

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

Antonio C. B. de Araújo, Eduardo S. Hori and Sigurd Skogestad*

Department of Chemical Engineering,
Norwegian University of Science and Technology (NTNU),
Trondheim, Norway

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Abstract

This paper describes the design of a control structure for a large-scale process, the HDA plant. A steady-state “top-down” analysis and optimization of the process¹ was used to select 16 sets of candidate “self-optimizing” primary (economic) variables. In this paper, we focus on the remaining “bottom-up” steps dealing with 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. In order to carry out the analysis, steady-state and dynamic models are necessary and Aspen PlusTM and Aspen DynamicsTM are used extensively. The final control structure is robust and yields good dynamic performance.

Keywords: HDA process, control structure design, regulatory control layer, production rate, supervisory control layer, Aspen PlusTM, Aspen DynamicsTM.

* Author to whom correspondences should be addressed: Department of Chemical Engineering, Sem Saelandsvei 4, NTNU Gloschaugen, 7491, Trondheim, Norway, Phone: +47-7359-4154, Fax: +47-7359-4080, e-mail: skoge@chemeng.ntnu.no.

1 Introduction

In a previous paper¹ the top-down part of the plantwide design procedure of Skogestad² was applied to the HDA process. The result was ten candidate sets of self-optimizing primary controlled variables (y_1). The present paper deals with the bottom-up part, where the following steps are considered (see Table 1):

- 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 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 controllability of the linearized model of the process such as the existence of right half plane transmission zeros (RHP zeros) and relative gain array (RGA).

In step 6, we choose a decentralized supervisory control layer design since, as seen later, this layer appears to be non-interacting and also suitable for the HDA process where the active constraints remain constant despite of the set of disturbances considered¹.

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

Previous work on the regulatory control structure for the HDA process includes Luyben³, the original work by Brognaux⁴, and more recently Qiu and Krishnaswamy⁵ 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 in Luyben³ to design the entire control structure of the HDA process. Luyben’s³ structure 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 time scale (see Figure 1). The layers are linked by the controlled variables, whereby the set points are computed by the upper layer and implemented by the lower layer.

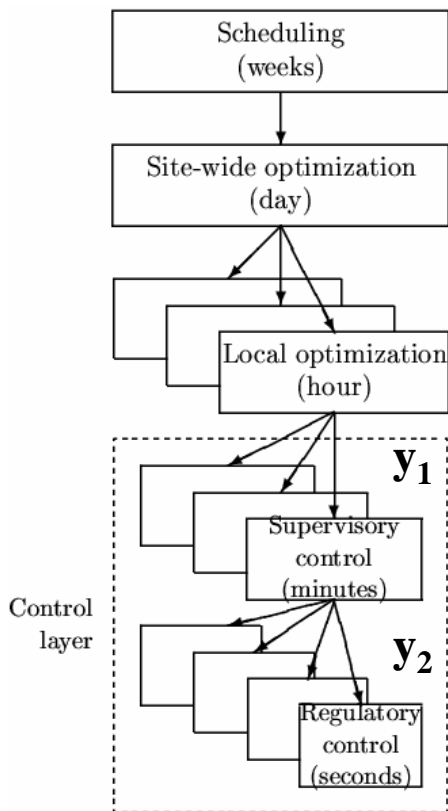


Figure 1: Typical control hierarchy in a chemical plant.

Control structure design is also known as plantwide control and deals with 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 Skogestad² which has two main points:

- I. *Top-down analysis*, including definition 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).

Table 1: Plantwide control structure design procedure.

Step
(I) Top-down analysis
<p>1. <i>Definition of operational objectives:</i> Identify operational constraints, and preferably identify a scalar cost function J to be minimized.</p> <p>2. <i>Manipulated variables u and degrees of freedom:</i> Identify dynamic and steady-state degrees of freedom (DOF).</p> <p>3. <i>Primary controlled variables:</i> Which (primary) variables $y_1 = c$ should we control?</p> <ul style="list-style-type: none"> - Control active constraints. - Remaining DOFs: control variables for which constant set points give small (economic) loss when disturbances occur (self-optimizing control). <p>4. <i>Production rate:</i> Where should the production rate be set? This is a very important choice as it determines the structure of remaining inventory control system.</p>
(II) Bottom-up design (with given primary controlled c and manipulated u variables)
<p>5. <i>Regulatory control layer:</i> <i>Purpose:</i> "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 ($y_1 = c$). <i>Main structural issue:</i></p> <ul style="list-style-type: none"> - Selection of secondary controlled variables (measurements) y_2. - Pairing of these y_2 with manipulated variables u_2. <p>6. <i>Supervisory control layer:</i> <i>Purpose:</i> 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. <i>Main structural issue:</i></p> <ul style="list-style-type: none"> - 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. <p>7. <i>Optimization layer:</i> <i>Purpose:</i> Identify active constraints and compute optimal set points c_s for controlled variables. <i>Main structural issue:</i> Do we need real-time optimization (RTO)?</p> <p>8. <i>Validation:</i> Nonlinear dynamic simulation of the plant.</p>

Steps 1-3 are thoroughly discussed in Araujo *et al.*¹ and applied to the primary variable selection of the HDA process.

2.1 Production rate manipulator

The decision on 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 are controlled since a self-consistent inventory control requires⁷⁸ (see Figure 2):

- Use outflow for inventory control downstream of the location where the production rate is set, and
- Use inflow for inventory control upstream of this location.

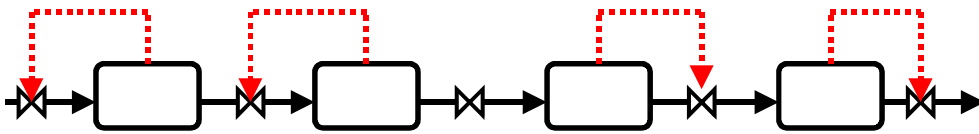


Figure 2: General representation of inventory control (with production rate set inside the plant).

We distinguish between two main modes of operation:

- **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 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 feed rate is increased, one eventually reaches a constraint (a bottleneck) where further increase is 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 should be used also 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) which may be affected by whether inflow or outflow is used for level

control⁹. Second, stabilization of the unit may require the “active” use of some flow variable, and thus prevent 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, close to maximum bottleneck flow) can be achieved.

2.2 Regulatory control layer

We define the regulatory control system as the layer in the control hierarchy which has operation as its main purpose, and which normally contains the control loops that must be in service in order 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 which keeps a set of measurements y_2 at given set points. This is a cascaded control system where the values of these set points 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 controllers¹⁰.

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:

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 .

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 the ones related to active constraints and the unconstrained degrees of freedom) are compositions which are often unreliable and delayed. Therefore, in addition to the regulatory control layer, we sometimes need to 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 failure of any of the primary (composition) loops. Since 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 considerations¹⁰. 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 set points y_{1s} , using as degrees of freedom the set points $y'_{1,sp}$ 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. MPC. Decentralized single-loop configuration is the simplest and it is preferred for non-interacting process and cases where active constraints remain constant. Advantages with decentralized control are:

- + Tuning may be done on-line;
- + None or minimal model requirements;

+ Easy to fix and change.

On the other hand, the disadvantages are:

- Need to determine pairing;
- Performance loss compared to multivariable control;
- Complicated logic required for reconfiguration when 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 a RGA-analysis may be useful, and the rule is pair such that the resulting transfer matrix is close to identity matrix at the crossover expected frequency, provided the element is not negative at steady-state¹⁰.

2.4 Optimization layer (RTO)

The purpose of the optimization is to identify the active constraints and recompute optimal set points y_{1s} for the controlled variables. The main structural issue is to decide if it is necessary to use real-time optimization (RTO). Real-time optimization 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

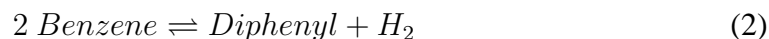
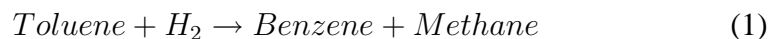
Finally, after having determined a plantwide control structure, it is recommended to validate the structure, for example, using nonlinear dynamic simulation of the plant.

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 (Figure 3). This reactant mixture is first preheated in a feed-effluent heat exchanger (FEHE) using the reactor effluent stream and then heated in a furnace before being fed to an adiabatic plug-flow reactor.

A main reaction and a side reaction take place in the reactor:



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 flow from the compressor discharge containing unconverted hydrogen and methane is purged to avoid 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 consisting 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 (however not the same as) Luyben's model³. We, in this paper, used essentially the same parameters as in Luyben³ e.g., numbers of stages in the distillation columns, 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 Araujo *et al.*¹, while in Luyben³ the steady-state is defined differently. A schematic flowsheet of the Aspen DynamicsTM model without the control loops is depicted in Figure 3. The stream table for the nominally optimal operating point taken from Araujo *et al.*¹ is shown in Table 2. The entire set of files can be found in Sigurd Skogestad's home page at <http://www.nt.ntnu.no/users/skoge/>.

Note that the conversion of toluene in the reactor is high (about 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. The design of the control structure for each of the two sections is therefore performed separately.

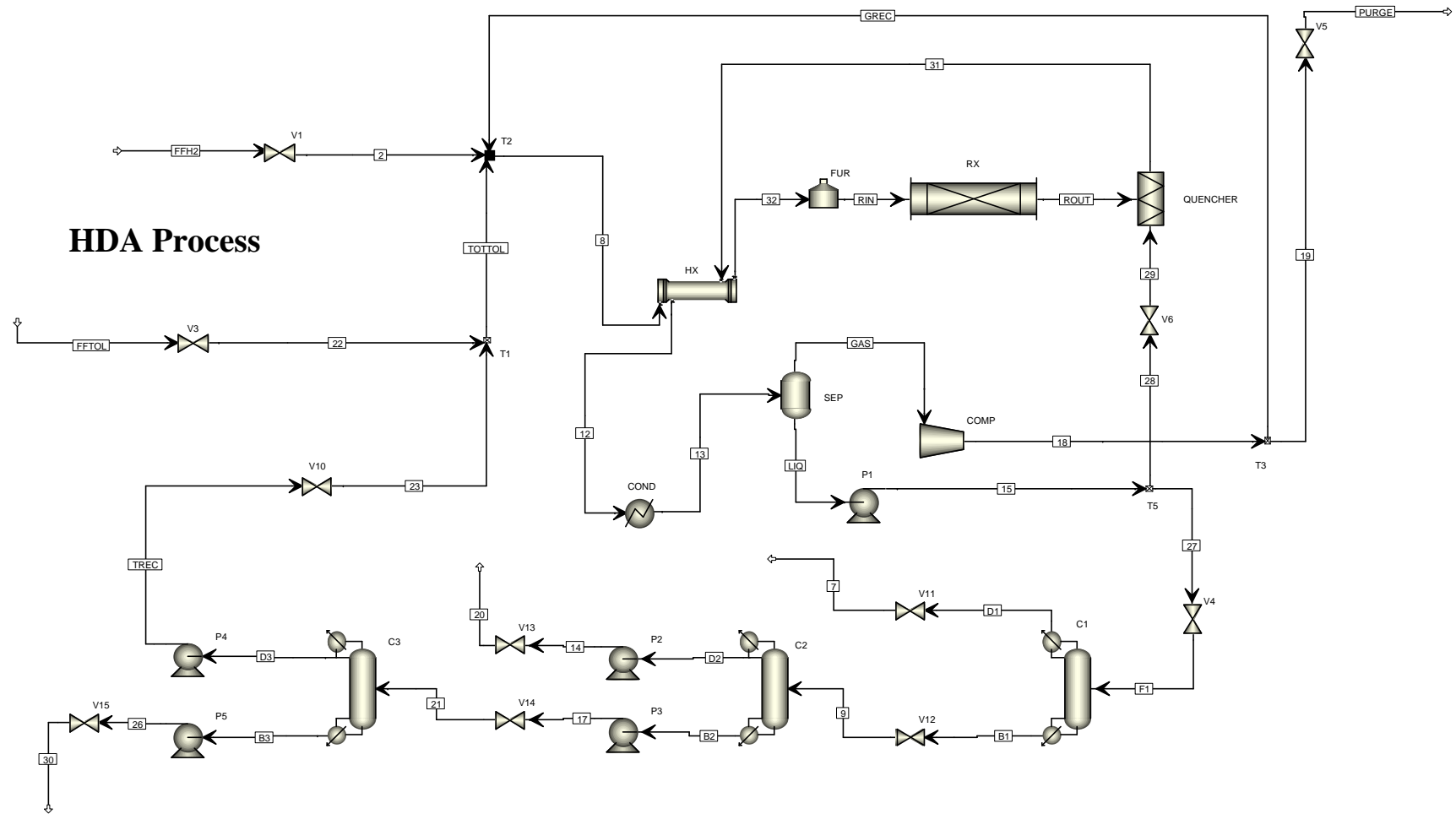


Figure 3: HDA Aspen DynamicsTM process flowsheet.

Table 2: Stream table for the nominally optimum operating point for the HDA process. See Figure 3 for the stream names.

Stream	2	7	8	9	12	13	14	15	17	18	19	20	21	22	23	26	27	28	29	30
Mole Flow [lbmol/h]																				
Hydrogen	433.37	1.0841	1809.1	0	1519.4	1519.4	0	1.7618	0	1517.7	141.9	0	0	0	0	0	1.0841	0.6777	0.6777	0
Methane	13.403	14.438	2910.1	0	3219	3219	0	23.464	0	3195.5	298.78	0	0	0	0	0	14.438	9.0258	9.0258	0
Benzene	0	0.0016	45.023	276.36	498.76	498.76	276.33	449.13	0.0329	49.631	4.6405	276.33	0.0329	0	0.0329	0	276.36	172.77	172.77	0
Toluene	0	0	316.8	15.946	26.948	26.948	0.0831	25.914	15.862	1.0342	0.0967	0.0831	15.862	300	15.859	0.0038	15.946	9.9684	9.9684	0.0038
Diphenyl	0	0	0.0101	9.43	15.328	15.328	0	15.325	9.43	0.0031	0.0003	0	9.43	0	0.0073	9.4227	9.43	5.8951	5.8951	9.4227
Mole Fraction																				
Hydrogen	0.97	0.0698	0.3561	0	0.2878	0.2878	0	0.0034	0	0.3186	0.3186	0	0	0	0	0	0.0034	0.0034	0.0034	0
Methane	0.03	0.9301	0.5727	0	0.6097	0.6097	0	0.0455	0	0.6708	0.6708	0	0	0	0	0	0.0455	0.0455	0.0455	0
Benzene	0	1E-04	0.0089	0.9159	0.0945	0.0945	0.9997	0.8711	0.0013	0.0104	0.0104	0.9997	0.0013	0	0.0021	0	0.8711	0.8711	0.8711	0
Toluene	0	0	0.0623	0.0528	0.0051	0.0051	0.0003	0.0503	0.6263	0.0002	0.0002	0.0003	0.6263	1	0.9975	0.0004	0.0503	0.0503	0.0503	0.0004
Diphenyl	0	0	2E-06	0.0313	0.0029	0.0029	0	0.0297	0.3724	6E-07	6E-07	0	0.3724	0	0.0005	0.9996	0.0297	0.0297	0.0297	0.9996
Total Flow [lbmol/h]	446.77	15.524	5081.1	301.74	5279.5	5279.5	276.41	515.6	25.325	4763.9	445.42	276.41	25.325	300	15.899	9.4264	317.26	198.33	198.33	9.4264
Total Flow [lb/h]	1081.2	233.3	82839	24475	98286	98286	21561	40155	2914.1	58131	5435.2	21561	2914.1	27600	1462.7	1451.4	24709	15447	15447	1451.4
Temperature [°F]	100.11	-93.394	120.25	235.26	357.67	95	223.92	95.359	333	124.89	124.89	224.02	325.6	100.27	289.14	566.56	95.359	95.359	95.578	565.56
Pressure [psi]	555	50	530	31.714	477.4	477	80	530	84	555	555	50	30.75	555	555	82	530	530	487.4	32
Vapor Fraction	1	1	0.932	0.4557	1	0.9023	0	0	0	1	1	0	0.0337	0	0	0	0	0	0	0.005
Enthalpy [MBtu/h]	-0.3551	-0.4846	-88.217	9.8177	-68.617	-90.323	7.2579	10.044	0.8809	-99.2	-9.2752	7.2579	0.8809	1.8353	0.2276	0.7991	6.1802	3.8635	3.8635	0.7991

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Stream	31	32	B1	B2	B3	D1	D2	D3	F1	FFH2	FFTOL	GAS	GREC	LIQ	PURGE	RIN	ROUT	TOTTOL	TREC
Mole Flow [lbmol/h]																			
Hydrogen	1519.4	1809.1	0	0	0	1.0841	0	0	1.0841	433.37	0	1517.7	1375.8	1.7618	141.9	1809.1	1518.8	0	0
Methane	3219	2910.1	0.0003	0	0	14.438	0	0	14.438	13.403	0	3195.5	2896.7	23.464	298.78	2910.1	3210	0	0
Benzene	498.76	45.023	276.36	0.0329	0	0.0016	276.33	0.0329	276.36	0	0	49.631	44.99	449.13	4.6405	45.023	325.99	0.0329	0.0329
Toluene	26.948	316.8	15.946	15.862	0.0038	0	0.0831	15.859	15.946	0	300	1.0342	0.9375	25.914	0.0967	316.8	16.98	315.86	15.859
Diphenyl	15.328	0.0101	9.43	9.43	9.4227	0	0	0.0073	9.43	0	0	0.0031	0.0028	15.325	0.0003	0.0101	9.4331	0.0073	0.0073
Mole Fraction																			
Hydrogen	0.2878	0.3561	0	0	0	0.0698	0	0	0.0034	0.97	0	0.3186	0.3186	0.0034	0.3186	0.3561	0.2989	0	0
Methane	0.6097	0.5727	1E-06	0	0	0.9301	0	0	0.0455	0.03	0	0.6708	0.6708	0.0455	0.6708	0.5727	0.6317	0	0
Benzene	0.0945	0.0089	0.9159	0.0013	0	1E-04	0.9997	0.0021	0.8711	0	0	0.0104	0.0104	0.8711	0.0104	0.0089	0.0642	0.0001	0.0021
Toluene	0.0051	0.0623	0.0528	0.6263	0.0004	0	0.0003	0.9975	0.0503	0	1	0.0002	0.0002	0.0503	0.0002	0.0623	0.0033	0.9999	0.9975
Diphenyl	0.0029	2E-06	0.0313	0.3724	0.9996	0	0	0.0005	0.0297	0	0	6E-07	6E-07	0.0297	6E-07	2E-06	0.0019	2E-05	0.0005
Total Flow [lbmol/h]	5279.5	5081.1	301.74	25.325	9.4264	15.524	276.41	15.899	317.26	446.77	300	4763.9	4318.5	515.6	445.42	5081.1	5081.1	315.9	15.899
Total Flow [lb/h]	98286	82839	24475	2914.1	1451.4	233.3	21561	1462.7	24709	1081.2	27600	58131	52695	40155	5435.2	82839	82839	29063	1462.7
Temperature [°F]	1150	1004.8	371.4	332.65	565.54	-83.814	223.52	283.61	97.982	100	100	94.979	124.89	94.979	123.85	1201.2	1277.2	110.72	288.76
Pressure [psi]	487.4	510	154	34	32	150	30	30	160	605	605	476	555	476	505	500	496	555	675
Vapor Fraction	1	1	0	0	0	1	0	0	0.0293	1	0	1	1	0	1	1	1	0	0
Enthalpy [MBtu/h]	-7.2542	-26.854	9.8177	0.8801	0.7981	-0.4846	7.2521	0.2222	6.1802	-0.3551	1.8353	-100.36	-89.925	10.033	-9.2752	-11.118	-11.118	2.0629	0.2276

3.2 Selection of primary controlled variables (Mode I)

Araujo *et al.*¹ report that there are 20 manipulated variables available for control, 7 of which have only a dynamic effect since 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. Quencher outlet temperature $T_{quencher} = 1150^{\circ}\text{F}$ (upper bound).
2. Separator temperature $T_{sep} = 95^{\circ}\text{F}$ (lower bound).
3. Fresh toluene feed rate $F_{tol} = 300\text{lbmol/h}$ (upper bound).
4. Reactor inlet pressure $P_{rin} = 500\text{psi}$ (upper bound).
5. Hydrogen to aromatic ratio in reactor inlet $rH_2 = 5$ (lower bound).

In addition, for the distillation columns, it was decided to control compositions¹. However, for the overhead in the stabilizer this is not a good choice. The small value of $x_{D,ben}^{stab}$ used in Araujo *et al.*¹ leads to cryogenic conditions which is 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, $T_1^{stab} = 77^{\circ}\text{F}$. 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. Condenser temperature at stabilizer column $T_1^{stab} = 77^{\circ}\text{F}$ (lower bound).
7. Methane mole fraction in stabilizer bottoms $x_{B,met}^{stab} = 10^{-6}$ (“optimal” value).
8. Benzene mole fraction in benzene column distillate $x_{D,ben}^{bc} = 0.9997$ (lower bound).
9. Benzene mole fraction in benzene column bottoms $x_{B,ben}^{bc} = 0.0013$ (“optimal” value).
10. Diphenyl mole fraction in toluene column distillate $x_{D,dip}^{tc} = 0.0005$ (“optimal” value).
11. Toluene mole fraction in toluene column bottoms $x_{B,tol}^{tc} = 0.0004$ (“optimal” value).

The “optimal” values for the distillation columns were found as a trade-off between maximizing the recovery of valuable component and minimizing energy consumption¹.

As the benzene column distillate is essentially composed by benzene and toluene only, we control in practice the toluene mole fraction in the benzene column distillate $x_{D,tol}^{bc}$ instead of $x_{D,ben}^{bc}$ 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 trade-off makes the optimum flat¹. In practice, temperature control will therefore 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 3¹. Note that all the best candidates involve compositions and that they all involve controlling inert in the reactor inlet (mixer T2 outlet). The approach is to select the set with the best steady-state cost (here Set I), unless there turns out to be other factors related to implementation that clashes this choice.

3.3 Maximum throughput (Mode II)

As mentioned, we consider two modes of operation:

- **Mode I: Given feed rate (F_{tol}).** The optimal operation for this case is described in Araujo *et al.*¹ and the main results were given in the previous Section.
- **Mode II: 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 by Araujo *et al.*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 find 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 4 and the profit J as a function of F_{tol} is shown graphically in Figure 4.

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

Table 3: Candidate sets of controlled variables with small losses (Mode I).

Set	Variables	Average loss ^(*) [k\$/year]
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

(*) The average loss is calculated with each variable in the set kept at its nominal optimal set point and taking into account also its implementation error.

Table 4: Re-optimizing with variable toluene feed rate F_{tol} .

Variable	Nominal	Maximum	Reached at F_{tol} (lbmol/h)	Comments
Compressor power (hp)	454.39	545.27 (+20%)	380 (+27%)	
Furnace heat duty (MBtu)	16.26	24.39 (+50%)	393 (+31%) ¹	Bottleneck
Cooler heat duty (MBtu)	21.57	32.36 (+50%)	410 (+37%) ^{1,2}	Bottleneck ²
Reactor outlet temperature (°F)	1277	1300	420 (+40%) ^{1,2,3}	Bottleneck ^{2,3}
Distillation heat duties		(+50%)	Up to 450 (+50%)	Max. not reached ⁴

¹ With compression power at maximum.

² Disregarding maximum furnace heat duty.

³ Disregarding maximum cooler heat duty.

⁴ The constraints on the heat duties of the distillation columns (reboiler and condenser) were not reached for F_{tol} up to 450 lbmol/h.

From Table 4, 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 as 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 as a further increase in F_{tol} with Q_{fur} at its maximum, causes infeasible operation. This may be explained because an increase in feed rate with a fixed furnace heat duty results in a decrease in the reactor temperature, reducing conversion of toluene, which leads to a build-up 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, since maximum conversion is already favored by the economics (and 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 cooler heat duty or reactor outlet temperature, which according to Table 4 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 $Q_{fur} = Q_{fur,max}$ for optimal operation and production rate should be set at this location.

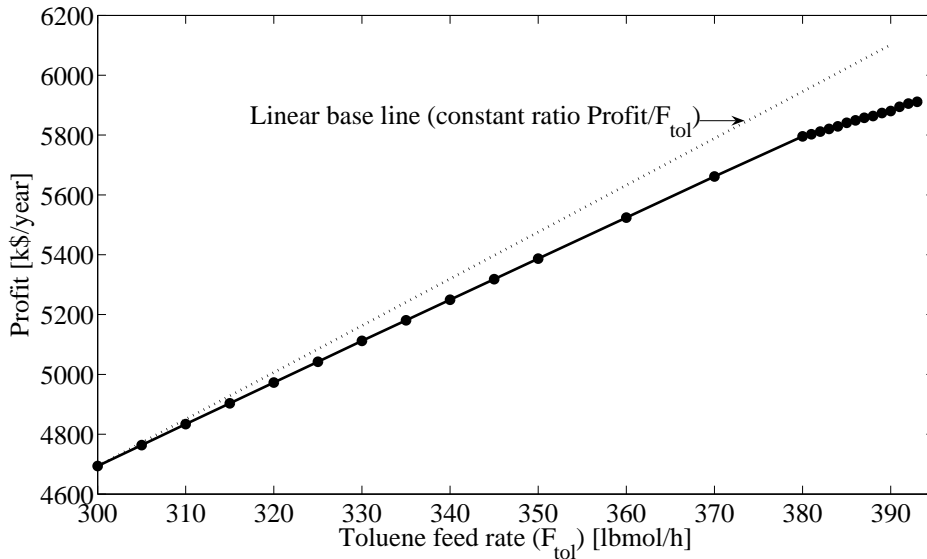


Figure 4: Optimization of the HDA process with variable toluene feed rate. The compressor power reaches its maximum at $F_{tol} = 380$ lbmol/h and the furnace heat duty becomes a bottleneck at $F_{tol} = 393$ lbmol/h.

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 found that mixer outlet inert (methane) mole fraction $x_{mix,met}$ is present in all candidate sets (see Table 3) and in order to minimize reconfiguration of loops when switching from one mode of operation to another (from Mode I to Mode II and converse), it would be desirable to select $x_{mix,met}$ as the self-optimizing controlled variable. Fortunately, the loss by keeping $x_{mix,met}$ at its nominally optimal set point in Mode II is acceptable as shown in Table 5. Thus, we decide to select $x_{mix,met}$ as the unconstrained “self-optimizing” controlled variables also in Mode II.

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 $Q_{fur} = Q_{fur,max}$. However, the reactor is unstable and the furnace heat duty is the most favorable input for closing a stabilizing

Table 5: Mode II - Maximum production rate (Mode II): Loss by selecting $x_{mix,met}$ as the unconstrained “self-optimizing” controlled variables.

Case	Description	Optimal		Loss ^(*)
		$x_{mix,met}$	Profit [k\$/year]	[k\$/year]
Nominal	$F_{tol} = 393$ lbmol/h	0.5555	5931.2	0
D1	Fresh gas feed rate methane mole fraction from 0.03 to 0.08	0.5254	6316.4	175.8
D2	Hydrogen to aromatics ratio in reactor inlet from 5.0 to 5.5	0.4943	6249.6	329.0
D3	Reactor inlet pressure [psi] from 500 to 507	0.5643	6198.7	181.0
D4	Quencher outlet temperature [°F] from 1150 to 1170	0.5381	6371.5	190.4
D5	Product purity in the benzene column distillate from 0.9997 to 0.9980	0.5202	6531.1	277.3
n_y	Implementation error of 0.0001 in $x_{mix,met}$	0.5556	5977.5	46.3

(*) Loss with fixed $x_{mix,met} = 0.5555$ (nominal optimum).

temperature loop. We must accept some “back off” 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 Mode I and Mode II. In Mode II, we use a duty controller that keeps the furnace heat duty at a given value (back off) 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 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_{rin}) because Q_{fur} has a direct effect on T_{rin} (with a small effective delay). In addition, there is a lower limit of $1150^{\circ}F$ 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 need to be stabilized. Since the throughput manipulator is at the feed, the inventory control for the columns are set up assuming 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_{rin} which is an active constraint and must be controlled at its nominal optimal set point for optimal operation. There are three manipulated variables that can effectively be used to control P_{rin} , 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} but since 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, since 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 since F_{hyd} directly affects the mass balance of the process. Second, the compressor is an expensive and delicate piece of equipment, so 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_{rin} .

The pressures in the distillation columns need also be controlled and we use condenser heat duty as manipulated variables. An exception is made for the stabilizer where 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.

Since 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 to the quencher. We use the flow rate of the cold liquid stream from the separator as the manipulated variable.

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 small¹¹. 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, as the temperature slope at this stage is very small, this may give difficult control problems dynamically, so we decide to

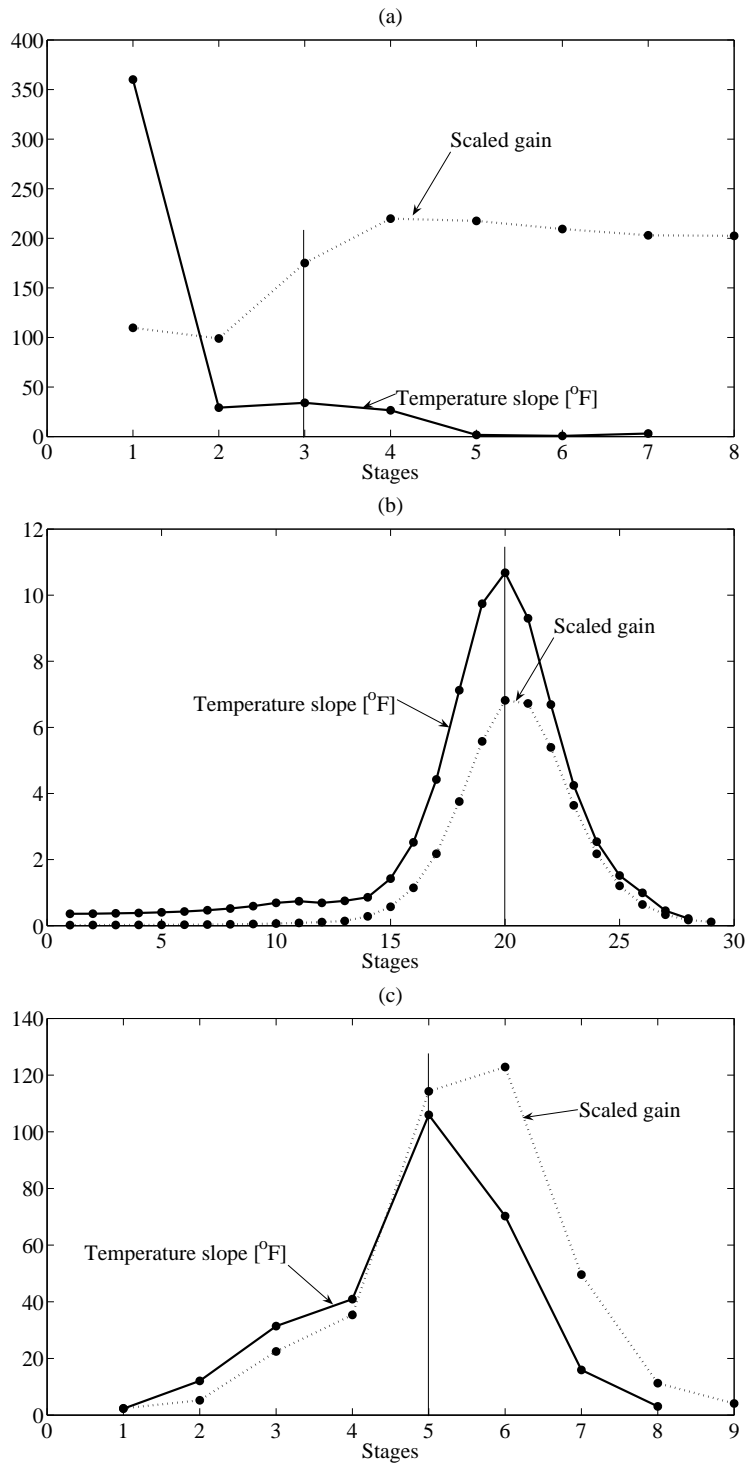


Figure 5: Temperature slope (solid line) and scaled gain (dotted line) for distillation columns. Temperature should be controlled at a location where both are sufficiently large. (a) Results for stabilizer; (b) Results for benzene column; (c) Results for toluene column.

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 Figures 5b and c. Therefore, for the benzene column we control 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 toluene feed rate F_{tol} and hydrogen feed rate F_{hyd} .

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. We here focus on the reactor-recycle system as the distillation column units are not critical for the economics in this case (first, because the loss for composition change is small¹ 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 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 need to control 3 compositions in Mode I ($rH_2, x_{mix,met}$, and $x_{quen,tol}$) and 2 compositions in Mode II (rH_2 and $x_{mix,met}$). The composition control will be slow because of measurement delays, so, as 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} , $T_{rin,sp}$, and W_s . In Mode II, W_s is fixed at its maximum and is therefore not available, and also in Mode I we choose not use W_s at this relatively fast time scale.

Once more, the maximum gain rule¹⁰ 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 6 for Mode I.

As seen from Table 6, the economic loss by controlling $u'_1 = \{F_{hyd}, T_{rin,sp}, W_s\}$ (Set VII) is almost the same as 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.

Table 6: Local analysis for possible “intermediate” regulatory control: Maximum (scaled) singular rule of best sets of candidate controlled variables (W_s is assumed constant).

Set	Controlled variables	$\underline{\sigma}(S_1 G J_{uu}^{-1/2}) \cdot 1000$
I	FEHE hot side outlet temperature ($T_{fhe,hs}$) Fresh gas feed rate (F_{hyd})	0.4939
II	FEHE hot side outlet temperature ($T_{fhe,hs}$) Mixer outlet flow rate (F_{mix})	0.4937
III	FEHE hot side outlet temperature ($T_{fhe,hs}$) Separator vapor outlet flow rate ($F_{sep,vap}$)	0.4929
IV	FEHE hot side outlet temperature ($T_{fhe,hs}$) Quencher outlet flow rate (F_{quen})	0.4923
V	Reactor outlet temperature (T_{rout}) Fresh gas feed rate (F_{hyd})	0.4911
VI	Reactor outlet temperature (T_{rout}) Mixer outlet flow rate (F_{mix})	0.4909
VII	Furnace outlet temperature (T_{rin}) Fresh gas feed rate (F_{hyd})	0.4907
VIII	Furnace outlet temperature (T_{rin}) Mixer outlet flow rate (F_{mix})	0.4906
IX	Reactor outlet temperature (T_{rout}) Separator vapor outlet flow rate ($F_{sep,vap}$)	0.4900
X	Furnace outlet temperature (T_{rin}) Separator vapor outlet flow rate ($F_{sep,vap}$)	0.4895

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 hydrogen feed rate F_{hyd} .
- RR2. Reactor inlet pressure P_{rin} with purge flow F_{purge} .
- RR3. Flow control of toluene feed rate F_{tol} .
- RR4. Quencher outlet temperature $T_{quencher}$ with cooling flow from separator $F_{sep,liq}$.
- RR5. Reactor inlet temperature T_{rin} with furnace heat duty Q_{fur} .
- RR6. Separator temperature T_{sep} with cooler heat duty Q_{cool} .
- RR7. Separator level using its liquid outlet flow rate to the distillation section.

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

- RD1. Stabilizer pressure P_{stab} with distillate flow rate D_{stab} .
- RD2. Benzene column pressure P_{bc} with condenser heat duty Q_{cond}^{bc} .
- RD3. Toluene column pressure P_{tc} with condenser heat duty Q_{cond}^{tc} .
- RD4. Temperature at stage 3 T_3^{stab} with reboiler heat duty Q_{reb}^{stab} in the stabilizer.
- RD5. Temperature at stage 20 T_{20}^{bc} with reboiler heat duty Q_{reb}^{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 condenser heat duty Q_{cond}^{stab} in the stabilizer.
- RD8. Reboiler sump level with bottoms flow rate B_{stab} in the stabilizer.
- 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.
- 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 back-off).

The aim of the supervisory control layer is to keep the active constraints and unconstrained (self-optimizing) controlled variables at constant set points. For the unconstrained controlled variables, we select in Mode I to control Set I in Table 3, 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 $x_{mix,met}$.

We here consider in detail Mode I. With the regulatory control in place, there are still 9 composition loops (3 compositions in the reactor-recycle section and 2 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 DynamicsTM. A linearization script defining controlled and manipulated variables can be easily written in Aspen DynamicsTM and the linear state-space model with constant matrices A, B, C, and D generated by the code are exported to MatLabTM 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, $u = [L_{stab} \ T_{3,sp}^{stab}]$ and $y = [T_1^{stab} \ x_{B,met}^{stab}]$ 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_1^{stab}) and the set point of the temperature controller at stage 3 ($T_{3,sp}^{stab}$) with methane mole fraction in bottoms ($x_{B,met}^{stab}$).

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

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

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

As for the toluene column, since 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_5^{tc}). This gives a steady-state RGA matrix (with $u = [Q_{reb}^{tc} T_{5,sp}^{tc}]$ and $y = [x_{B,tol}^{tc} x_{D,dip}^{tc}]$)

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

and the chosen pairing is reboiler heat duty (Q_{reb}^{tc}) with toluene mole fraction in bottoms ($x_{B,tol}^{tc}$) and the set point of the temperature controller at stage 5 ($T_{5,sp}^{tc}$) with diphenyl mole fraction in distillate ($x_{D,dip}^{tc}$).

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

$$u = \{T_{rin,sp}; W_s; F_{hyd,sp}\} \quad (3)$$

and controlled variables

$$y = \{rH_2; x_{mix,met}; x_{quen,tol}\} \quad (4)$$

need to be designed, where $T_{rin,sp}$ is the set point of the temperature controller at the reactor inlet, $F_{hyd,sp}$ is the set point 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 quencher outlet.

To check the controllability of the 3×3 system ($\hat{g}_{3 \times 3}$), we obtain the zeros, and found two pairs of RHP-zeros ($250 \pm 908i$ and $588 \pm 346i$ rad/h), but these are located quite far into the right-half plane (corresponding to an effective delay at about $\frac{1}{250}$ h = 0.24min) and will not cause any performance limitations. We also found that the RHP-zeros 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 loops¹², but 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 (hydrogen to aromatic ratio at reactor inlet) since we might expect $F_{hyd,sp}$ to have a large and direct effect on rH_2 . However, the steady-state RGA analysis matrix

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

suggests this should be avoided due to pairing on negative steady-state RGA elements. To avoid pairing on negative RGA elements, we must pair $T_{rin,sp}$ with $x_{quen,tol}$; W_s with rH_2 ; and $F_{hyd,sp}$ with $x_{mix,met}$. Figure 6 shows the RGA number ($\|\Lambda_{reac} - I_3\|_{sum}$)¹⁰ as a function of frequency for these pairings, and we find that the dynamic interactions are also small.

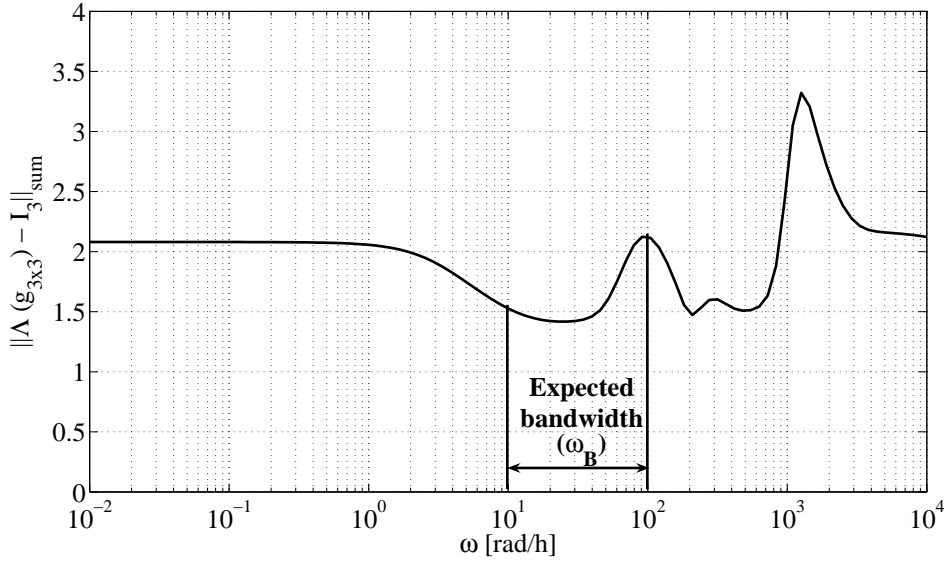


Figure 6: RGA number as a function of frequency for reaction section with pairing $T_{rin,sp} - x_{quen,tol}$; $W_s - rH_2$; and $F_{hyd,sp} - x_{mix,met}$.

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. Toluene mole fraction at quencher outlet $x_{quen,tol}$ with set point of the reactor temperature controller $T_{rin,sp}$.

SR2. Methane mole fraction at mixer outlet $x_{mix,met}$ with set point of the hydrogen feed rate flow controller $F_{hyd,sp}$.

SR3. Hydrogen to aromatic ratio at reactor inlet rH_2 with compressor power W_s .

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

SD1. Toluene mole fraction in bottoms $x_{B,tol}^{tc}$ with reboiler heat duty Q_{reb}^{tc} in the toluene column.

SD2. Benzene mole fraction in bottoms $x_{B,ben}^{bc}$ with the set point of the temperature controller at stage 20 $T_{20,sp}^{bc}$ in the benzene column.

SD3. Toluene mole fraction in distillate $x_{D,tol}^{bc}$ with reflux rate L_{bc} in the benzene column.

SD4. Methane mole fraction in bottoms $x_{B,met}^{stab}$ with the set point of the temperature controller at stage 3 $T_{3,sp}^{stab}$ in the stabilizer.

SD5. Diphenyl mole fraction in distillate $x_{D,dip}^{tc}$ with the set point of the temperature controller at stage 5 $T_{5,sp}^{tc}$ in the toluene column.

SD6. Condenser temperature T_1^{stab} 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 set point. For Mode II, F_{tol} controls the furnace heat duty $Q_{fur,sp} = Q_{fur,max} - Q_{fur,backoff}$ (non-optimal strategy), where $Q_{fur,backoff}$ is the back-off (input resetting) from the maximum furnace heat duty to avoid that it saturates, which may give instability because of loss of stabilizing temperature control. This back-off value must be found 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 assure active constraint control).
3. Use $T_{rin,sp}$ to control $x_{mix,met}$ and change the set point 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 7 and 8. Note that only the loops $F_{hyd,sp} - rH_2$ and $F_{tol,sp} - Q_{fur}$ need to be retuned.

3.6.3 Controller tuning

The lower layer loops selected above are closed and tuned one at the time in a sequential manner (starting with the fastest loops). Aspen DynamicsTM 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 rules¹³ to design the PI-controllers:

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

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, gain K_c and integral time τ_I , are given in Tables 7 and 8 for the reactor-recycle section and distillation section, respectively. See also Figures 7 and 8 for the controller tag.

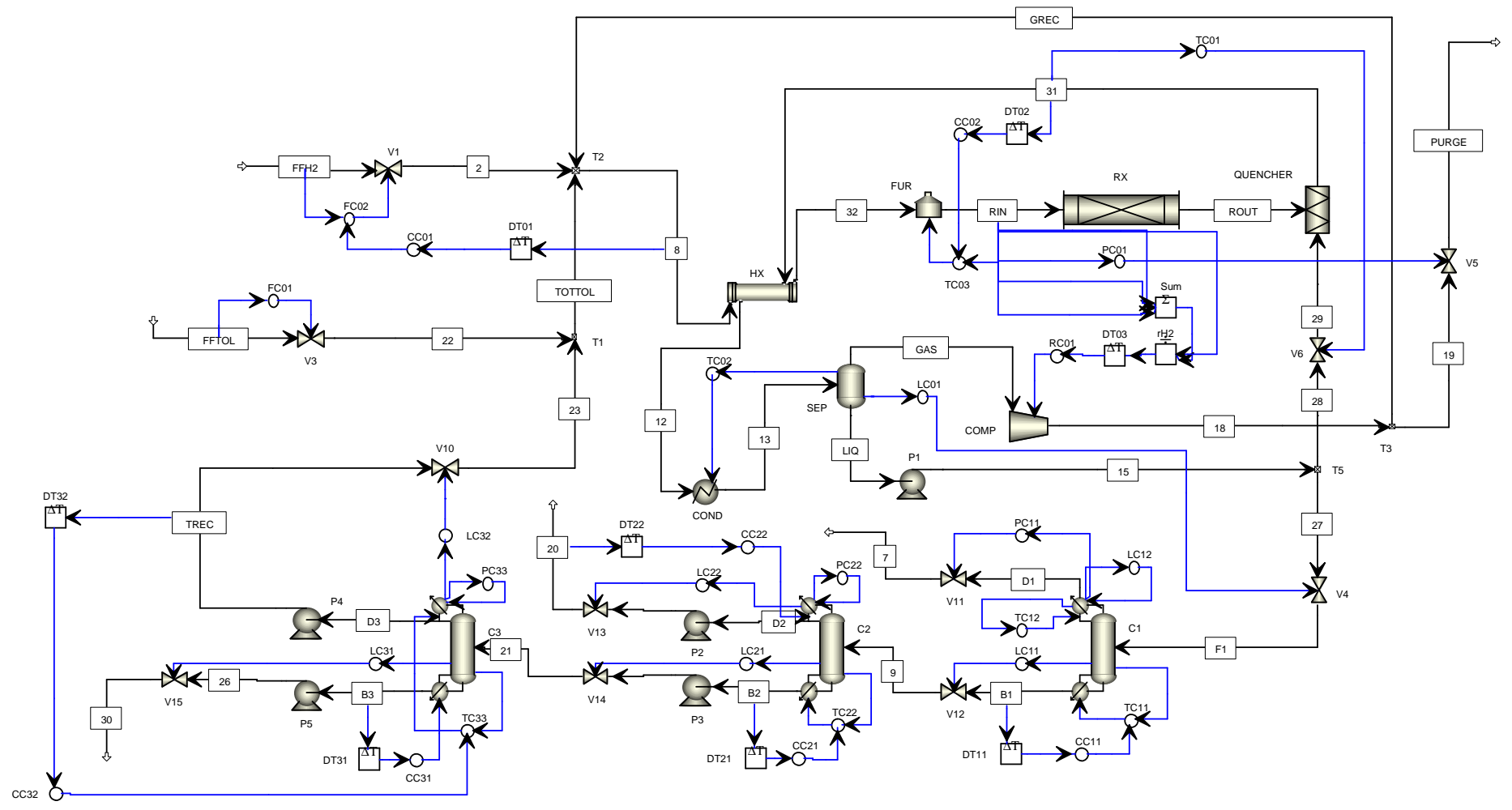


Figure 7: Mode I: HDA Aspen DynamicsTM process flowsheet with controllers installed.

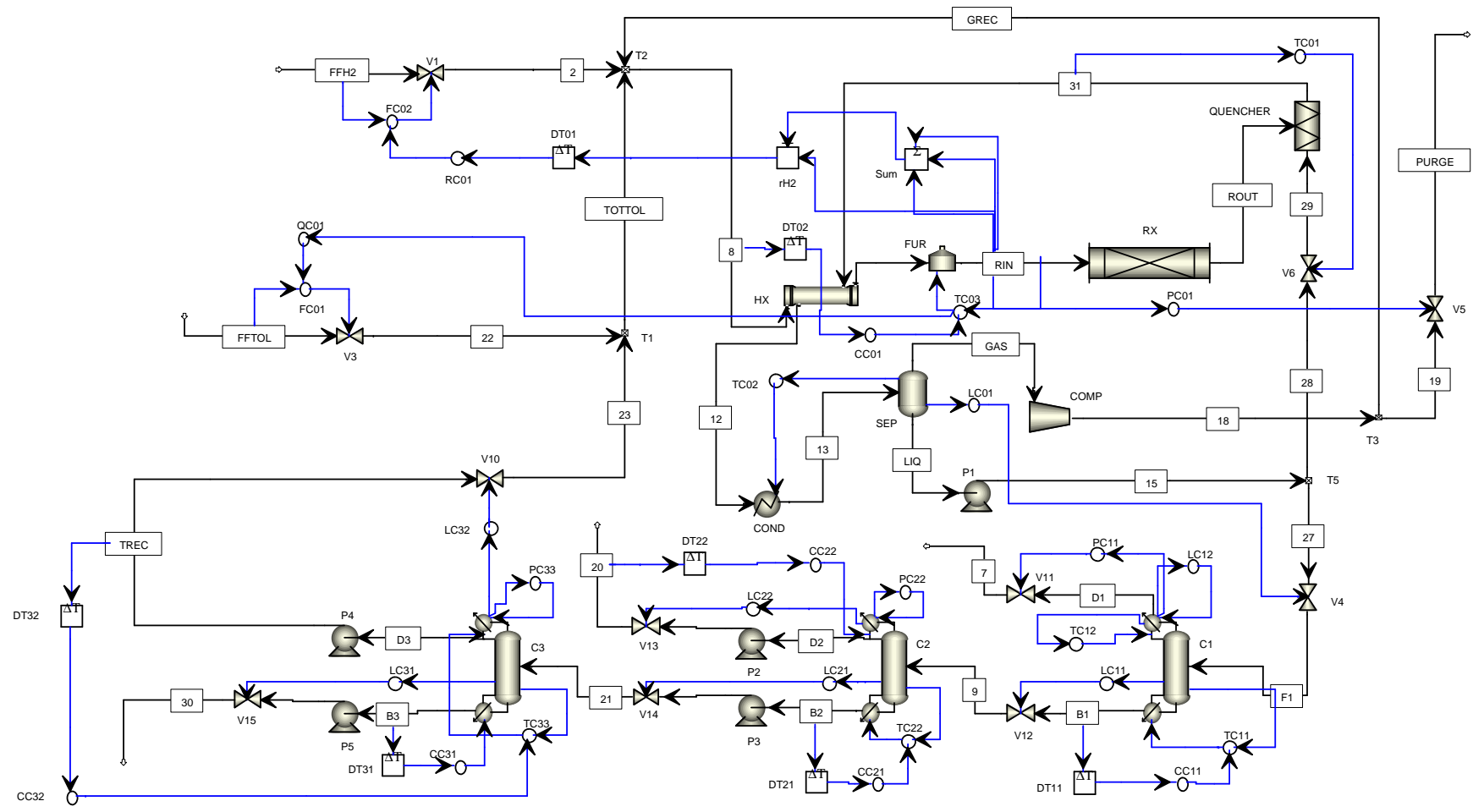


Figure 8: Mode II: HDA Aspen DynamicsTM process flowsheet with controllers installed.

Table 7: Tuning parameters for the reactor-recycle section (Modes I and II).

No.	Loop		Tag ^a	PI-controller parameters	
	Input	Output		K_c (%/%)	τ_I (min)
RR1	V_1	F_{hyd}	FC02	3.08	0.65
RR2	V_5	P_{rin}	PC01	144.7	0.80
RR3	V_3	F_{tol}	FC01	3.13	0.57
RR4	V_6	$T_{quencher}$	TC01	34.98	0.47
RR5	Q_{fur}	T_{rin}	TC03	9.83	0.67
RR6	Q_{cool}	T_{sep}	TC02	1.36	0.80
RR7	M_{sep}	$F_{sep,liq}$	LC01	2	-
SR1 ^b	$T_{rin,sp}$	$x_{quen,tol}$	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	$T_{rin,sp}$	$x_{mix,met}$	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.

3.7 Structure of the optimization layer

Since we obtained a design that takes care of 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 in this study with the one proposed by Luyben³ for Mode I of operation. They are both based on the same underlying Aspen model but Luyben³ consider a different steady-state operating point. However, a good control structure should not depend on the operating point. In order to have a consistent basis for comparison, we use the steady-state considered in this paper but maintain the original tuning settings determined by Luyben³. Figures 9 through 12 compares the results for the disturbances in Table 9.

Table 8: Tuning parameters for the distillation section (Modes I and II).

No.	Input	Loop		PI-controller parameters	
		Output	Tag ^a	K_c (%/%)	τ_I (min)
RD1	V_{11}	P_{stab}	PC11	122.02	0.80
RD2	Q_{cond}^{tc}	P_{tc}	PC33	56.30	0.80
RD3	Q_{cond}^{bc}	P_{bc}	PC22	21.047	0.80
RD4	Q_{reb}^{stab}	T_3^{stab}	TC11	1.23	0.80
RD5	L_{tc}	T_5^{tc}	TC33	110.44	1.12
RD6	Q_{reb}^{bc}	T_{20}^{bc}	TC22	5.82	4.8
RD7	M_D^{stab}	Q_{cond}^{stab}	LC11	2	-
RD8	M_B^{stab}	B_{stab}	LC12	2	-
RD9	M_D^{bc}	D_{bc}	LC21	20	-
RD10	M_B^{bc}	B_{bc}	LC22	2	-
RD11	M_D^{tc}	D_{tc}	LC31	2	-
RD12	M_B^{tc}	B_{tc}	LC32	20	-
SD1	Q_{reb}^{tc}	$x_{B,tol}^{tc}$	CC31	40.96	16.19
SD2	$T_{20,sp}^{bc}$	$x_{B,ben}^{bc}$	CC21	6.69	4.56
SD3	L_{bc}	$x_{D,tol}^{bc}$	CC22	432.64	25.60
SD4	$T_{3,sp}^{stab}$	$x_{B,met}^{stab}$	CC11	5611.33	1.74
SD5	$T_{5,sp}^{tc}$	$x_{D,dip}^{tc}$	CC32	56.95	52.61
SD6	L_{stab}	T_1^{stab}	TC12	4243.41	0.8

^a See tags in Figures 7 and 8.

Table 9: Disturbances for dynamic simulations of the HDA process.

#	Variable	Nominal ^(*)	Disturbance (Δ)
Dyn1	Toluene feed rate (F_{tol})	300 lbmol/h	+30 lbmol/h (+10%)
Dyn2	Toluene feed rate (F_{tol})	300 lbmol/h	-30 lbmol/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

(*) This refers to the optimal nominal considered in this work.

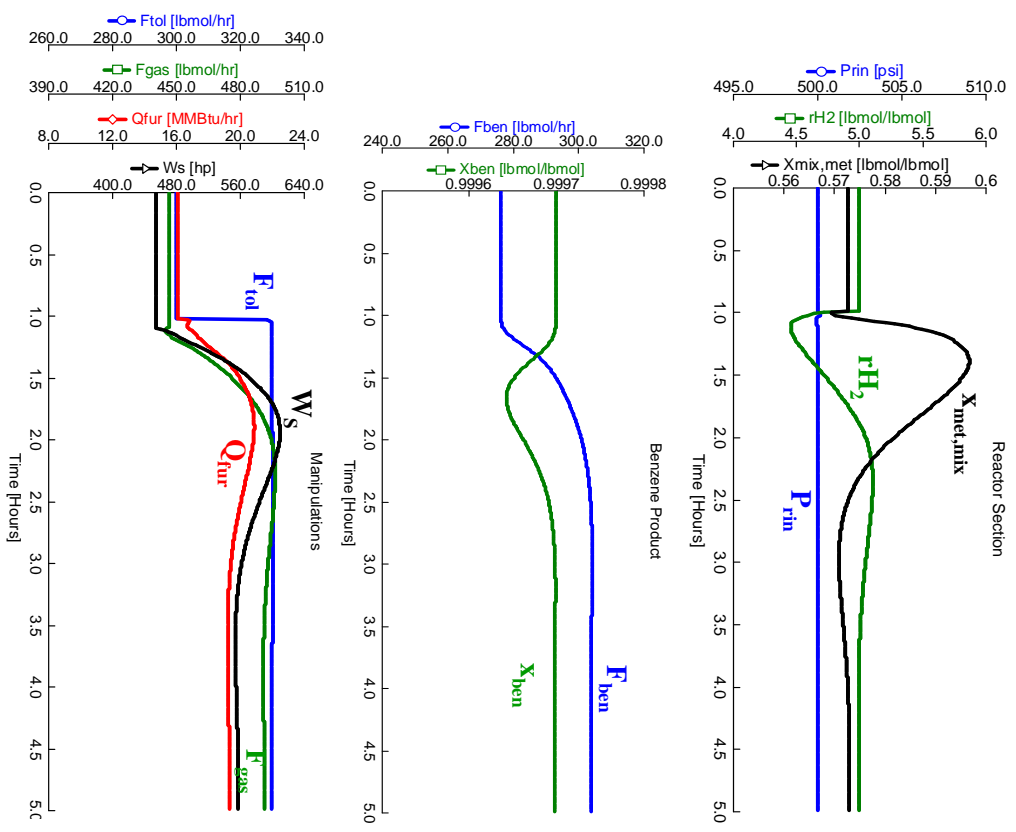
From Figures 9 - 12, we can see that the structure of Luyben³ is not optimal (or even feasible) in some cases, specifically, in response to material and/or component mass balances disturbances, since the hydrogen-to-aromatic ratio at reactor inlet rH_2 and product purity $x_{D,ben}^{bc}$, which are active constraints, are not controlled. The hydrogen-to-aromatic ratio rH_2 in the structure by Luyben³ gives a much higher offset variation than the product purity $x_{D,ben}^{bc}$ 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, Luyben³ does not consider using compressor power W_s as a degree of freedom (it is actually assumed constant) in contrast with our control structure that makes use of W_s for long term control. Economically, this can result in economic losses since in some cases it has been used excessively (see, e.g., Figure 10).

However, in general, the dynamic responses of the two control structures are similar with essentially the same settling time (about 4 hours) 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 back-off 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.

Configuration in this work



Luyben's configuration

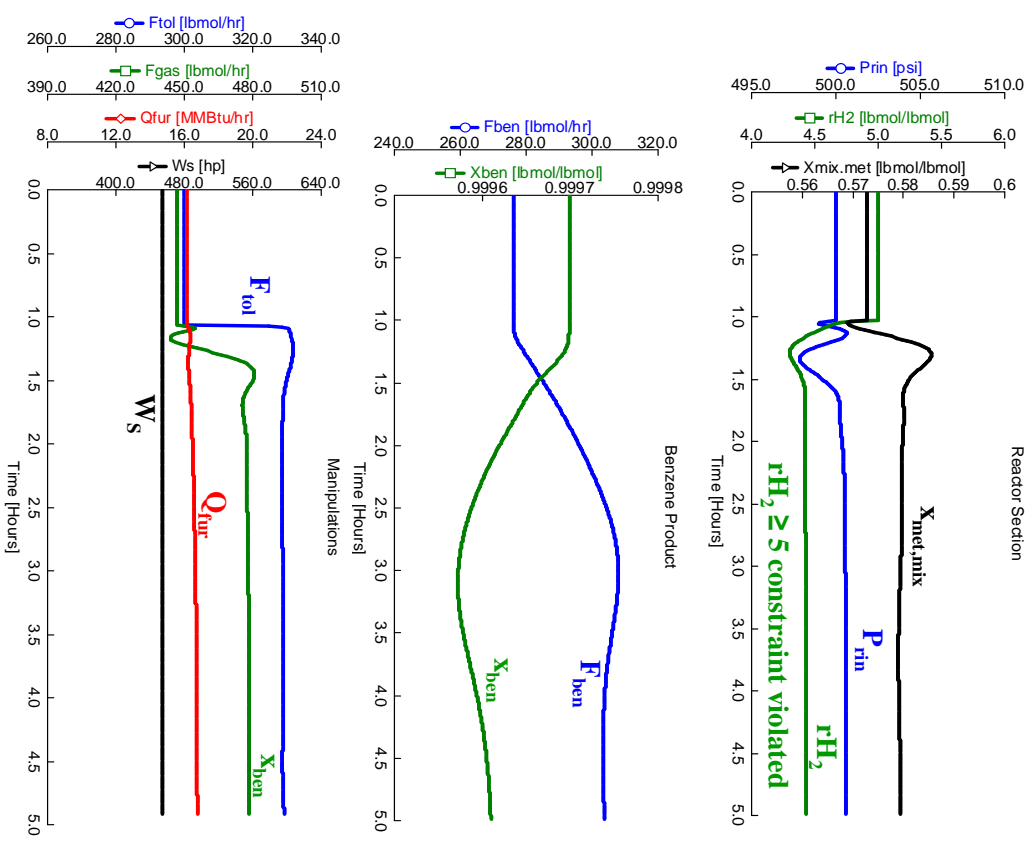


Figure 9: Mode I: Dynamic response of selected variables for disturbance Dyn1: +10% increase in F_{tol} .

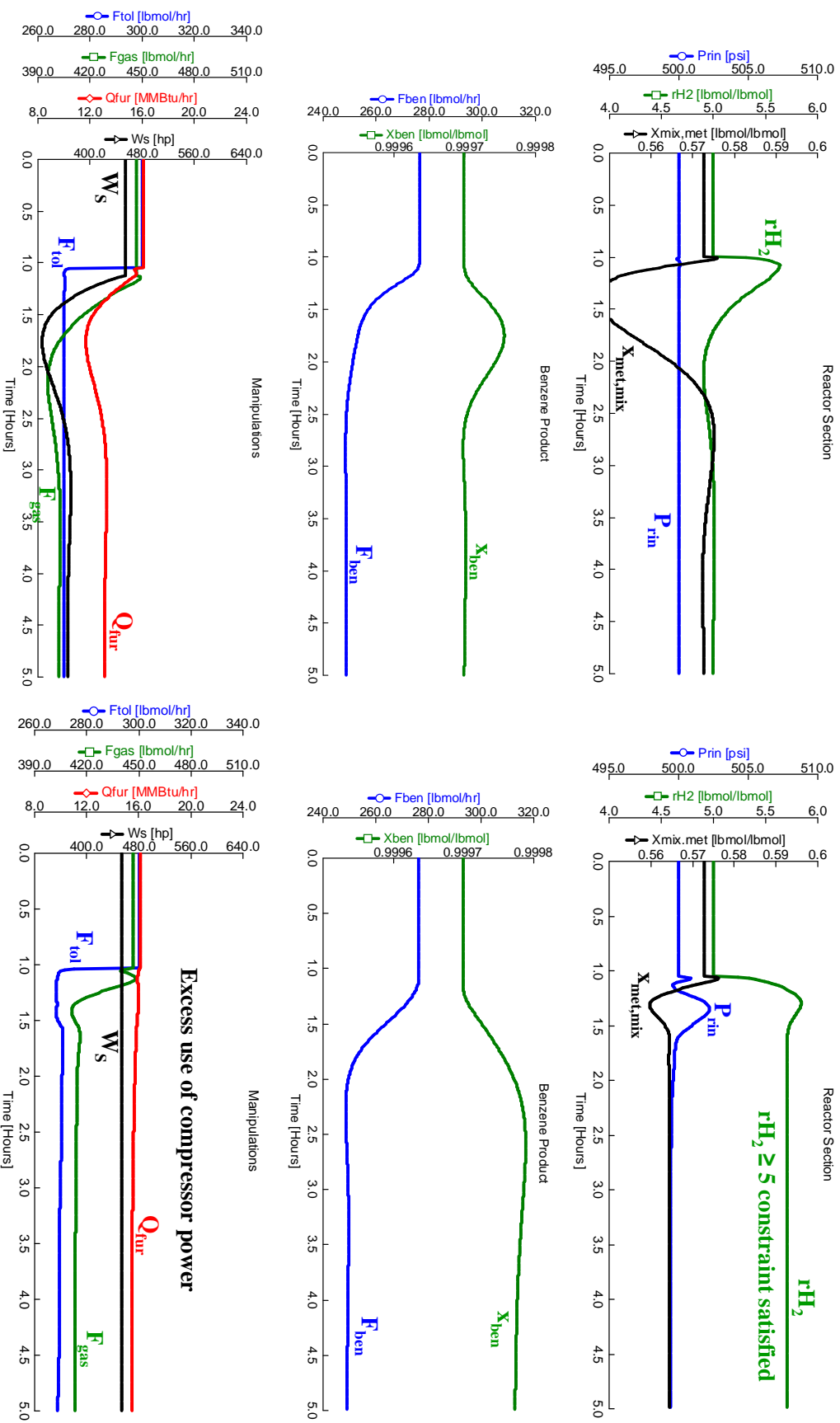
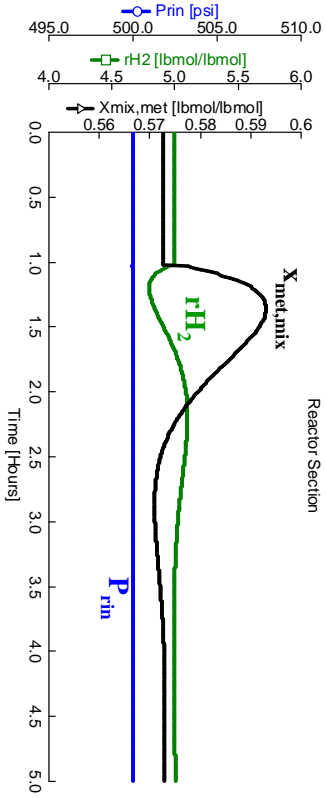
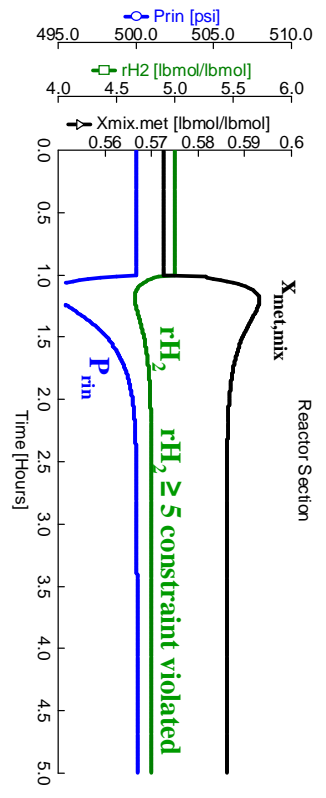


Figure 10: Mode I: Dynamic response of selected variables for disturbance Dyn2: -10% increase in F_{tol} .

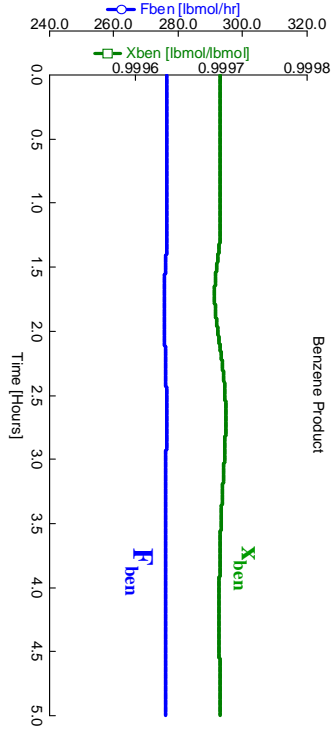
Configuration in this work



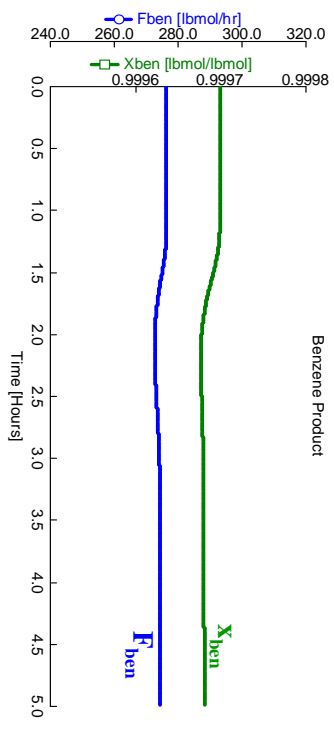
Luyben's configuration



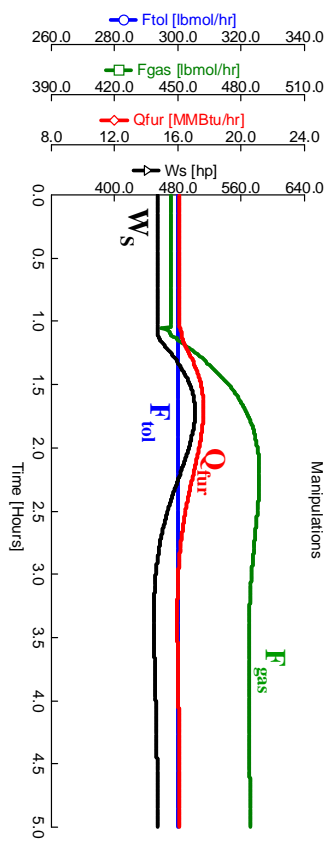
Benzene Product



Benzene Product



Manipulations



Manipulations

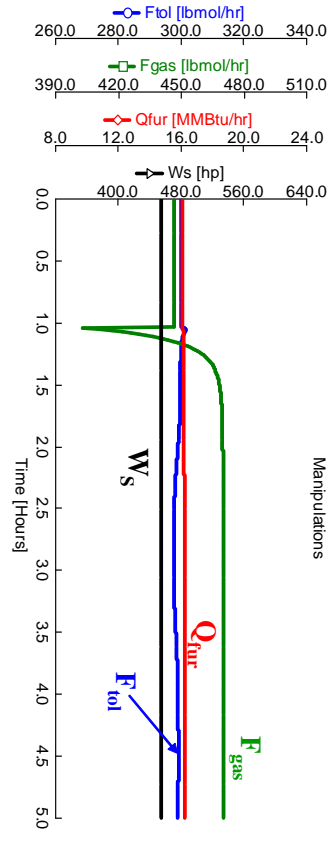
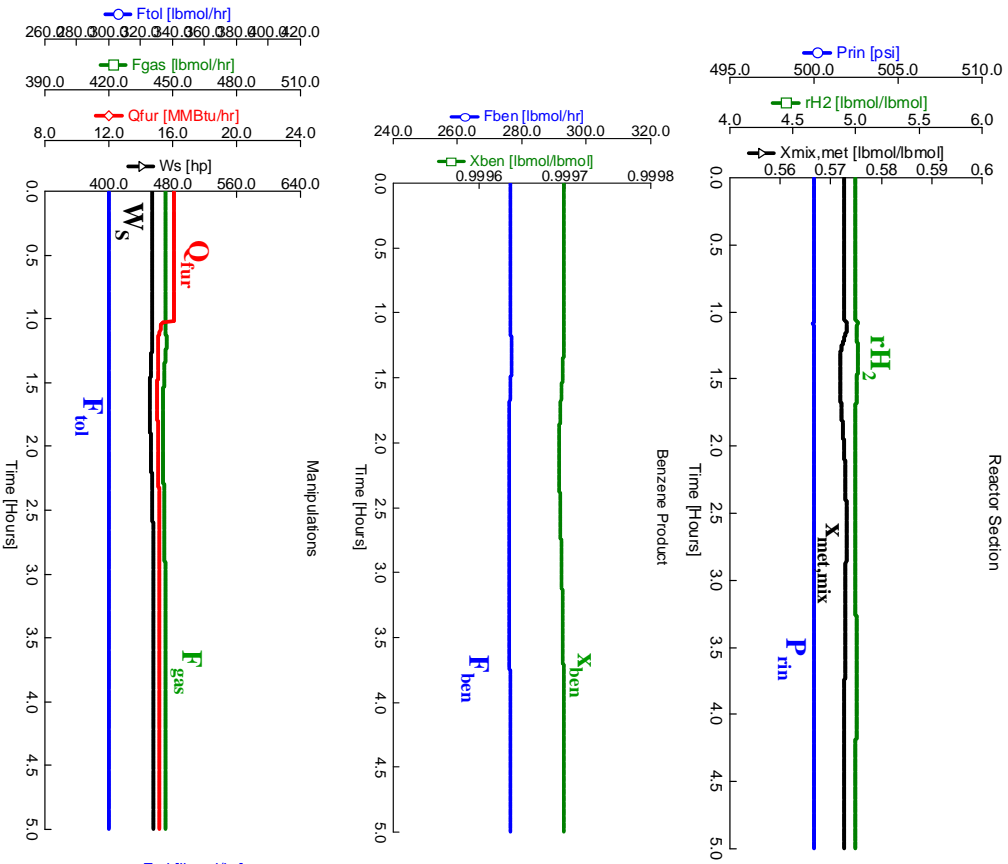


Figure 11: Mode I: Dynamic response of selected variables for disturbance Dyn3: +0.05 increase in x_{met} .

Configuration in this work



Luyben's configuration

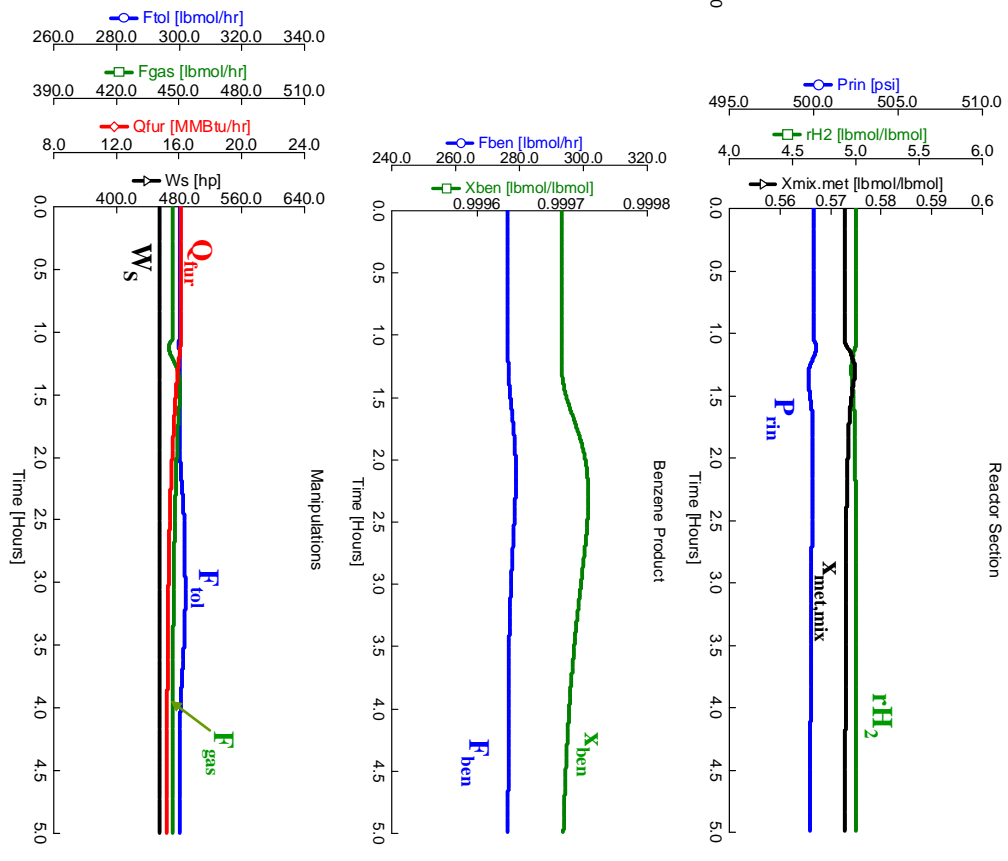


Figure 12: Mode I: Dynamic response of selected variables for disturbance Dyn4: +20°F increase in $T_{quencher}$.

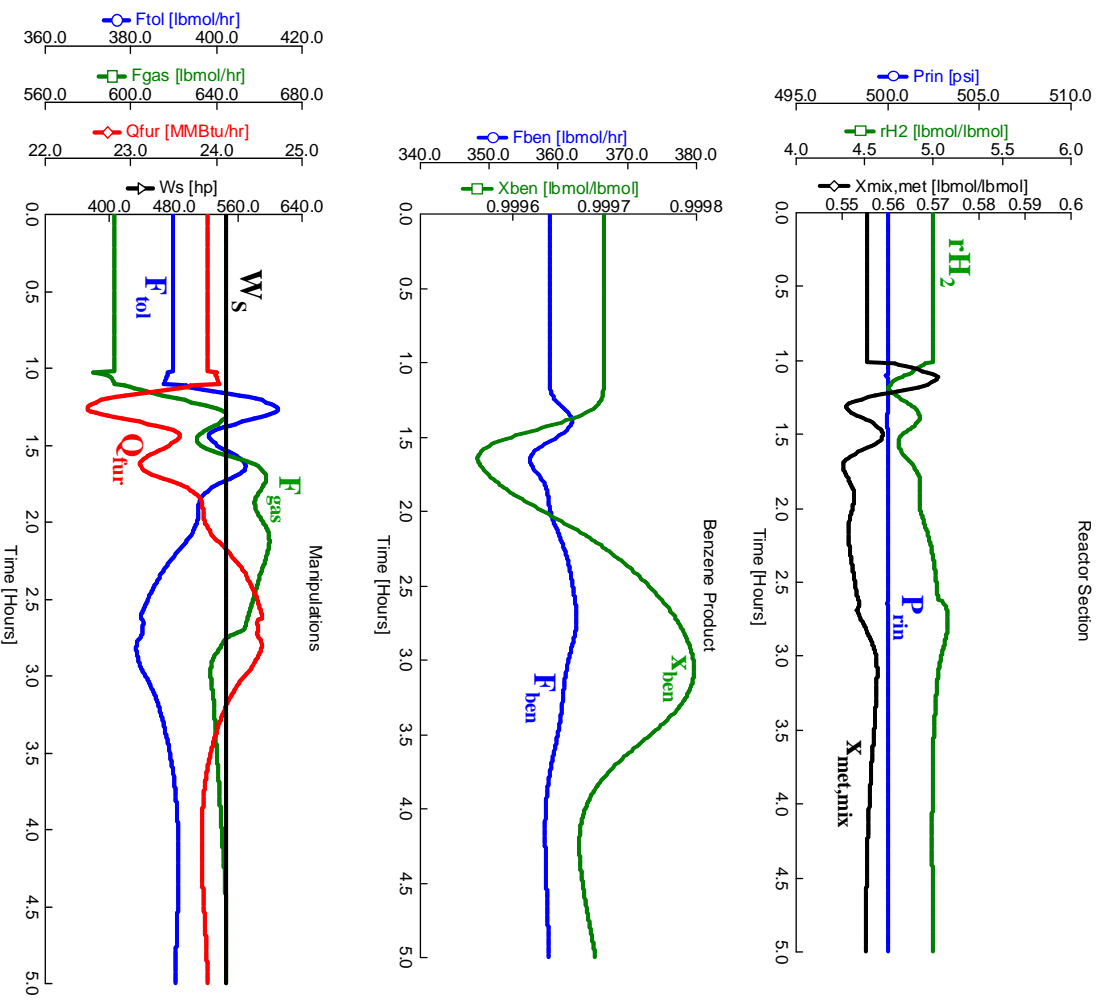


Figure 13: Mode II (configuration in this work): Dynamic response of selected variables for disturbance Dyn3: +0.05 increase in x_{met} .

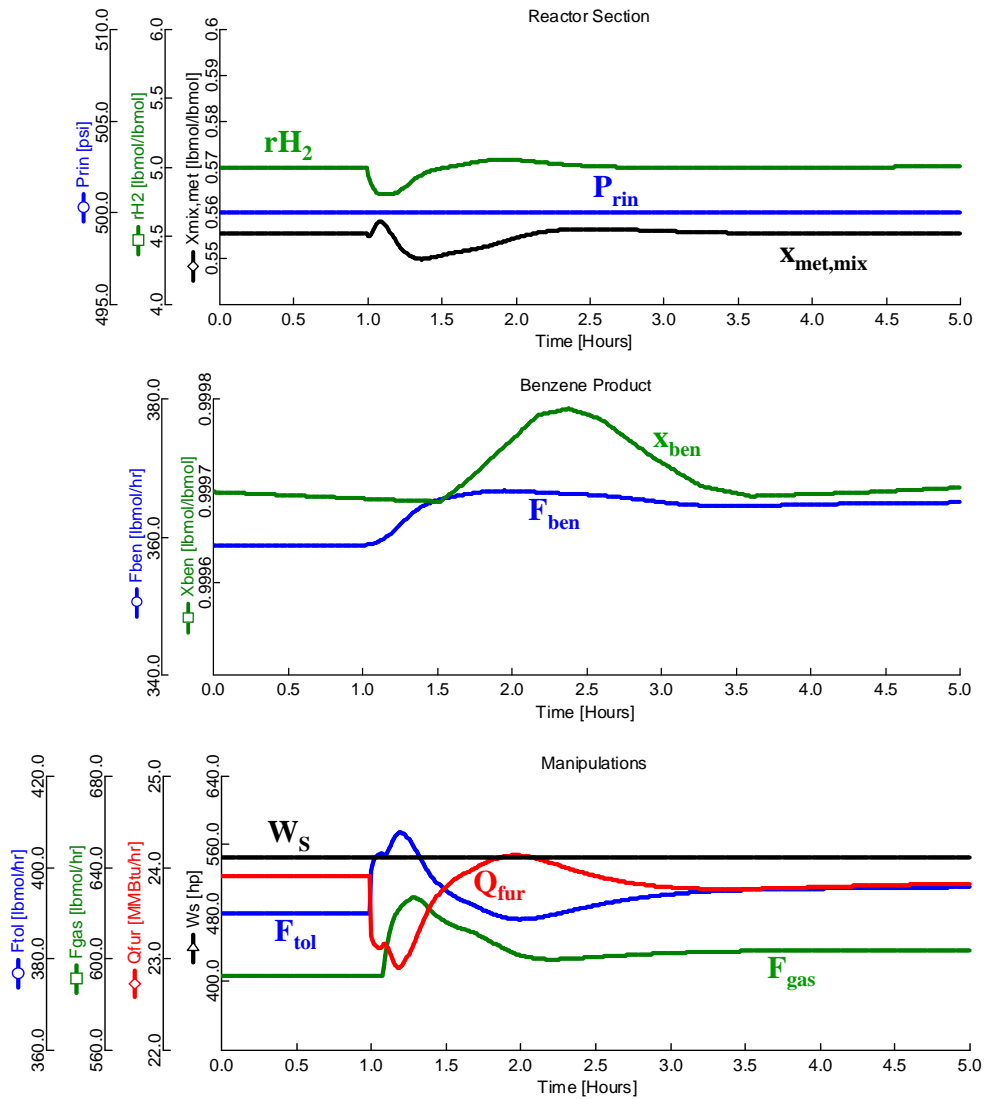


Figure 14: Mode II (configuration in this work): Dynamic response of selected variables for disturbance Dyn4: $+20^{\circ}\text{F}$ increase in $T_{quencher}$.

5 Conclusion

This paper has discussed control structure design for the HDA process using the design procedure of Skogestad² with emphasis on the regulatory control layer. For this process, the bottleneck for maximum production rate (Mode II) was found 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 seen 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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