol} (FC01) and for the hydrogen feed rate F_{hyd} (FC02). These flow controllers also allow the introduction of a ratio controller, with the setpoint for F_{hyd}/F_{tol} being set by an outer loop. Although ratio control was not used in the simulations, it is recommended, to improve the response with respect to changes and disturbances in F_{tol}.

3.5.5. Possible "Intermediate" Regulatory Layer. The primary controlled variables (y_1) that we want to control for economic reasons are given in Section 3.2. Here, we focus on the reactor−recycle system, because the distillation column units are not critical for the economics in this case (first, because the loss for composition change is small[1] and, second, because they are not bottlenecks (see Section 3.3)). The question here is: Do we need any intermediate regulatory layer, or will control of

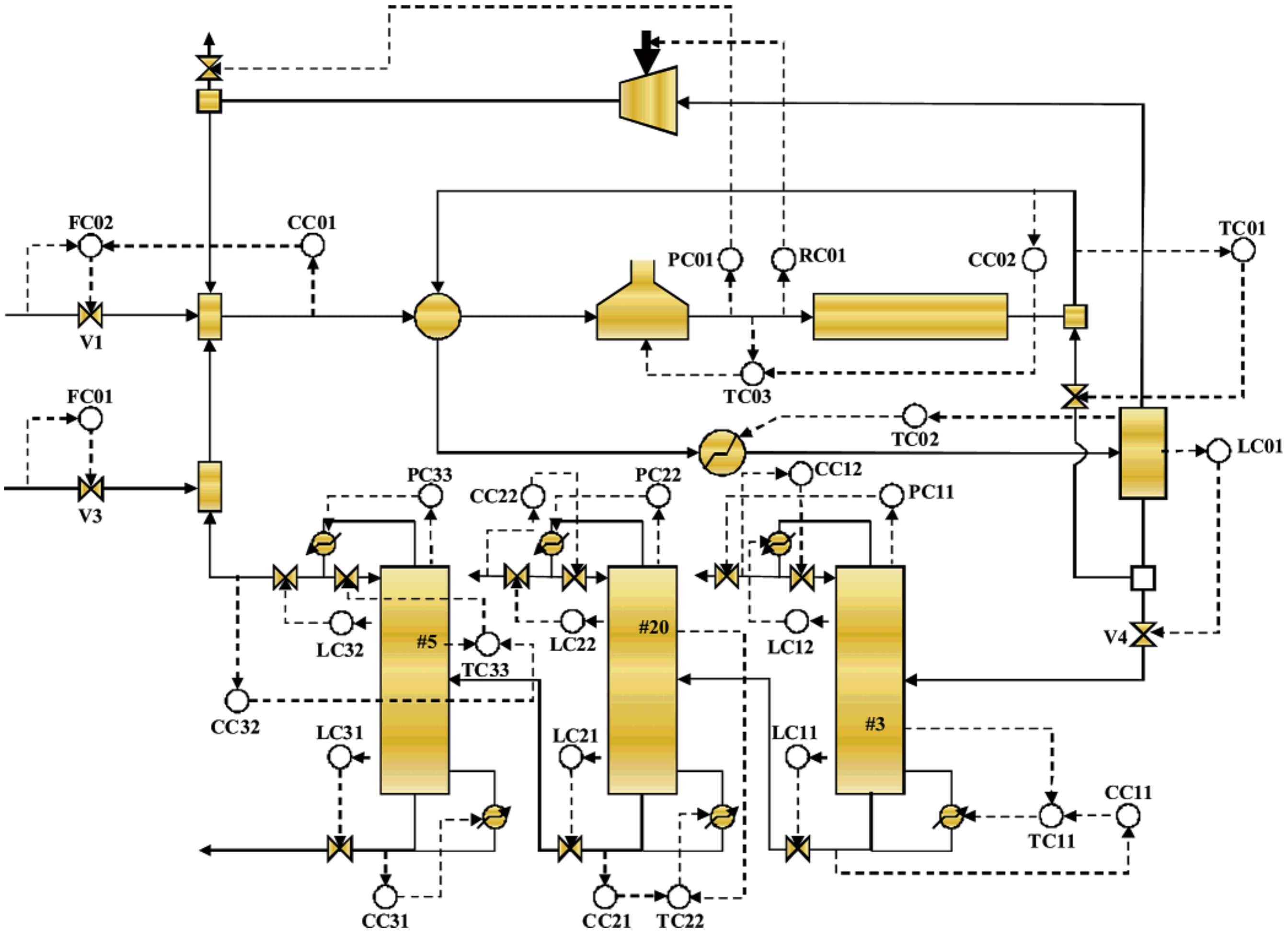

Figure 7. Mode I: HDA process flowsheet with controllers installed.

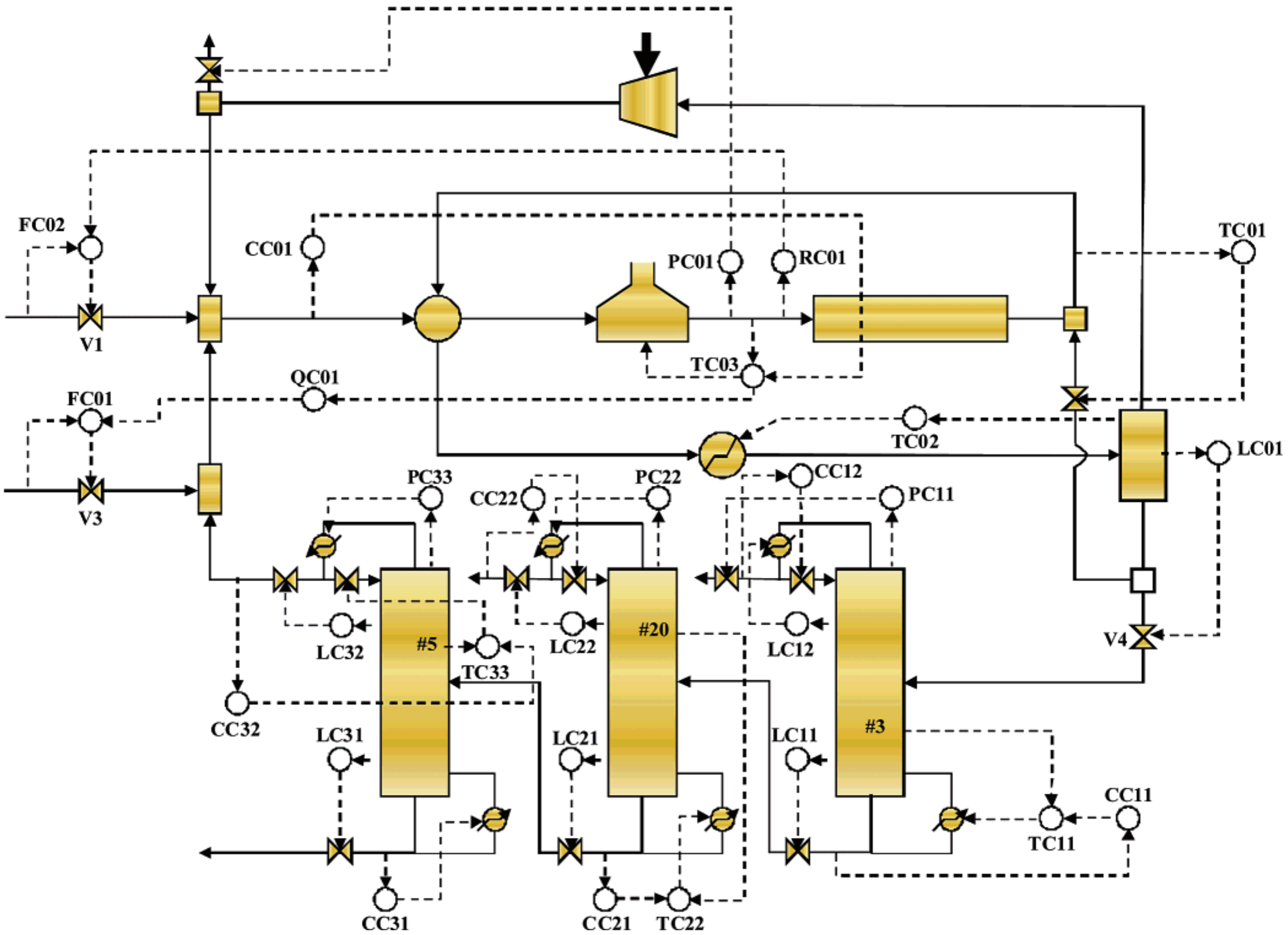

Figure 8. Mode II: HDA process flowsheet with controllers installed.

the secondary controlled variables y_2 indirectly result in "acceptable" control of the primary controlled variables y_1? If we compare the variables controlled in the regulatory control layer (designed so far) with the primary controlled variables, then we still must control three compositions in mode I (rH_2, $x_{\mathrm{mix,met}}$, and $x_{\mathrm{quen,tol}}$) and two compositions in mode II (rH_2 and $x_{\mathrm{mix,met}}$). The composition control will be slow, because of measurement delays; therefore, as previously mentioned in Section 2.2.2, we may introduce an intermediate layer where we control the extra variables y_1' which are easier to control on the intermediate time scale. The degrees of freedom (manipulated variables u_1') are F_{hyd}, $T_{\mathrm{r,in,sp}}$, and W_s. In mode II, W_s is fixed at its maximum and therefore, is not available; in mode I, we choose not to use W_s at this relatively fast time scale.

Once more, the maximum gain rule[10] is used to decide which variables should be controlled. We chose not to use compressor power W_s at the intermediate time scale. The candidate controlled variables y_1' are chosen to be temperatures, flows, and pressures in the reaction section (compositions are ruled out for obvious reasons) as well as the three manipulated variables themselves. The result of the maximum gain rule analysis is seen in Table 5 for mode I.

As seen from Table 5, the economic loss by controlling $u_1' = \{F_{\mathrm{hyd}}, T_{\mathrm{r,in,sp}}, W_s\}$ (set VII) is almost the same as that for the best set in the table (set I). Thus, we decide that there is no benefit of an additional "intermediate" layer for indirect composition control in this case.

3.5.6. Summary on the Regulatory Control Layer. In summary, we have decided to close the following regulatory loops in the reactor−recycle section (modes I and II): RR1, flow control of the hydrogen feed rate (F_{hyd}); RR2, reactor inlet pressure ($P_{\mathrm{r,in}}$) with purge flow (F_{purge}); RR3, flow control of the toluene feed rate (F_{tol}); RR4, quencher outlet temperature (T_{quencher}) with cooling flow from the separator ($F_{\mathrm{sep,liq}}$); RR5, reactor inlet temperature ($T_{\mathrm{r,in}}$) with furnace heat duty (Q_{fur}); RR6, separator temperature (T_{sep}) with cooler heat duty (Q_{cool}); and RR7, separator level, using its liquid outlet flow rate to the distillation section).

As for the distillation section, we have decided on the following regulatory control structure (modes I and II):

RD1, stabilizer pressure (P_{stab}) with a distillate flow rate (D_{stab});

RD2, benzene column pressure (P_{bc}) with condenser heat duty $Q_{\mathrm{cond}}^{\mathrm{bc}}$;

RD3, toluene column pressure (P_{tc}) with condenser heat duty $Q_{\mathrm{cond}}^{\mathrm{tc}}$;

RD4, temperature at stage 3 (T_3^{stab}) with reboiler heat duty $Q_{\mathrm{reb}}^{\mathrm{stab}}$ in the stabilizer;

RD5, temperature at stage 20 (T_{20}^{bc}) with reboiler heat duty $Q_{\mathrm{reb}}^{\mathrm{bc}}$ in the benzene column;

RD6, temperature at stage 5 (T_5^{tc}) with reflux rate L_{tc} in the benzene column;

RD7, reflux drum level with the condenser heat duty $Q_{\mathrm{cond}}^{\mathrm{stab}}$ in the stabilizer;

RD8, reboiler sump level with bottoms flow rate B_{stab} in the stabilizer;

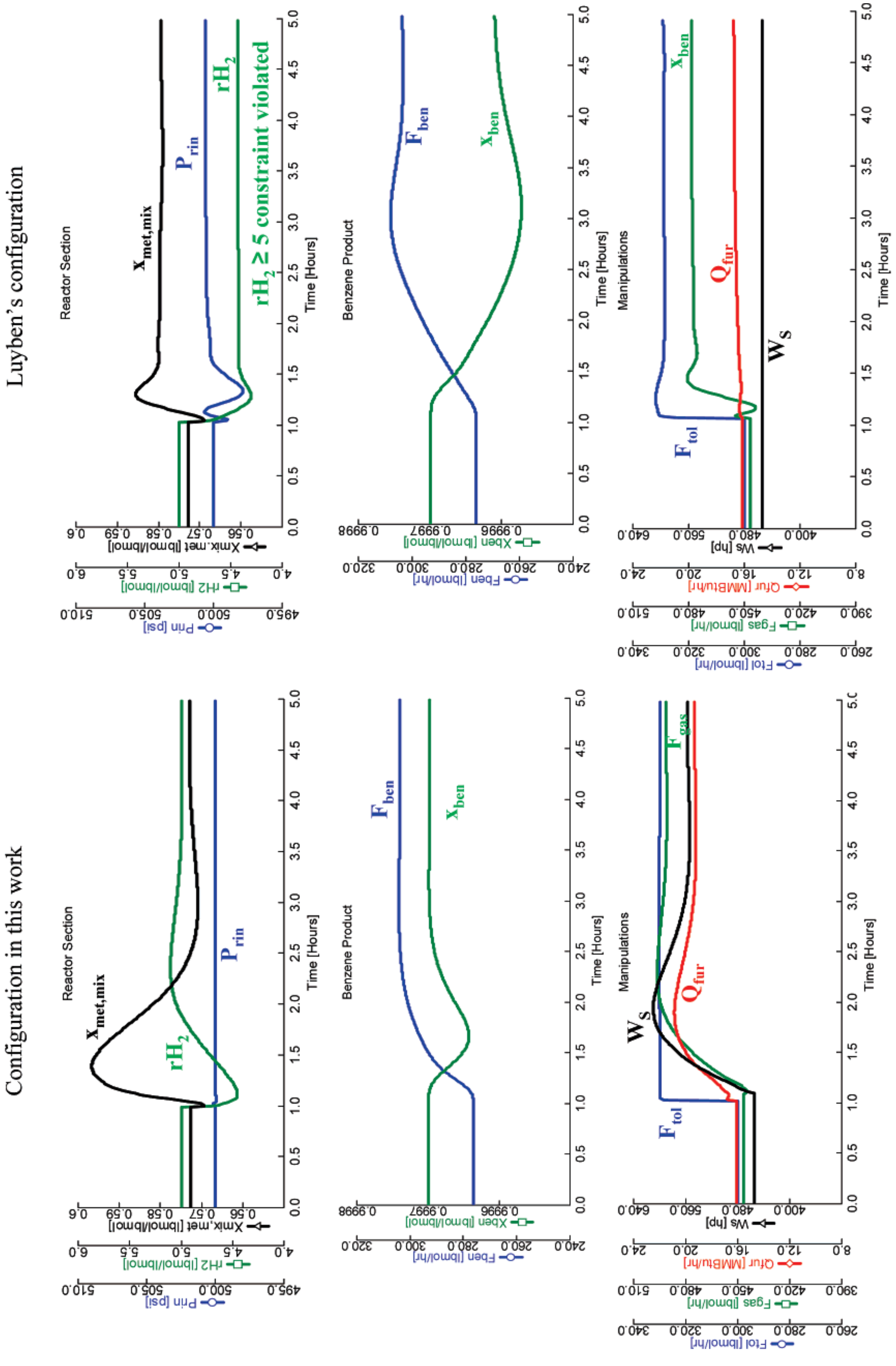

Figure 9. Mode I: Dynamic response of selected variables for disturbance Dyn1: +10% increase in F_{tol}.

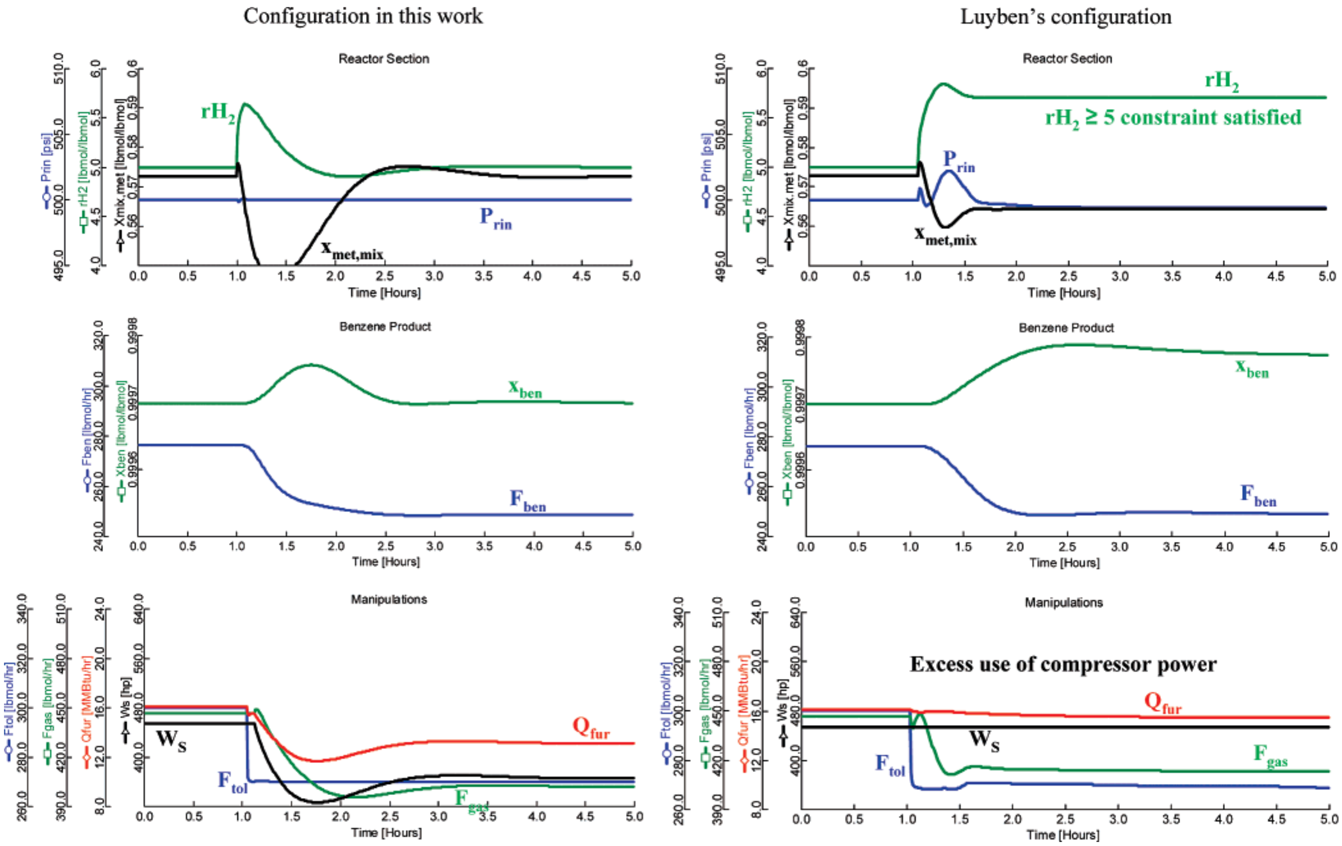

Figure 10. Mode I: Dynamic response of selected variables for disturbance Dyn2: −10% increase in F_{tol}.

RD9, reflux drum level with distillate flow rate D_{bc} in the benzene column;

RD10, reboiler sump level with bottoms flow rate B_{bc} in the benzene column;

RD11, reflux drum level with distillate flow rate D_{tc} in the toluene column; and

RD12, reboiler sump level with bottoms flow rate B_{tc} in the toluene column.

3.6. Structure of the Supervisory Control Layer. The production rate manipulator is selected as the toluene feed rate. In mode I, it is fixed, and in mode II, it is adjusted to give the desired maximum furnace duty (with some backoff).

The intention of the supervisory control layer is to keep the active constraints and unconstrained (self-optimizing) controlled variables at constant setpoints. For the unconstrained controlled variables, we select in mode I to control set I in Table 2, i.e., mixer outlet inert (methane) mole fraction ($x_{mix,met}$) and quencher outlet toluene mole fraction ($x_{quen,tol}$). In mode II, the compression power W_s is not available as a degree of freedom, and we only control $x_{mix,met}$.

Here, we consider mode I in detail. With the regulatory control in place, there are still nine composition loops (three compositions in the reactor−recycle section and two in each distillation column) to be closed in the supervisory layer. We first consider a decentralized structure and proceed with a more-detailed analysis based on RGA methods, which requires a linear model of the process, and for this, we use the linearization capabilities of Aspen Dynamics. A linearization script defining the controlled and manipulated variables can be easily written in Aspen Dynamics and the linear state-space model with constant matrices A, B, C, and D generated by the code are exported to a MatLab program, to be used in the linear analysis.

We start with the distillation columns taken one at the time. The steady-state RGA matrix tells us, in all cases, to use the expected pairing where reflux controls the top product. For the stabilizer, $u = [L_{stab}\ T^{stab}_{3,sp}]$ and $y = [T^{stab}_{1}\ x^{stab}_{B,met}]$, and the RGA matrix

$$\Lambda_{stab}(0) = \begin{bmatrix} 0.9844 & 0.0156 \\ 0.0156 & 0.9844 \end{bmatrix}$$

suggests to pair reflux rate (L_{stab}) with condenser temperature (T^{stab}_{1}) and the setpoint of the temperature controller at stage 3 ($T^{stab}_{3,sp}$) with methane mole fraction in bottoms ($x^{stab}_{B,met}$).

The steady-state RGA matrix for the benzene column (with $u = [L_{bc}\ T^{bc}_{20,sp}]$ and $y = [x_{D,tol}{}^{bc}\ x^{bc}_{B,ben}]$),

$$\Lambda_{bc}(0) = \begin{bmatrix} 1.8457 & -0.8457 \\ -0.8457 & 1.8457 \end{bmatrix}$$

indicates the pairing should be the reflux rate (L_{bc}) with the benzene mole fraction in the distillate ($x^{bc}_{D,tol}$) and the setpoint of the temperature controller at stage 20 ($T^{bc}_{20,sp}$) with the benzene mole fraction in bottoms ($x^{bc}_{B,ben}$).

As for the toluene column, because the stream of interest is the distillate (recycle of toluene to the process), we choose to use reflux rate (L_{tc}) to control the temperature at stage 5 (T^{tc}_{5}). This gives a steady-state RGA matrix (with $u = [Q^{tc}_{reb}\ T^{tc}_{5,sp}]$ and $y = [x^{tc}_{B,tol}\ x^{tc}_{D,dip}]$) of

$$\Lambda_{tc}(0) = \begin{bmatrix} 1.3187 & -0.3187 \\ -0.3187 & 1.3187 \end{bmatrix}$$

and the chosen pairing is the reboiler heat duty (Q^{tc}_{reb}) with the

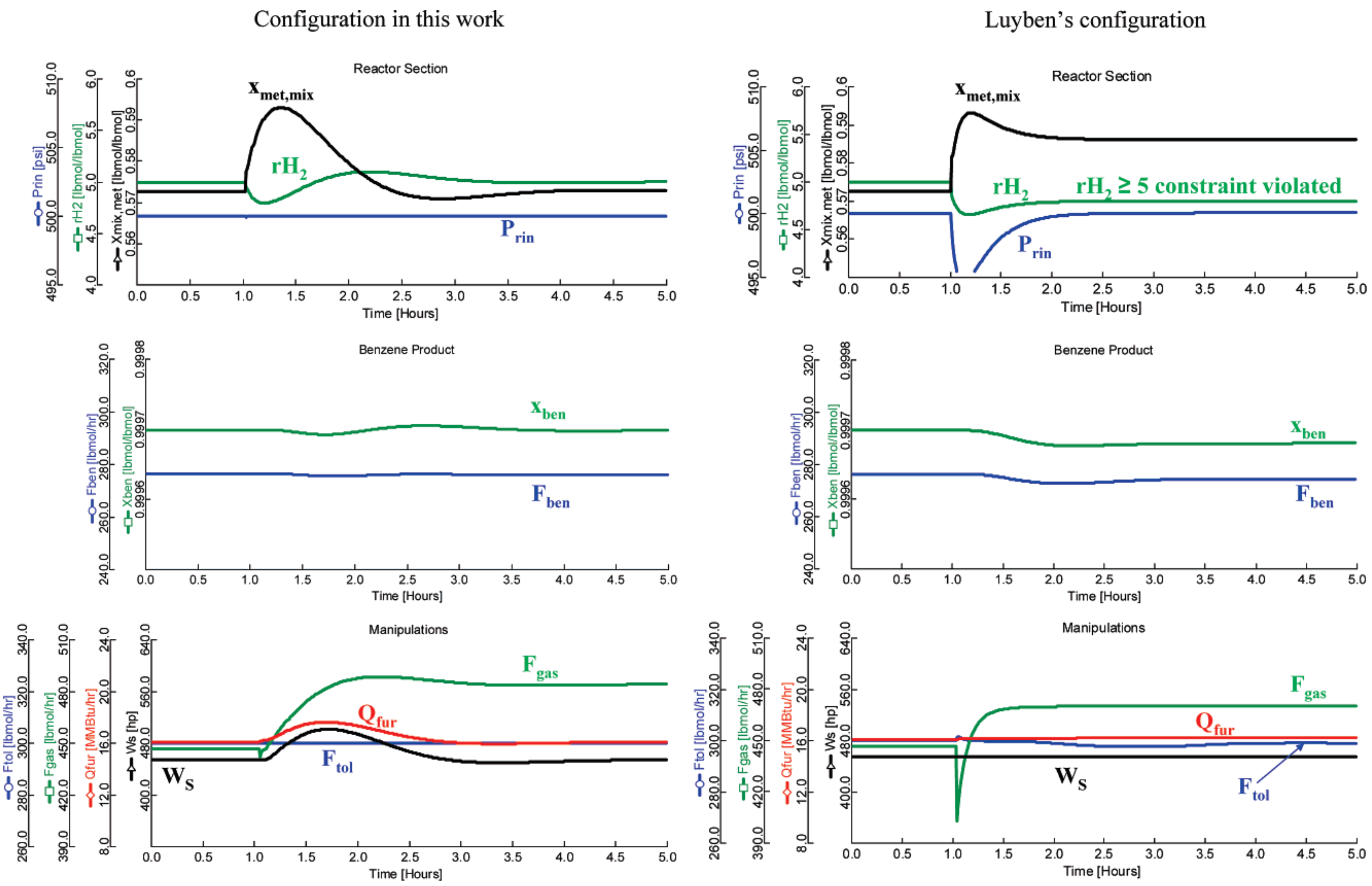

Figure 11. Mode I: Dynamic response of selected variables for disturbance Dyn3: +0.05 increase in x_{met}.

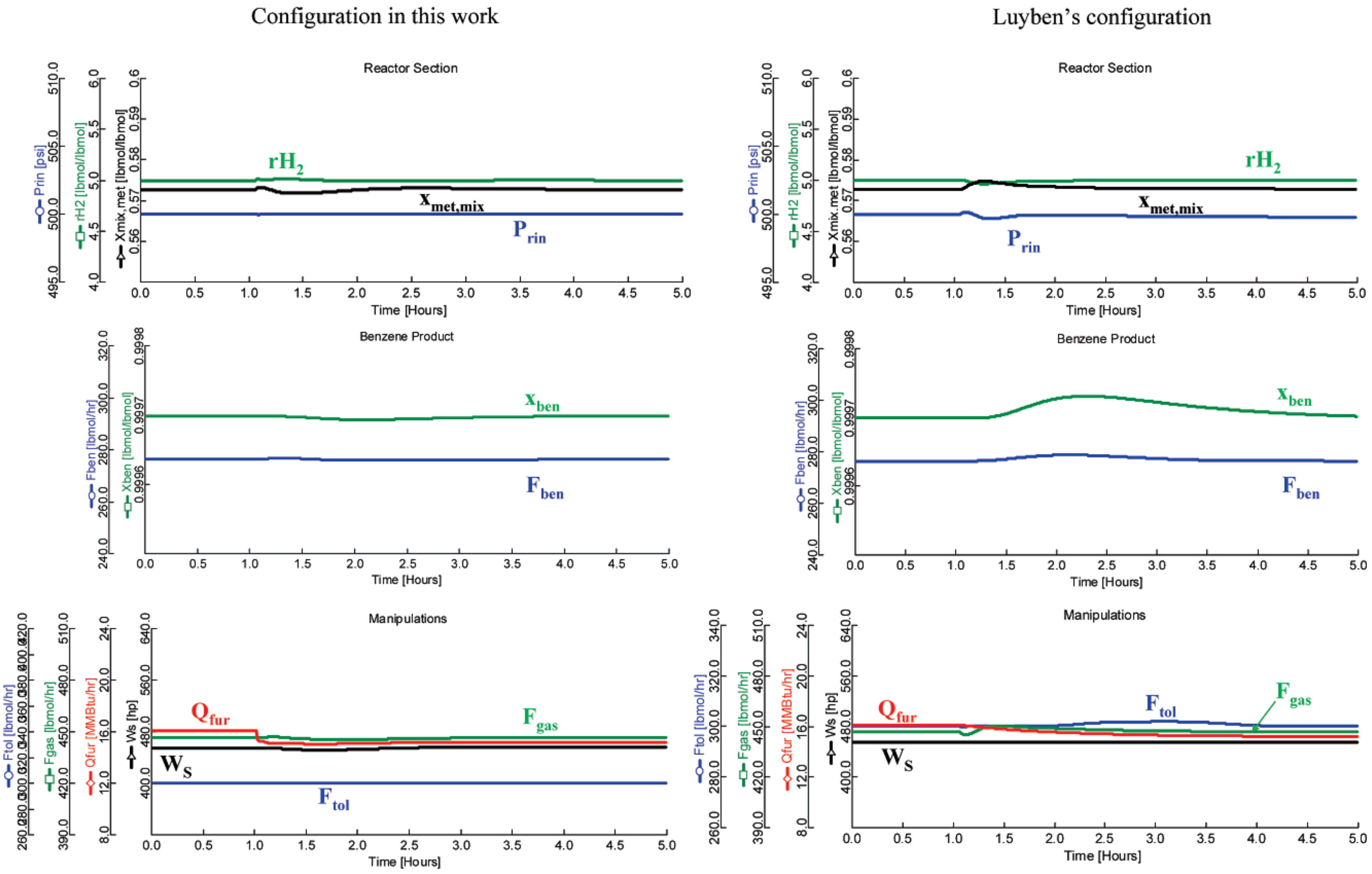

Figure 12. Mode I: Dynamic response of selected variables for disturbance Dyn4: +20 °F increase in $T_{quencher}$.

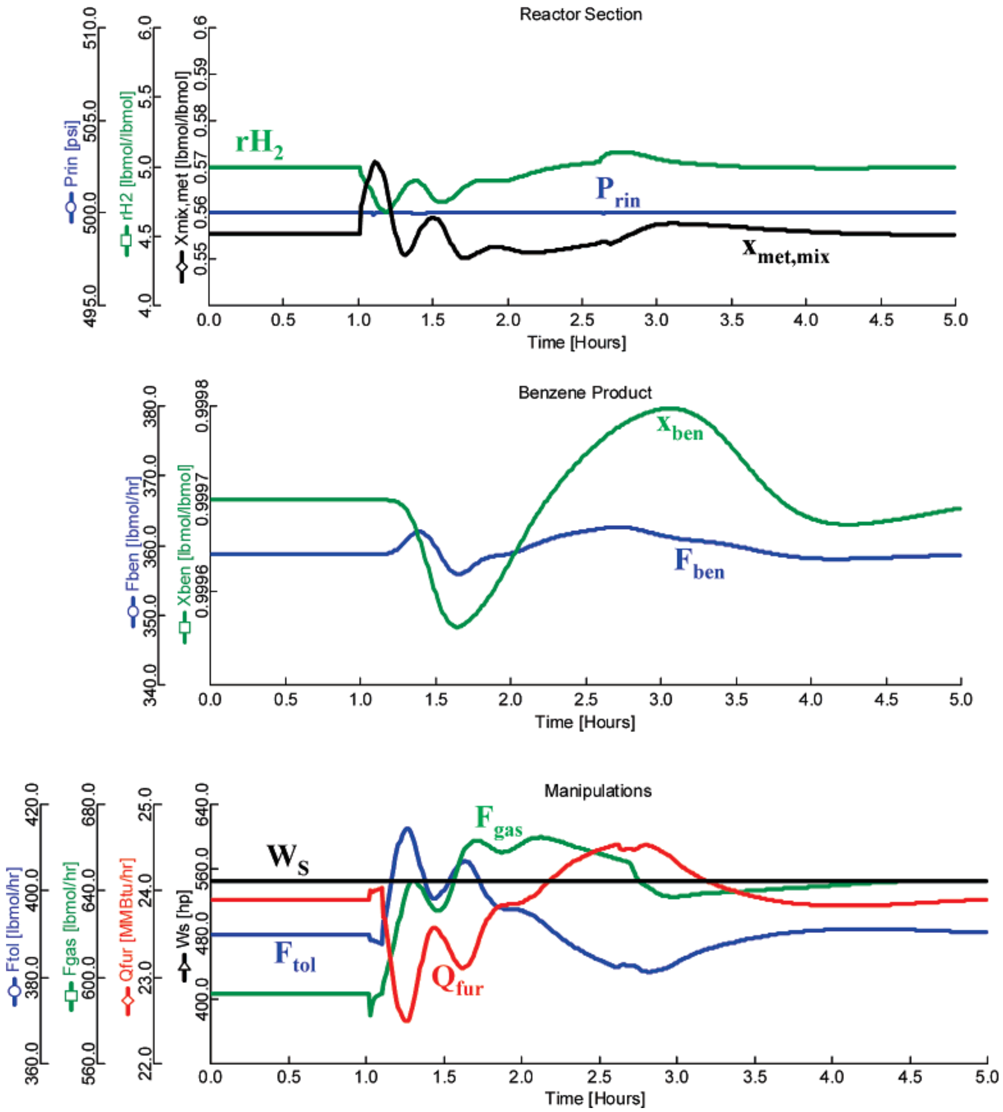

Figure 13. Mode II (configuration in this work): Dynamic response of selected variables for disturbance Dyn3: +0.05 increase in x_{met}.

Table 8. Disturbances for Dynamic Simulations of the HDA Process

No.	variable	nominal[a]	disturbance, Δ
Dyn1	toluene feed rate, F_{tol}	300 lb-mol/h	+30 lb-mol/h (+10%)
Dyn2	toluene feed rate, F_{tol}	300 lb-mol/h	−30 lb-mol/h (−10%)
Dyn3	methane mole fraction in hydrogen feed rate, x_{met}	0.03	+0.05
Dyn4	quencher outlet temperature, $T_{quencher}$	1150 °F	+20 °F

[a] This refers to the optimal nominal considered in this work.

toluene mole fraction in bottoms ($x^{tc}_{B,tol}$) and the setpoint of the temperature controller at stage 5 ($T^{tc}_{5,sp}$) with the diphenyl mole fraction in the distillate ($x^{tc}_{D,dip}$).

For the reactor−recycle section, a control configuration for the remaining 3 × 3 partially controlled system (denoted here as $\hat{g}_{3\times3}$) with the available manipulations

$$u = \{T_{r,in,sp}; W_s; F_{hyd,sp}\} \tag{3}$$

and controlled variables

$$y = \{rH_2; x_{mix,met}; x_{quen,tol}\} \tag{4}$$

must be designed, where $T_{r,in,sp}$ is the setpoint of the temperature controller at the reactor inlet, $F_{hyd,sp}$ is the setpoint of the hydrogen feed rate flow controller, $x_{mix,met}$ is the methane mole fractions at mixer outlet, and $x_{quen,tol}$ is the toluene mole fraction at the quencher outlet.

To check the controllability of the 3 × 3 system ($\hat{g}_{3\times3}$), we obtain the zeroes and found two pairs of RHP zeroes (250 ± 908i and 588 ± 346i rad/h); however, these are located quite far into the RHP (corresponding to an effective delay at approximately $^1/_{250}$ h = 0.24 min) and will not cause any performance limitations. We also found that the RHP zeroes were moved closer to the origin (becoming more restrictive) by loosening the control (using lower gains) in the regulatory loops. This indicates that we have paired on negative steady-state gains in the lower loops;[12] however, this is not a problem as long as the regulatory loops do not fail (e.g., saturate) and are sufficiently fast.

At first sight, it seems reasonable to pair $F_{hyd,sp}$ with rH_2 (the hydrogen-to-aromatic ratio at the reactor inlet), because we might expect $F_{hyd,sp}$ to have a large and direct effect on rH_2. However, the steady-state RGA analysis matrix

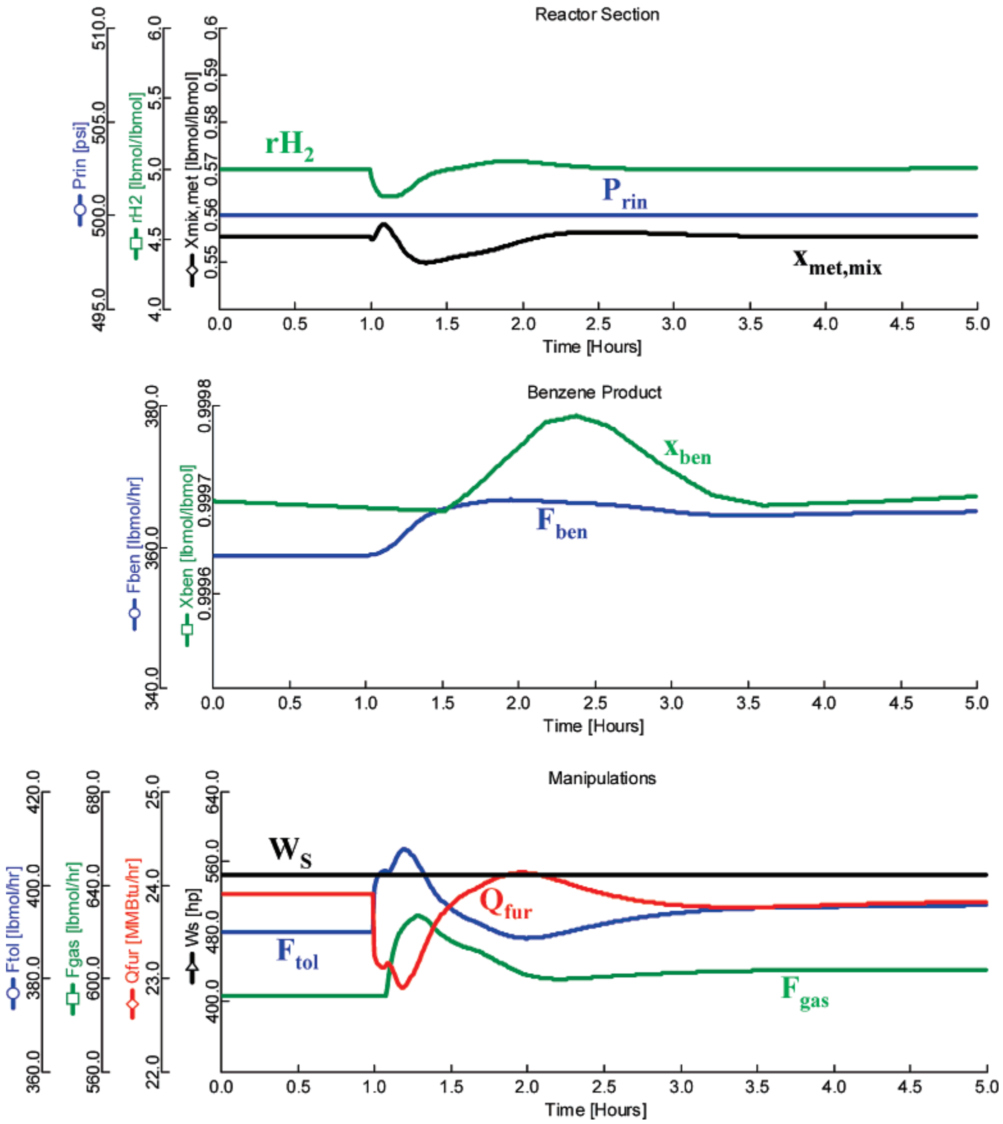

Figure 14. Mode II (configuration in this work): Dynamic response of selected variables for disturbance Dyn4: +20 °F increase in T_{quencher}.

$$\Lambda_{\mathrm{reac}}(0) = \begin{bmatrix} -0.3736 & 1.1774 & 0.1962 \\ 0.5032 & -0.1439 & 0.6407 \\ 0.8704 & -0.0335 & 0.1631 \end{bmatrix}$$

suggests that this should be avoided, because of pairing on negative steady-state RGA elements. To avoid pairing on negative RGA elements, we must pair $T_{\mathrm{r,in,sp}}$ with $x_{\mathrm{quen,tol}}$; W_{s} with $r\mathrm{H}_2$; and $F_{\mathrm{hyd,sp}}$ with $x_{\mathrm{mix,met}}$. Figure 6 shows the RGA number ($||\Lambda_{\mathrm{reac}} - I_3||_{\mathrm{sum}}$),[10] as a function of frequency for these pairings, and we find that the dynamic interactions are also small.

3.6.1. Summary on the Supervisory Control Layer. In summary, we close the following supervisory control loops in the reactor−recycle section (mode I):

SR1, the toluene mole fraction at the quencher outlet $x_{\mathrm{quen,tol}}$ with the setpoint of the reactor temperature controller ($T_{\mathrm{rmin,sp}}$);

SR2, the methane mole fraction at the mixer outlet $x_{\mathrm{mix,met}}$ with the setpoint of the hydrogen feed rate flow controller ($F_{\mathrm{hyd,sp}}$); and

SR3, the hydrogen-to-aromatics ratio at the reactor inlet ($r\mathrm{H}_2$) with compressor power (W_{s}).

In addition, in the distillation section, we close the following supervisory loops (modes I and II):

SD1, the toluene mole fraction in the bottoms ($x^{\mathrm{tc}}_{\mathrm{B,tol}}$) with reboiler heat duty $Q^{\mathrm{tc}}_{\mathrm{reb}}$ in the toluene column;

SD2, the benzene mole fraction in the bottoms $x^{\mathrm{bc}}_{\mathrm{B,ben}}$ with the setpoint of the temperature controller at stage 20 $T^{\mathrm{bc}}_{20,\mathrm{sp}}$ in the benzene column;

SD3, the toluene mole fraction in the distillate ($x^{\mathrm{bc}}_{\mathrm{D,tol}}$) with the reflux rate L_{bc} in the benzene column;

SD4, the methane mole fraction in the bottoms ($x^{\mathrm{stab}}_{\mathrm{B,met}}$) with the setpoint of the temperature controller at stage 3 $T^{\mathrm{stab}}_{3,\mathrm{sp}}$ in the stabilizer;

SD5, the diphenyl mole fraction in the distillate ($x^{\mathrm{tc}}_{\mathrm{D,dip}}$) with the set point of the temperature controller at stage 5 $T^{\mathrm{tc}}_{5,\mathrm{sp}}$ in the toluene column; and

SD6, the condenser temperature (T^{stab}_1) with reflux rate L_{stab} in the stabilizer.

3.6.2. Switching between Mode I and Mode II. For mode I, the strategy is to keep the toluene feed rate (F_{tol}) constant at its nominally optimal setpoint. For mode II, F_{tol} controls the furnace heat duty:

$$Q_{\mathrm{fur,sp}} = Q_{\mathrm{fur,max}} - Q_{\mathrm{fur,backoff}} \text{ (nonoptimal strategy)}$$

where $Q_{\mathrm{fur,backoff}}$ is the backoff (input resetting) from the maximum furnace heat duty to avoid that it saturates, which may give instability, because of the loss of stabilizing temperature control. This back-off value must be determined based on the expected disturbances for the reactor temperature control loop.

Switching from mode I to mode II may be accomplished through the following logic steps:

(1) Break the loop between W_s and rH_2 and fix the compressor power W_s at its maximum.

(2) Use $F_{hyd,sp}$ to control rH_2 (to ensure active constraint control).

(3) Use $T_{r,in,sp}$ to control $x_{mix,met}$ and change the setpoint of $x_{mix,met}$ from its nominally optimal value in mode I (0.5724) by its nominally optimal value in mode II (0.5555).

(4) Use $F_{tol,sp}$ to control Q_{fur} (production rate manipulation).

(5) Tune the loops with the parameters listed in Tables 6 and 7. (Note that only the loops $F_{hyd,sp}-rH_2$ and $F_{tol,sp}-Q_{fur}$ must be retuned.)

3.6.3. Controller Tuning. The lower layer loops selected previously are closed and tuned one at the time in a sequential manner (starting with the fastest loops). Aspen Dynamics has an open-loop test capability that was used to determine a first-order plus delay model from u to y. Based on the model parameters, we used the SIMC tuning rules[13] to design the PI controllers:

$$K_c = \frac{1}{k}\frac{\tau}{\tau_c + \theta}, \qquad \tau_I = \min[\tau, 4(\tau_c + \theta)] \tag{5}$$

where k, τ, and θ are the gain, time constant, and effective time delay, respectively. In our case, we choose $\tau_c = 3\theta$ to give smooth control with acceptable performance, in terms of disturbance rejection.

The controllers parameters—the gain K_c and integral time τ_I—are given in Tables 6 and 7 for the reactor−recycle section and distillation section, respectively. (Also see Figures 7 and 8 for the controller tag.)

3.7. Structure of the Optimization Layer. Because of the fact that we obtained a design that addresses important disturbances (self-optimizing control structure) with acceptable loss, on-line optimization is not needed.

4. Dynamic Simulations

In this section, we compare the control structure designed for mode I of operation with the small recycle flow scheme proposed by Luyben.[3] They are both based on the same underlying Aspen model, but Luyben[3] considered a different steady-state operating point. However, a good control structure should not be dependent on the operating point. To have a consistent basis for comparison, we use the steady-state considered in this paper but maintain the original tuning settings determined by Luyben.[3] Figures 9−12 present a comparison of the results for the disturbances in Table 8.

From Figures 9−12, we can see that the structure of Luyben[3] is not optimal (or even feasible) in some cases, specifically, in response to material and/or component mass balances disturbances, because the hydrogen-to-aromatic ratio at the reactor inlet rH_2 and product purity $x^{bc}_{D,ben}$, which are active constraints, are not controlled. The hydrogen-to-aromatic ratio rH_2 in the structure by Luyben[3] gives a much higher offset variation than the product purity $x^{bc}_{D,ben}$, which contributes to increase the economic loss of this control structure. This ratifies the benefit of having a control structure that gives (near) optimal steady-state operation, which is the goal of any enterprise.

Moreover, Luyben[3] did not consider using compressor power W_s as a degree of freedom (it is actually assumed to be constant), in contrast with our control structure that makes use of W_s for long-term control. Economically, this can result in economic losses, because, in some cases, it has been used excessively (see, e.g., Figure 10).

However, generally, the dynamic responses of the two control structures are similar with essentially the same settling time (∼4 h) and with small oscillations, which shows that, although based on different steady-state consideration, they are, to some extent, robust to the considered disturbances.

For mode II of operation, we found that a backoff in furnace heat duty (Q_{fur}) from 100% to 98% takes care of all the assumed disturbances without saturation of Q_{fur}. The simulation results for disturbances Dyn3 and Dyn4 are depicted in Figures 13 and 14. As one can see, the responses are not as good as those of mode I of operation, but they are still satisfactory if we consider that practically no controller retune from mode I was performed. Adaptive schemes could improve the response, but this is not considered in this paper.

5. Conclusion

This paper has discussed control structure design for the HDA process, using the design procedure of Skogestad,[2] with emphasis on the regulatory control layer. For this process, the bottleneck for maximum production rate (mode II) was determined to be the furnace heat duty (Q_{fur}). However, this heat duty is needed to stabilize the reactor, so the throughput manipulator was selected as the toluene feed rate (F_{tol}). The final regulatory control layer shows good dynamic responses, as observed from the simulation results. One reason for this is that the systematic procedure ensures that the process does not drift away from its nominally optimal operating point. The pairing decisions discussed in the design of the regulatory layer could be essentially decided on more-practical terms, even though they are not truly quantitative. Note that no "intermediate" control layer was needed in the hierarchy, which contributes to a low complexity of the overall control structure.

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