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Application of plantwide control to the HDA process. I—steady-state optimization and self-optimizing control

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Abstract

This paper describes the application of self-optimizing control to a large-scale process, the HDA plant. The idea is to select controlled variables which when kept constant lead to minimum economic loss. First, the optimal active constraints need to be controlled. Next, controlled variables need to be found for the remaining unconstrained degrees of freedom. In order to avoid the combinatorial problem related to the selection of outputs/measurements for such large plants, a local (linear) analysis based on singular value decomposition (SVD) is used for pre-screening. This is followed by a more detailed analysis using the nonlinear model. Note that a steady-state model, in this case one built in Aspen Plus™, is sufficient for selecting controlled variables. A dynamic model is required to design and test the complete control system which include regulatory control. This is considered in the part II of the series.
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Keywords: HDA process; Self-optimizing control; Selection of controlled variable; Aspen Plus™

1. Introduction

This paper deals with the selection of controlled variables for the HDA process. One objective is to avoid the combinatorial control structure issue for such large-scale processes by using local methods based on the singular value decomposition (SVD) of the linearized model of the process.

The selection of controlled variables is based on steady-state economics and use the ideas of self-optimizing control to find the best set(s). Self-optimizing control is when an acceptable (economic) loss can be achieved using constant set points for the controlled variables, without the need to reoptimize when disturbances occur (Skogestad, 2000). The constant set point policy is simple but will not be optimal (and thus have a positive loss) as a result of the following two factors: (1) disturbances, i.e., changes in (independent) variables and parameters that cause the optimal set points to change, and (2) implementation errors, i.e., differences between the setpoints and the actual values of

the controlled variables (e.g., because of measurement errors or poor control). The effect of these factors (or more specifically the loss) depends on the choice of controlled variables, and the objective is to find a set of controlled variables for which the loss is acceptable.

The HDA process (Fig. 1) was first presented in a contest which the American Institute of Chemical Engineers arranged to find better solutions to typical design problems (McKetta, 1977). It has been exhaustively studied by several authors with different objectives, such as steady-state design, controllability and operability of the dynamic model and control structure selection and controller design.

This paper is organized as follows: Section 2 examines previous proposed control structures for the HDA process. Section 3 shortly introduces the self-optimizing control technique. Section 4 describes the HDA process and the features of the model used in the present article. Section 5 summarizes the results found by applying the self-optimizing control procedure and the SVD analysis to the selection of controlled variables for the HDA process. A discussion of the results is found in Section 6 followed by a conclusion in Section 7.

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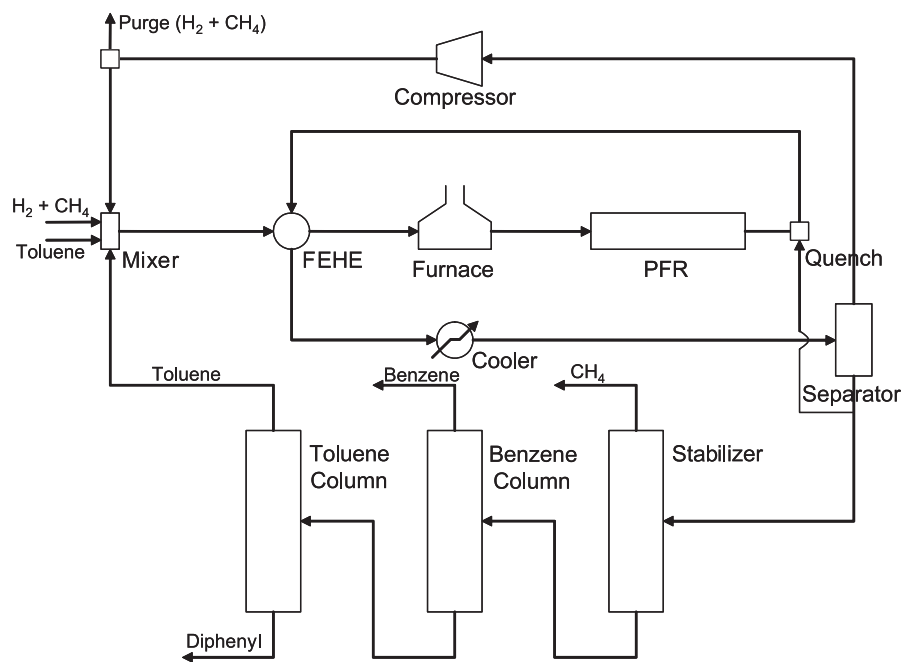*E-mail address:* sigurd.skogestad@chemeng.ntnu.no (S. Skogestad).

Fig. 1. HDA process flowsheet.

2. Previous work on the HDA process

Stephanopoulos (1984) followed the approach proposed by Buckley (1964) based on material balance and product quality control. He used an HDA plant model where steam is generated from the effluent of the feed-effluent heat exchanger (FEHE) through a series of steam coolers. From the material balance viewpoint, the selected controlled variables of choice were fresh toluene feed flow rate (production rate control), recycle gas flow rate, hydrogen contents in the recycle gas, purge flow rate, and quencher flow rate. Product quality is controlled through product compositions in the distillation columns and the controlled variables selected are product purity in benzene column and reactor inlet temperature.

Later, Douglas (1988) used another version of the HDA process to demonstrate a steady-state procedure for flowsheet design.

Brognaux (1992) implemented both a steady-state and dynamic model of the HDA plant in Speedup™ based on the model developed by Douglas (1988) and used it as an example to compute operability measurements, define control objectives, and perform controllability analysis. He found that it is optimal to control the active constraints found by optimization.

Wolff (1994) used an HDA model based on Brognaux (1992) to illustrate a procedure for operability analysis. He concluded that the HDA process is controllable provided the instability of the heat-integrated reactor is resolved. After some additional heuristic consideration, the controlled variables were selected to be the same as used by Brognaux (1992).

Ng and Stephanopoulos (1996) used the HDA process to illustrate how plantwide control systems can be synthesized based on a hierarchical framework. The selection of controlled variables is performed somehow heuristically by prioritizing the implementation of the control objectives. In other words, it is necessary to control the material balances of hydrogen, methane and toluene, the energy balance is controlled by the amount of energy added to the process (as fuel in the furnace, cooling water, and steam), production rate, and product purity.

Cao et al. used the HDA process as a case study in several papers, but mainly to study input selection, whereas the focus of the present paper is on output selection. In Cao and Biss (1996), Cao and Rossiter (1997), Cao, Rossiter, and Owens (1997a), and Cao and Rossiter (1998) issues involving input selection are discussed. Cao, Rossiter, and Owens (1997b) considered input and output selection for control structure design purposes using the SVD. Cao, Rossiter, and Owens (1998) applied a branch and bound algorithm based on local (linear) analysis. All the papers by Cao et al. utilize the same controlled variables selected heuristically by Wolff (1994). Cao, Rossiter, Edwards, Knechtel, and Owens (1998) discuss the importance of modeling in order to achieve the most effective control structure and improves the HDA process model for such purpose.

Ponton and Laing (1993) presented a unified heuristic hierarchical approach to process and control system design based on the ideas of Douglas (1988) and used the HDA process throughout. The controlled variables selected at each stage are: toluene flow rate, hydrogen concentration in the reactor, and methane contents in the compressor inlet (feed and product rate control stage); separator liquid stream outlet temperature and toluene contents at the bottom of the toluene column (recycle structure, rates and compositions stage); and separator pressure, benzene

contents at stabilizer overhead, and toluene contents at benzene column overhead are related to product and intermediate stream composition stage. The stages related to energy integration and inventory regulation do not cover the HDA process directly, so no controlled variables are assigned at these stages.

Luyben, Tyréus, and Luyben (1998) applied a heuristic nine-step procedure together with dynamic simulations to the HDA process and concluded that control performance is worse when the steady-state economic optimal design is used. They chose to control the inventory of all components in the process (hydrogen, methane, benzene, toluene, and diphenyl) to ensure that the component material balance are satisfied; the temperatures around the reactor are controlled to ensure exothermic heat removal from the process; total toluene flow or reactor inlet temperature (it is not exactly clear which one was selected) can be used to set production rate and product purity by the benzene contents in the benzene column distillate. Luyben (2002) uses the rigorous commercial flowsheet simulators Hysys^{TM}, Aspen Plus^{TM} and Aspen Dynamics^{TM} to propose a heuristic-based control structure for the HDA process.

Herrmann, Spurgeon, and Edwards (2003) consider the HDA process to be an important test-bed problem for design of new control structures due to its high integration and non-minimum phase behavior. They re-implemented Brognaux (1992)'s model in Aspen Custom Modeler^{TM} and design a model-based, multivariable H_∞ controller for the process. They considered the same controlled variables used by Wolff (1994).

Konda, Rangaiah, and Krishnaswamy (2005) used an integrated framework of simulation and heuristics and proposed a control structure for the HDA process. A Hysys^{TM} model of the plant was built to assist the simulations. They selected fresh toluene feed flow rate to set production rate, product purity at benzene column distillate to fulfill the product specification, overall toluene conversion in the reactor to regulate the toluene recycle loop, ratio of hydrogen to aromatics and quencher outlet temperature to fulfill process constraint, and methane contents in the purge stream to avoid its accumulation in the process.

Table 1 summarizes the selection of (steady state) controlled variables by various authors. It seems clear that the systematic selection of controlled variable for this plant has not been fully investigated although the process has been extensively considered by several authors. In this work, a set(s) of controlled variables for the HDA process is to be systematically selected.

3. Selection of controlled variables using self-optimizing control

The selection of primary controlled variables is considered here. The objective is to achieve self-optimizing control where fixing the primary controlled variables c at constant setpoints c_s indirectly leads to near-optimal operation (see Fig. 2).

More precisely (Skogestad, 2004):

> Self-optimizing control is when one can achieve an acceptable loss with constant setpoint values for the controlled variables without the need to re-optimize when disturbances occur.

For continuous processes with infrequent grade changes, like the HDA process, a steady-state analysis is usually sufficient because the economics can be assumed to be determined by the steady-state operation.

It is assumed that the optimal operation of the system can be quantified in terms of a scalar cost function (performance index) J_0, which is to be minimized with respect to the available degrees of freedom u_0,

$$\min_{u_0} J_0(x, u_0, d) \tag{1}$$

subject to the constraints

$$g_1(x, u_0, d) = 0; \quad g_2(x, u_0, d) \leqslant 0. \tag{2}$$

Here d represents all of the disturbances, including exogenous changes that affect the system (e.g., a change in the feed), changes in the model (typically represented by changes in the function g_1), changes in the specifications (constraints), and changes in the parameters (prices) that enter in the cost function and the constraints. x represents the internal variables (states). One way to approach this problem is to evaluate the cost function for the expected set of disturbances and implementation errors. The main steps of this procedure are as follows (Skogestad, 2000):

1. Degree of freedom analysis.
2. Definition of optimal operation (cost and constraints).
3. Identification of important disturbances (typically, feed flow rates, active constraints and input error).
4. Optimization.
5. Identification of candidate controlled variables c.
6. Evaluation of loss for alternative combinations of controlled variables (loss imposed by keeping constant set points when there are disturbances or implementation errors), including feasibility investigation.
7. Final evaluation and selection (including controllability analysis).

To achieve optimal operation, the active constraints are chosen to be controlled. The difficult issue is to decide which unconstrained variables c to control.

Unconstrained problem: The original independent variables $u_0 = u', u$ are divided into the "constraint" variables u' (used to satisfy the active constraints $g_2' = 0$) and the remaining unconstrained variables u. The value of u' is then a function of the remaining independent variables (u and d). Similarly, the states x are determined by the value of the remaining independent variables. Thus, by solving the

Table 1
Steady-state controlled variables selected by various authors

		(1)	(2)	(3)	(4)	(5)	(6)	(7)
	Number of steady-state (economic) controlled variables[a]	8	7	6	8	8	9	13
Y20[b]	Fresh toluene feed rate (active constraint)[c]	x			x		x	x
Y71	Recycle gas flow rate	x						
Y48	Recycle gas hydrogen mole fraction	x						
Y49	Recycle gas methane mole fraction			x	x	x	x	
Y62	Reactor inlet pressure (active constraint)							x
Y68	Compressor power	x	x	x	x	x	x	
Y72	Total toluene flow rate to the reaction section					x		
Y28	Mixer outlet methane mole fraction							x
Y5	Reactor inlet temperature	x	x			x		
Y19	Separator temperature (active constraint)		x		x		x	x
Y64	Separator pressure		x	x	x		x	
Y70	Hydrogen to aromatics ratio at the reactor inlet (active constraint)		x				x	x
Y73	Hydrogen mole fraction in the reactor outlet				x			
Y69	Overall toluene conversion in the reactor						x	
Y27	Quencher flow rate	x						
Y16	Quencher outlet temperature (active constraint)					x	x	x
Y26	Purge flow rate	x						
Y46	Separator liquid toluene mole fraction							x
Y74	Hydrogen mole fraction in stabilizer distillate			x				
Y53	Benzene mole fraction in stabilizer distillate				x			x
Y54	Methane mole fraction in stabilizer bottoms							x
Y55	Benzene product purity (active constraint)	x	x	x		x	x	x
Y56	Benzene mole fraction in benzene column bottoms							x
Y75	Production rate (benzene column distillate flow rate)		x					
Y76	Temperature in an intermediate stage of the benzene column					x		
Y77	Temperature in an intermediate stage of the toluene column					x		
Y78	Toluene mole fraction in toluene column distillate			x				x
Y58	Toluene mole fraction in toluene column bottoms				x			
Y57	Diphenyl mole fraction in toluene column distillate							x

Note: (1) Stephanopoulos (1984); (2) Brognaux (1992), Wolff (1994), Cao et al., Herrmann et al. (2003); (3) Ng and Stephanopoulos (1996); (4) Ponton and Laing (1993); (5) Luyben et al. (1998), Luyben (2002); (6) Konda et al. (2005); (7) This work.

[a] The total number of steady-state degrees of freedom is 13, so there are additional controlled variables, or fixed inputs, which are not clearly specified by some authors.

[b] Y-variables refer to candidates in Table 4.

[c] Active constraints found in this work.

model equations ($g_1 = 0$), and for the active constraints ($g'_2 = 0$), one may formally write $x = x(u, d)$ and $u' = u'(u, d)$ and one may formally write the cost as a function of u and d: $J = J_0(x, u_0, d) = J_0[x(u, d), u'(u, d), u, d] = J(u, d)$. The remaining unconstrained problem in reduced space then becomes

$$\min_u J(u, d), \tag{3}$$

where u represents the set of remaining unconstrained degrees of freedom. This unconstrained problem is the basis for the local method introduced below.

3.1. Degrees of freedom analysis

It is paramount to determine the number of steady-state degrees of freedom because this in turns determines the number of steady-state controlled variables that need to be chosen. To find them for complex plants, it is useful to sum the number of degrees for individual units as given in Table 2 (Skogestad, 2002).

3.2. Local (linear) method

In terms of the unconstrained variables, the loss function around the optimum can be expanded as

$$L = J(u, d) - J_{opt}(d) = \tfrac{1}{2}\|z\|_2^2 \tag{4}$$

with $z = J_{uu}^{1/2}(u - u_{opt}) = J_{uu}^{1/2}G^{-1}(c - c_{opt})$, where G is the steady-state gain matrix from the unconstrained degrees of freedom u to the controlled variables c (yet to be selected) and J_{uu} the Hessian of the cost function with respect to the u. Truly optimal operation corresponds to $L = 0$, but in general $L > 0$. A small value of the loss function L is desired as it implies that the plant is operating close to its optimum. The main issue here is not to find the optimal set points, but rather to find the right variables to keep constant.

Assuming that each controlled variable c_i is scaled such that $\|e_c'\| = \|c' - c_{opt}'\|_2 \leqslant 1$, the worst case loss is given by (Halvorsen, Skogestad, Morud, & Alstad, 2003):

$$L_{max} = \max_{\|e_c\|_2 \leqslant 1} L = \frac{1}{2} \frac{1}{\underline{\sigma}(S_1 G J_{uu}^{-1/2})^2}, \tag{5}$$

where S_1 is the matrix of scalings for c_i:

$$S_1 = diag\left\{\frac{1}{span(c_i)}\right\}, \tag{6}$$

Fig. 2. Typical control hierarchy in a chemical plant.

where $span(c_i) = \Delta c_{i,opt}(d) + n_i$ ($\Delta c_{i,opt}(d)$ is the variation of c_i due to variation in disturbances and n_i is the implementation error of c_i).

It may be cumbersome to obtain the matrix J_{uu}, and if it is assumed that each "base variable" u has been scaled such that a unit change in each input has the same effect on the cost function J (such that the Hessian J_{uu} is a scalar times unitary matrix, i.e., $J_{uu} = \alpha U$), then (5) becomes

$$L_{max} = \frac{\alpha}{2} \frac{1}{\underline{\sigma}(S_1 G)^2}, \tag{7}$$

where $\alpha = \underline{\sigma}(J_{uu})$.

Thus, to minimize the loss, L, $\underline{\sigma}(S_1 G J_{uu}^{-1/2})$ should be maximized or alternatively maximize $\underline{\sigma}(S_1 G)$; the latter is the original minimum singular value rule of Skogestad (2000).

Originally, a MatLab^{TM} model was used to obtain the optimal variation $\Delta c_{opt}(d)$, the steady-state gain matrix G and the Hessian J_{uu}, but in the present version Aspen Plus^{TM} is used instead (see the Appendix for details). The use of a commercial flowsheet simulator like Aspen Plus^{TM} demonstrates the practical usefulness of the approach.

4. HDA process description

In the HDA process, fresh toluene (pure) and hydrogen (97% hydrogen and 3% methane) are mixed with recycled toluene and hydrogen (Fig. 1). This reactant mixture is first preheated in a FEHE using the reactor effluent stream and then to the reaction temperature in a furnace before being fed to an adiabatic plug-flow reactor.

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

$$Toluene + H_2 \rightarrow Benzene + Methane, \tag{8}$$

$$2\,Benzene \rightleftharpoons Diphenyl + H_2. \tag{9}$$
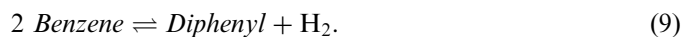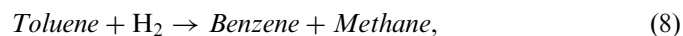
The reactor effluent is quenched by a portion of the recycle separator liquid flow to prevent coking, and further cooled in the FEHE and cooler before being fed to the vapor–liquid separator. Part of the vapor containing unconverted hydrogen and methane is purged to avoid accumulation of methane within the process while the remainder is compressed and recycled to the process. The liquid from the separator is
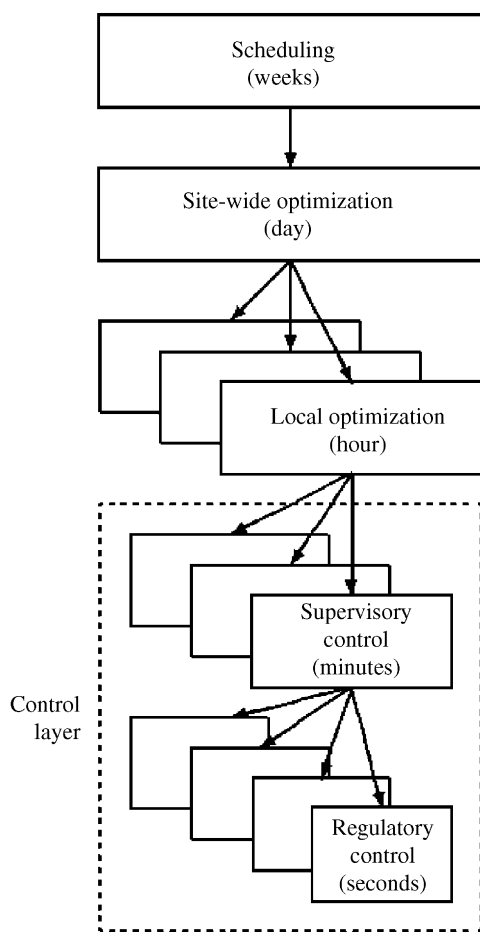
Table 2
Typical number of steady-state degrees of freedom for some process units

Process unit	DOF
Each external feed stream	1 (feedrate)
Splitter	$n - 1$ split fractions (n is the number of exit streams)
Mixer	0
Compressor, turbine, and pump	1 (work)
Adiabatic flash tank	0[a]
Liquid phase reactor	1 (holdup)
Gas phase reactor	0[a]
Heat exchanger	1 (duty or net area)
Columns (e.g., distillation) excluding heat exchangers	0[a] + number of side streams

[a] Add 1 degree of freedom for each extra pressure that is set (need an extra valve, compressor, or pump), e.g., in flash tank, gas phase reactor, or column.

processed in the separation section consisting of three distillation columns. The stabilizer column removes small amounts of hydrogen and methane in the overhead product, and the benzene column takes the benzene product in the overhead. Finally, in the toluene column, unreacted toluene is separated from diphenyl and recycled to the process.

4.1. Details of the HDA process model in Aspen Plus™

The model of the HDA process used in this paper is a modified version of the model developed by Luyben (2002). A schematic flowsheet of the Aspen Plus™ model is depicted in Fig. 3 and the corresponding stream table is shown in Table 3.

Details of this model can be found in Luyben (2002). The main difference between the model in this paper and Luyben's lies on the distillation train. As optimization of the entire plant is difficult for this problem, it has been decided to first optimize the distillation train separately (see Section 5.4.1). The distillation train may then be represented by simple material balances with given specifications. This was implemented in Aspen Plus™ using an Excel™ spreadsheet, and optimization of the remaining plant is then relatively simple.

5. Results

This section describes the self-optimizing control procedure applied to the HDA process model in Aspen Plus™ starting with the degree of freedom analysis.

5.1. Step 1. Degree of freedom analysis

It is considered 20 manipulated variables (Table 6), 70 candidate measurements (the first 70 in Table 4), and 12 disturbances (Table 8). The 20 manipulated variables correspond to 20 dynamic degrees of freedom. However, at steady state there are only 13 degrees of freedom because there are seven liquid levels that need to be controlled which have no steady-state effect. This is confirmed by the alternative steady-state degree of freedom analysis in Table 5.

With 13 degrees of freedom and 70 candidate controlled variables, there are $\binom{70}{13} = 70!/13!57! = 4.7466 \times 10^{13}$ (!) control structures, without including the alternative ways of controlling liquid levels. Clearly, an analysis of all of them is intractable. To avoid this combinatorial explosion, the active constraints are first determined, which should be controlled to achieve optimal operation, and then a local analysis to eliminate further sets is applied.

5.2. Step 2. Definition of optimal operation

The following profit function $(-J)$ (M\$/year) given by Douglas (1988)'s economic potential (EP) is to be maximized:

$$(-J) = (p_{ben}D_{ben} + p_{fuel}Q_{fuel}) - (p_{tol}F_{tol} + p_{gas}F_{gas}$$
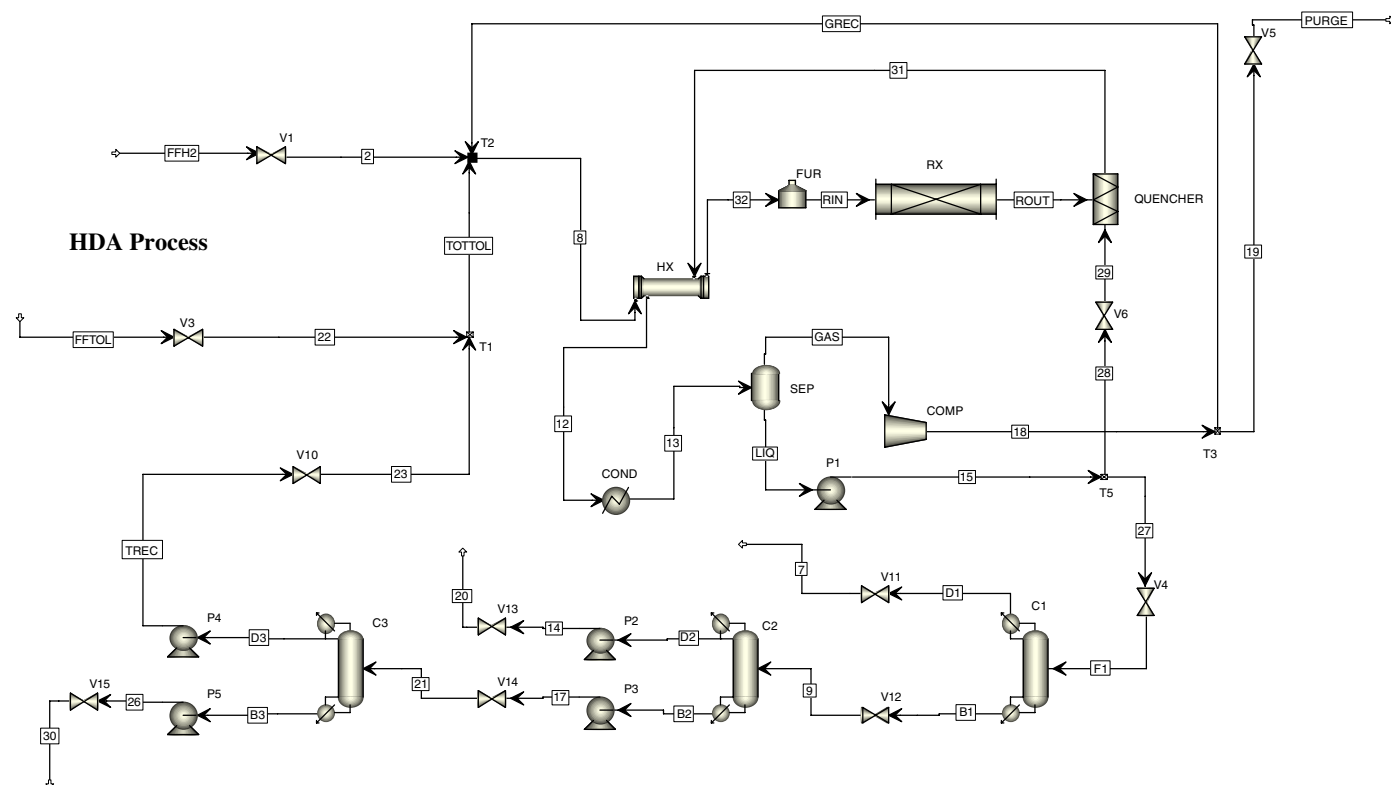$$+ p_{fuel}Q_{fur} + p_{cw}Q_{cw} + p_{pow}W_{pow} + p_{stm}Q_{stm}) \quad (10)$$

Fig. 3. HDA Aspen Plus™ process flowsheet.

Table 3
Stream table for the nominally optimal operating point for the HDA process

Stream	2	7	8	9	12	13	14	15	17	18	19	20	21	22	23	26	27	28	29	30
Mole flow [lb mol/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 [lb mol/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
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 [M Btu/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

Stream	31	32	B1	B2	B3	D1	D2	D3	F1	FFH2	FFTOL	GAS	GREC	LIQ	PURGE	RIN	ROUT	TOTTOL	TREC
Mole flow [lb mol/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 [lb mol/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
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 [M Btu/h]	−7.2524	−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

See Fig. 3 for the stream names.

Table 4
Selected candidate controlled variables for the HDA process (excluding levels)

Y1	Mixer outlet temperature
Y2	FEHE hot side outlet temperature
Y3	Furnace inlet temperature
Y4	Furnace outlet temperature
Y5	Reactor section 1 temperature
Y6	Reactor section 2 temperature
Y7	Reactor section 3 temperature
Y8	Reactor section 4 temperature
Y9	Reactor section 5 temperature
Y10	Reactor section 6 temperature
Y11	Reactor section 7 temperature
Y12	Reactor section 8 temperature
Y13	Reactor section 9 temperature
Y14	Reactor section 10 temperature
Y15	Reactor section 11 temperature
Y16	Quencher outlet temperature (active constraint)
Y17	Compressor inlet temperature
Y18	Compressor outlet temperature
Y19	Separator temperature (active constraint)
Y20	Fresh toluene feed rate (active constraint)
Y21	Fresh gas feed flow rate
Y22	Mixer outlet flow rate
Y23	Quencher outlet flow rate
Y24	Separator vapor outlet flow rate
Y25	Separator liquid outlet flow rate
Y26	Purge flow rate
Y27	Flow of cooling stream to quencher
Y28	Mixer outlet hydrogen mole fraction
Y29	Mixer outlet methane mole fraction
Y30	Mixer outlet benzene mole fraction
Y31	Mixer outlet toluene mole fraction
Y32	Mixer outlet diphenyl mole fraction
Y33	Quencher outlet hydrogen mole fraction
Y34	Quencher outlet methane mole fraction
Y35	Quencher outlet benzene mole fraction
Y36	Quencher outlet toluene mole fraction
Y37	Quencher outlet diphenyl mole fraction
Y38	Separator overhead vapor hydrogen mole fraction
Y39	Separator overhead vapor methane mole fraction
Y40	Separator overhead vapor benzene mole fraction
Y41	Separator overhead vapor toluene mole fraction
Y42	Separator overhead vapor diphenyl mole fraction
Y43	Separator liquid outlet hydrogen mole fraction
Y44	Separator liquid outlet methane mole fraction
Y45	Separator liquid outlet benzene mole fraction
Y46	Separator liquid outlet toluene mole fraction
Y47	Separator liquid outlet diphenyl mole fraction
Y48	Gas recycle hydrogen mole fraction
Y49	Gas recycle methane mole fraction
Y50	Gas recycle benzene mole fraction
Y51	Gas recycle toluene mole fraction
Y52	Gas recycle diphenyl mole fraction
Y53	Benzene mole fraction in stabilizer distillate (active constraint)
Y54	Methane mole fraction in stabilizer bottoms (active constraint)
Y55	Benzene mole fraction in benzene column distillate (active constraint)
Y56	Benzene mole fraction in benzene column bottoms (active constraint)
Y57	Diphenyl mole fraction in toluene column distillate (active constraint)
Y58	Toluene mole fraction in toluene column bottoms (active constraint)
Y59	Mixer outlet pressure
Y60	FEHE hot side outlet pressure

Table 4 (*continued*)

Y61	Furnace inlet pressure
Y62	Reactor inlet pressure (active constraint)
Y63	Reactor outlet pressure
Y64	Separator pressure
Y65	Compressor outlet pressure
Y66	Furnace heat duty
Y67	Cooler heat duty
Y68	Compressor power
Y69	Toluene conversion at reactor outlet
Y70	Hydrogen to aromatic ratio in reactor inlet (active constraint)
Y71	Recycle gas flow rate
Y72	Total toluene flow rate to the reaction section
Y73	Hydrogen mole fraction in the reactor outlet
Y74	Hydrogen mole fraction in stabilizer distillate
Y75	Production rate (benzene column distillate flow rate)
Y76	Temperature in an intermediate stage of the benzene column
Y77	Temperature in an intermediate stage of the toluene column
Y78	Toluene mole fraction in toluene column distillate

Table 5
Steady-state degrees of freedom analysis based on Table 2

Process unit	DOF
External feed streams	$2 \times 1 = 2$
Splitters (purge and quench)	$2 \times 1 = 2$
Compressor	$1 \times 1 = 1$
Adiabatic flash[a] (quencher and separator)	$2 \times 0 = 0$
Gas phase reactor[a]	$1 \times 0 = 0$
Heat exchangers in recycle section[b] (furnace and cooler)	$2 \times 1 = 2$
Heat exchangers in three distillation columns	$3 \times 2 = 6$
Total	13

[a]Assuming no adjustable valves for pressure control (assume fully open valve before separator).
[b]The FEHE (feed effluent heat exchanger) duty is not a degree of freedom because there is no adjustable bypass.

subject to the constraints

1. Minimum production rate:
$$D_{benzene} \geqslant 265\, \text{lb mol/h}. \tag{11}$$

2. Hydrogen to aromatic ratio in reactor inlet (to prevent coking):
$$\frac{F_{H_2}}{(F_{benzene} + F_{toluene} + F_{diphenyl})} \geqslant 5. \tag{12}$$

3. Maximum toluene feed rate:
$$F_{toluene} \leqslant 300\, \text{lb mol/h}. \tag{13}$$

4. Reactor inlet pressure:
$$P_{reactor,in} \leqslant 500\, \text{psia}. \tag{14}$$

Table 6
List of manipulable variables

	Manipulated variable	Status in this work
U1	Fresh toluene feed rate	Steady state
U2	Fresh gas feed rate	Steady state
U3	Furnace heat duty	Steady state
U4	Cooler heat duty	Steady state
U5	Compressor power	Steady state
U6	Purge flow rate	Steady state
U7	Flow of cooling stream to quencher	Steady state
U8	Liquid flow to stabilizer	Dynamic only (level control)
U9	Stabilizer reflux rate	Steady state
U10	Stabilizer distillate rate	Dynamic only (level control)
U11	Stabilizer reboiler duty	Steady state
U12	Stabilizer bottoms rate	Dynamic only (level control)
U13	Benzene column reflux rate	Steady state
U14	Benzene column distillate rate	Dynamic only (level control)
U15	Benzene column reboiler duty	Steady state
U16	Benzene column bottoms rate	Dynamic only (level control)
U17	Toluene column reflux rate	Steady state
U18	Toluene column distillate rate	Dynamic only (level control)
U19	Toluene column reboiler duty	Steady state
U20	Toluene column bottoms rate	Dynamic only (level control)

5. Reactor outlet temperature:

$$T_{reactor,out} \leqslant 1300\,^\circ\text{F}. \tag{15}$$

6. Quencher outlet temperature:

$$T_{quencher,out} \leqslant 1150\,^\circ\text{F}. \tag{16}$$

7. Product purity at the benzene column distillate:

$$x_{D,benzene} \geqslant 0.9997. \tag{17}$$

8. Separator inlet temperature:

$$95\,^\circ\text{F} \leqslant T_{separator,in} \leqslant 105\,^\circ\text{F}. \tag{18}$$

9. Reactor inlet temperature (to get a high enough reaction rate):

$$T_{reactor,in} \geqslant 1150\,^\circ\text{F}. \tag{19}$$

10. In addition, all flows and concentrations must be non-negative.

It is assumed that all by-products (purge, stabilizer distillate, and toluene column bottom) are sold as fuel.
Here,

1. p_{ben}, p_{tol}, p_{gas}, p_{fuel}, p_{cw}, p_{pow}, and p_{stm} are the prices of benzene, fresh toluene feed, fresh gas feed, fuel to the furnace, cooling water, power to the compressor, and steam, respectively (see Table 7 for data);
2. D_{ben}, F_{tol}, F_{gas}, Q_{fur}, Q_{cw}, W_{pow}, and Q_{stm} are the flows of product benzene, fresh toluene feed, fresh gas

Table 7
Economic data for the HDA process based on Douglas (1988)

p_{ben}	9.04\$/lb mol
p_{tol}	6.04\$/lb mol
p_{gas}	1.32\$/lb mol
p_{fuel}	4.00×10^{-6}\$/Btu
p_{cw}	2.34×10^{-8}\$/Btu
p_{pow}	0.042\$/Bhp
p_{stm}	2.50×10^{-6}\$/Btu

(hydrogen) feed, energy fuel to the furnace, cooling water, power to the compressor, and steam, respectively;
3. $Q_{cw} = Q_{cw,cooler} + Q_{cw,stab} + Q_{cw,ben-col} + Q_{cw,tol-col}$;
4. $Q_{stm} = Q_{stm,stab} + Q_{stm,ben-col} + Q_{stm,tol-col}$;
5. Q_{fuel} is the fuel value of the by-product streams F_{purge}, D_{stab}, and $B_{tol-col}$;
6. 8150 h of operation per year.

5.3. Step 3. Identification of important disturbances

The 12 disturbances listed in Table 8 are considered. They include changes in the feed and in the active constraints.

5.4. Step 4. Optimization

5.4.1. Optimization of the distillation columns

The six steady-state degrees of freedom for the three distillation columns should ideally be used to optimize the profit for the entire plant, but as mentioned in Section 4, a simplified recovery model is used for the distillation columns when modeling the entire plant to make the optimization feasible. The error imposed by this is expected to be very small. The distillation columns were therefore optimized separately using detailed models. Assumed internal prices were defined to take care of the interaction with the remaining process. For distillation columns, to avoid product give-away, it is always optimal to have the most valuable product at its constraint. In the present case, there is only one product constraint, namely $x_{D,benzene} \geqslant 0.9997$, and this should always be active as benzene is the main (and most valuable) product. For the remaining distillation products, the optimal conditions were obtained by a trade-off between maximizing the recovery of valuable component and minimizing energy (favored by a large mole fraction). Fig. 4 shows the relations between the reboiler duty and the respective mole fraction of valuable component for each distillation column. When the mole fraction is less than about 10^{-3}, its economic effect on the recovery is small. In general, a good trade-off is achieved if there is a small mole fraction (about 10^{-3} or less) in the "flat" region.

The resulting "optimal" values for the five remaining degrees of freedom (product compositions) are given in Table 9.

Table 8
Disturbances to the process

		Nominal	Disturbance
D1	Fresh toluene feed rate (lb mol/h)	300	285
D2	Fresh toluene feed rate (lb mol/h)	300	315
D3	Fresh gas feed rate methane mole fraction	0.03	0.08
D4	Hydrogen to aromatic ratio in reactor inlet	5.0	5.5
D5	Reactor inlet pressure (psi)	500	520
D6	Quencher outlet temperature (°F)	1150	1170
D7	Product purity in the benzene column distillate	0.9997	0.9960
D8	Benzene mole fraction in stabilizer distillate	1×10^{-4}	3×10^{-4}
D9	Methane mole fraction in stabilizer bottoms	1×10^{-6}	5×10^{-6}
D10	Benzene mole fraction in benzene column bottoms	1.3×10^{-3}	2×10^{-3}
D11	Diphenyl mole fraction in toluene column distillate	0.5×10^{-3}	1×10^{-3}
D12	Toluene mole fraction in toluene column bottoms	0.4×10^{-3}	1×10^{-3}

The reason why the impurities in Table 9 are so small is that the columns in this paper have many stages so that it does not cost much energy to achieve higher purity. This also means that the optimal point is "flat" (which is good) as it is also illustrated by Fig. 5. For the stabilizer column, the separation is very simple and improving the purity has almost no penalty in terms of reboiler duty.

Note that it has been chosen to use product compositions as controlled variables (specifications) for the distillation columns. There are two reasons for this: First, with fixed product compositions only mass balances are needed to represent the distillation columns when simulating the overall process in Aspen Plus^{TM}. Second, compositions are good self-optimizing variables in most cases (e.g., Skogestad, 2000) also note that the product compositions should normally be given in terms of impurity of key components Luyben et al., 1998 as this avoids problems with non-unique specifications.

These six specifications for the distillation columns consumes six steady-state degrees of freedom. There are then $13 - 6 = 7$ degrees of freedom left.

5.4.2. Optimization of the entire process (reactor and recycle)

Optimization with respect to the seven remaining steady-state degrees of freedom was performed using an SQP algorithm in Aspen Plus^{TM}. Fig. 5 gives the effect of disturbances on the profit ($-J$). Note that disturbances D8–D12 in the distillation product compositions have almost no effect. This is expected, since the five distillation composition specifications (Table 9) are in the "flat" region and have practically no influence in the profit. A change in the given purity for the benzene product (disturbance D7) has, as expected, a quite large effect. The detailed results for disturbances D1 to D7 are summarized in Table 10.

From Table 10, five constraints are optimally active in all operating points:

Y16. Quencher outlet temperature (upper bound).
Y19. Separator temperature (lower bound).

Y20. Fresh toluene feed rate (upper bound).
Y62. Reactor inlet pressure (upper bound).
Y70. Hydrogen to aromatic ratio in reactor inlet (lower bound).

As expected, the benzene purity at the outlet of the process is kept at its bound for economic reasons. Moreover, fresh feed toluene is maintained at its maximum flow rate to maximize the profit. The separator inlet temperature is kept at its lower bound in order to maximize the recycle of hydrogen and to avoid the accumulation of methane in the process. Luyben's rule of keeping all recycle loops under flow control is not economically optimal in this process since it is best to let the recycle flow fluctuates.

All the five active constraints should be controlled to achieve optimal operation (Maarleveld & Rijnsdorp, 1970). Consequently, the remaining number of unconstrained degrees of freedom is 2 ($7 - 5 = 2$). This reduces the number of possible sets of controlled variables to $\binom{59}{2} = 59!/2!57! = 1711$, where the number 59 is found by subtracting from the initial 70 candidate measurements in Table 4 the six distillation specifications and five active constraints of the reactor and recycle process. However, this number is still too large to consider all alternatives in detail.

The next step uses local analysis to find promising candidate sets of two controlled variables.

5.5. Step 5. Identification of candidate controlled variables—local analysis

A branch-and-bound algorithm (Cao, Rossiter, & Owens, 1998) for maximizing the minimum singular value of $S_1 G J_{uu}^{-1/2}$ and $S_1 G$ was used to obtain the candidate sets of controlled variables (details on the calculation of S_1, G, and J_{uu} are given in the Appendix). Note that the steady-state gain matrix G is obtained with the five active constraints fixed at their optimal values. The minimum singular value of the 16 candidate sets are given
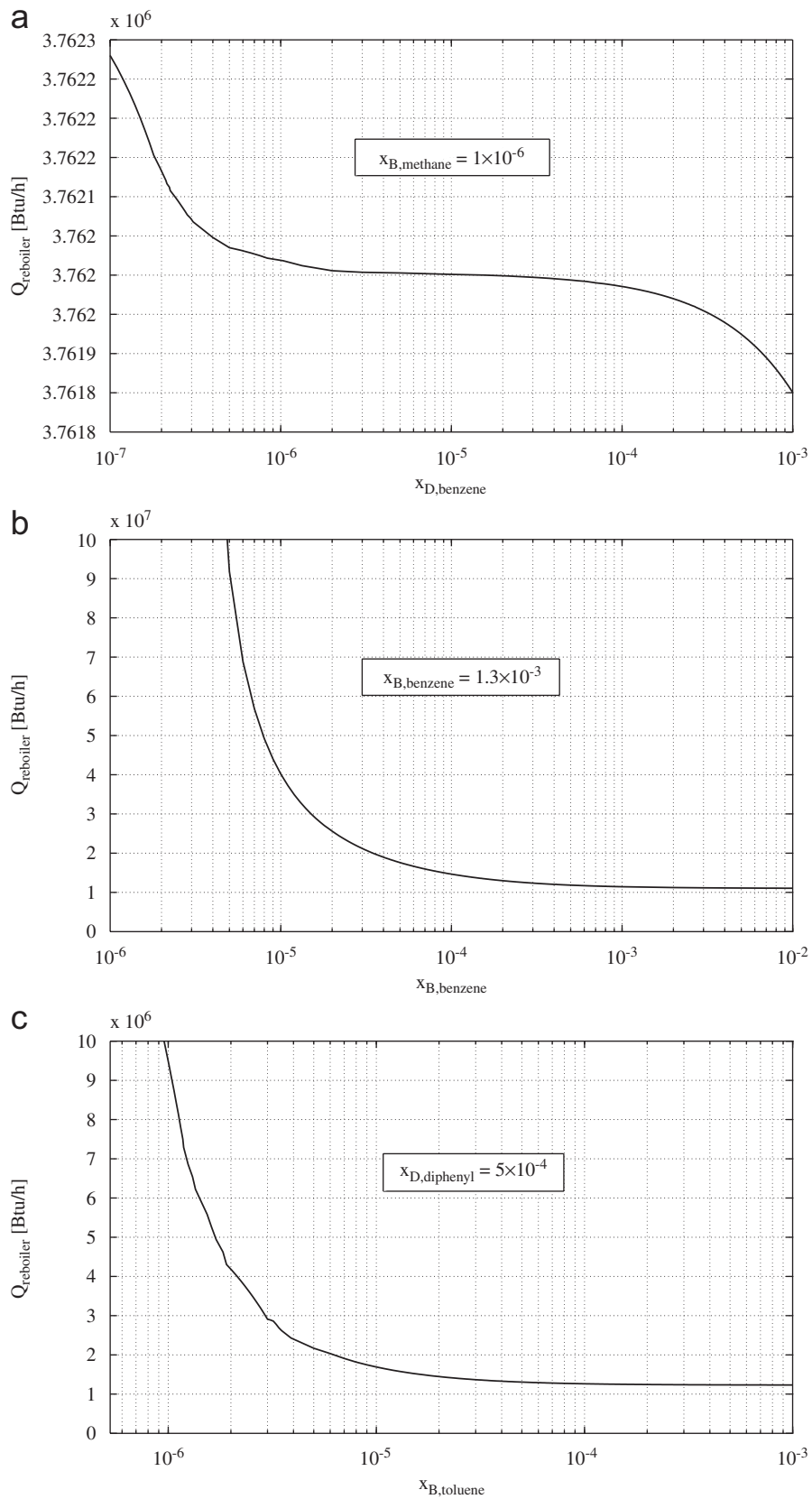
Fig. 4. Typical relations between reboiler duty and product purity: (a) stabilizer distillate; (b) benzene column bottoms; (c) toluene column bottoms.

in Table 12 and the 15 (out of 59) measurements involved in the 16 sets are listed in Table 11, with their nominally optimal values, the optimal variations, and assumed implementation errors (i.e., the total span is the sum of the optimal variation and the implementation error). From Table 12 it is seen that the same best 10 sets were identified for both criteria of maximizing $\underline{\sigma}(S_1 G J_{uu}^{-1/2})$ and $\underline{\sigma}(S_1 G)$. Also note the 10 best sets all include the reactor feed inert (methane) mole fraction (Y29) plus another composition (of benzene, toluene, or diphenyl) as controlled variable. The remaining six sets (XI–XVI) are some other common choices that are reasonable to consider, including inert (methane) recycle concentration (Y49), the furnace outlet temperature (Y4), the purge rate (Y26), and the compressor power (Y68). Set XII with fixed furnace outlet temperature (Y4) and inert (methane) concentration (Y49) is similar to the structure of Luyben (2002), although Luyben does not control all the active constraints.

Table 9
Specifications for distillation columns

Column/specification	Value	Comment
Stabilizer		
Y53 $x_{D,benzene}$	1×10^{-4}	(A)
Y54 $x_{B,methane}$	1×10^{-6}	(B)
Benzene column		
Y55 $x_{D,benzene}$	0.9997	Active constraint
Y56 $x_{B,benzene}$	1.3×10^{-3}	(A)
Toluene column		
Y57 $x_{D,diphenyl}$	0.5×10^{-3}	(C)
Y58 $x_{B,toluene}$	0.4×10^{-3}	(A)

(A) Determined by trade-off between energy usage and recovery (Fig. 4).
(B) $x_{B,methane}$ should be small to avoid methane impurity in distillate of benzene column.
(C) Diphenyl should not be recycled because it may reduce the available production rate if there is bottleneck in the plant.

5.6. Step 6. Detailed evaluation of the loss

The next step is to evaluate the loss for the promising sets of controlled variables in Table 12 by keeping constant setpoint policy when there are disturbances and/or implementation errors. The computations were performed on the nonlinear model in Aspen Plus™ for disturbances D1 through D7 (the losses for disturbances D8 to D12 are negligible, as discussed above) and the results are shown in Table 13.

As seen in Tables 12 and 13, the results from the linear and nonlinear analysis give the same ranking for the sets of candidate controlled variables, with the best sets having both the largest value of $\underline{\sigma}(S_1 G_{2 \times 2} J_{uu}^{-1/2})$ (as one would expect from (7)) and the lowest value of the actual loss. Note from Table 13 that all the structures were found to be feasible for the given disturbances.

Compared to the controlled structure proposed by Luyben (2002) the sets of controlled variables selected by the self-optimizing control approach give smaller economic losses. This is because the steady-state nominal point of Luyben (2002) is not optimal: it gives a profit of $(-J) = 3.955.2 \, \text{k\$/year}$, which is about 16% smaller than the nominally optimal operation (4693.4 k\$/year) found in this paper. First, Luyben (2002) considers only 12 degrees of freedom at steady state as compressor power is assumed fixed. Second, Luyben (2002) does not control all the active constraints in the process. Specifically, the hydrogen-to-aromatics ratio, which is an important variable in the process and should be kept at its lower bound of 5 (see (12)), is not controlled. Instead, Luyben (2002) controls inert (methane) composition in the recycle gas and reactor inlet temperature which results in large economic losses.

6. Discussion

In this paper, it has been considered the standard operation mode with given feed rate (indirectly, through an upper bound on toluene feed). Yet another important
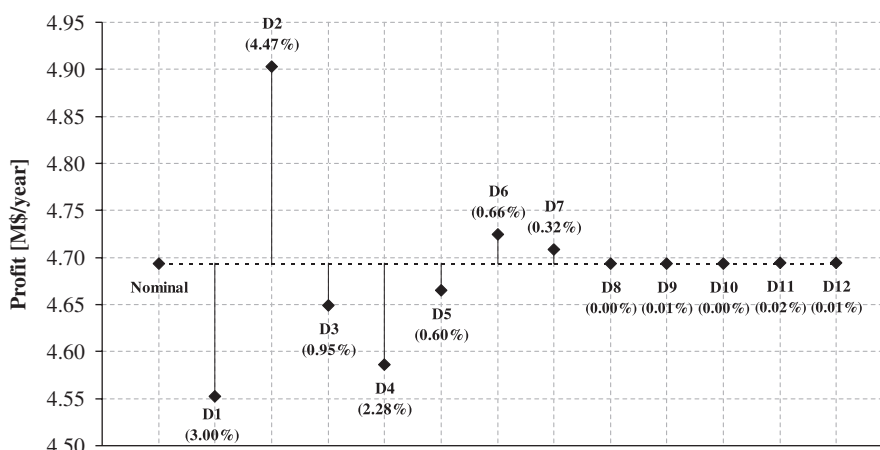

Fig. 5. Effect of disturbances (see Table 8) on optimal operation. Percentages in parentheses are changes with respect to the nominal optimum.

Table 10
Effect of disturbances on optimal values for selected variables

Variable	Unit	Nominal	D1	D2	D3	D4	D5	D6	D7
Profit	k\$/year	4693.4	4552.7	4903.2	4649.0	4585.6	4664.7	4722.5	4705.5
Y4	°F	1201.15	1198.20	1202.89	1204.66	1206.66	1196.44	1201.88	1199.33
Y15	°F	1277.21	1273.64	1279.25	1277.71	1279.65	1272.25	1276.89	1274.99
Y16[a]	°F	1150	1150	1150	1150	1150	1150	1170	1150
Y19[a]	°F	95	95	95	95	95	95	95	95
Y20[a]	lb mol/h	300	285	315	300	300	300	300	300
Y21	lb mol/h	446.59	431.29	470.33	476.29	460.03	446.75	444.73	445.46
Y26	lb mol/h	445.27	429.78	468.91	474.95	458.44	445.27	443.23	443.90
Y28		0.3558	0.3548	0.3577	0.3454	0.3703	0.3558	0.3526	0.3560
Y29		0.5729	0.5742	0.5707	0.5854	0.5622	0.5730	0.5767	0.5727
Y45		0.8721	0.8671	0.8703	0.8667	0.8792	0.8683	0.8692	0.8662
Y46		0.0491	0.0544	0.0511	0.5419	0.4534	0.5322	0.5205	0.5549
Y49		0.6710	0.6717	0.6691	0.6803	0.6534	0.6708	0.6737	0.6705
Y53[b]		1×10^{-4}	1×10^{-4}	1×10^{-4}	1×10^{-4}	1×10^{-4}	1×10^{-4}	1×10^{-4}	1×10^{-4}
Y54[b]		1×10^{-6}	1×10^{-6}	1×10^{-6}	1×10^{-6}	1×10^{-6}	1×10^{-6}	1×10^{-6}	1×10^{-6}
Y55[b]		0.9997	0.9997	0.9997	0.9997	0.9997	0.9997	0.9997	0.996
Y56[b]		1.3×10^{-3}	1.3×10^{-3}	1.3×10^{-3}	1.3×10^{-3}	1.3×10^{-3}	1.3×10^{-3}	1.3×10^{-3}	1.3×10^{-3}
Y57[b]		5×10^{-4}	5×10^{-4}	5×10^{-4}	5×10^{-4}	5×10^{-4}	5×10^{-4}	5×10^{-4}	5×10^{-4}
Y58[b]		4×10^{-4}	4×10^{-4}	4×10^{-4}	4×10^{-4}	4×10^{-4}	4×10^{-4}	4×10^{-4}	4×10^{-4}
Y62[a]	psi	500	500	500	500	500	520	500	500
Y68	hp	454.39	443.20	474.93	473.22	485.53	564.09	460.82	455.41
Y70[a]		5.0	5.0	5.0	5.0	5.5	5.0	5.0	5.0

[a] Active constraints.
[b] Distillation specification.

Table 11
Candidate controlled variables with small losses in local analysis

Variable	Name	Nominal optimal	Optimal variation	Implementation error	Total span
Y4	Furnace outlet temperature	1201.15	5.52	60.06	65.57
Y26	Purge flow rate	445.27	29.73	22.26	52
Y29	Mixer outlet inert (methane) mole fraction	0.5729	0.0125	0.0001	0.0126
Y30	Mixer outlet benzene mole fraction	0.0091	0.000068	0.0001	0.000168
Y35	Quencher outlet benzene mole fraction	0.0996	0.0059	0.0001	0.006
Y36	Quencher outlet toluene mole fraction	0.0031	0.0007	0.0001	0.0008
Y37	Quencher outlet diphenyl mole fraction	0.0033	0.0003	0.0001	0.0004
Y40	Separator overhead vapor benzene mole fraction	0.0107	0.000081	0.0001	0.000181
Y45	Separator liquid benzene mole fraction	0.8721	0.0071	0.0001	0.0072
Y46	Separator liquid toluene mole fraction	0.0491	0.0071	0.0001	0.0072
Y47	Separator liquid diphenyl mole fraction	0.0318	0.0023	0.0001	0.0024
Y49	Gas recycle inert (methane) mole fraction	0.6710	0.0175	0.0001	0.0176
Y50	Gas recycle benzene mole fraction	0.0107	0.000081	0.0001	0.000181
Y68	Compressor power	454.39	109.69	4.54	114.23
Y69	Toluene conversion at reactor outlet	0.9124	0.0076	0.01	0.0176

mode of operation is maximum throughput, which occurs when prices are such that it is optimum to maximize production.

Another point to stress is the consistency of the results with the empirical arguments made by Douglas (1988) which is that impurity levels should be controlled in order to avoid build-up of inerts in the system that eventually makes the process inoperable. This was accomplished when the inert (methane) concentration leaving the mixer (controlled variable Y29 above) was chosen to be controlled.

The final evaluation and selection of the control structure involves the selection of sets of controlled variables with acceptable loss, such as those shown in Table 13. These are then analyzed to see if they are adequate with respect to the expected dynamic control performance (input–output controllability). This, in addition to maximum throughput case and design of the regulatory layer, will be the focus of part II of the series where a dynamic analysis is used. No constraint on the stabilizer column condenser temperature was included. In practice one should avoid the cryogenic temperature on the

Table 12
Local analysis: minimum singular values for candidate sets of unconstrained controlled variables

Set	Variable 1	Variable 2	$1000 \times \underline{\sigma}(S_1 G_{2\times2})$	$1000 \times \underline{\sigma}(S_1 G_{2\times2} J_{uu}^{-1/2})$
Full[a]			6.2523	6.3436
I	Y29	Y36	2.2942	2.3331
II	Y29	Y69	2.2523	2.2761
III	Y29	Y45	2.2133	2.2545
IV	Y29	Y46	2.2102	2.2398
V	Y29	Y40	2.2072	2.2201
VI	Y29	Y50	2.1981	2.2199
VII	Y29	Y35	1.8452	1.8247
VIII	Y29	Y47	1.8344	1.8044
IX	Y29	Y30	1.7855	1.7851
X	Y29	Y37	1.7149	1.6825
XI	Y4	Y26	1.2439	1.2815
XII	Y4	Y49	0.2008	0.1957
XIII	Y26	Y49	1.3352	1.2902
XIV	Y4	Y68	0.1198	0.1201
XV	Y26	Y68	1.2196	1.2785
XVI	Y49	Y68	0.0198	0.0201

[a]With all 59 variables: $G_{full} = G_{59\times2}$.

Table 13
Loss in k\$/year caused by disturbances and implementation errors for the alternative sets of controlled variables from Table 12

Set	D1	D2	D3	D4	D5	D6	D7	n_{y1}[a]	n_{y2}	Average
I	70.40	5.37	14.41	4.57	12.85	12.57	9.66	5.33	3.37	15.39
II	86.16	10.91	25.78	18.98	27.11	13.31	17.77	5.33	33.58	26.55
III	100.01	13.22	35.40	26.66	55.52	13.60	21.82	5.33	10.92	31.39
IV	118.45	16.04	38.22	39.52	60.30	37.98	43.17	5.33	4.57	40.40
V	136.60	16.92	48.46	53.16	69.07	41.48	78.59	5.33	16.17	51.75
VI	143.54	19.70	48.47	58.17	79.12	51.23	106.07	5.33	12.02	58.18
VII	149.94	22.01	58.42	67.39	79.27	64.68	112.07	5.33	12.05	63.46
VIII	140.83	23.40	59.81	85.09	81.44	76.60	118.25	5.33	12.03	66.97
IX	150.37	25.25	67.70	96.31	83.30	85.55	136.07	5.33	3.40	72.59
X	151.61	31.07	70.11	99.91	88.29	106.15	141.18	5.33	4.19	77.54
XI	163.29	43.10	97.70	133.87	104.15	127.00	150.84	243.97	176.86	137.87
XII[b]	188.09	55.86	125.35	169.45	128.55	151.18	178.46	243.97	25.46	140.71
XIII	162.78	37.49	88.99	144.73	128.55	124.42	148.47	176.86	25.46	115.31
XIV	193.80	61.99	131.70	157.08	137.96	154.38	188.23	243.97	302.04	174.57
XV	179.48	43.24	89.21	183.32	155.35	122.78	159.47	176.86	302.04	156.86
XVI	233.26	188.87	259.70	364.56	186.68	171.82	224.66	25.46	302.04	217.45

[a]n_{y1} and n_{y2} are the implementation errors associated with each variable in the set.
[b]This is similar to the structure of Luyben (2002), but with control of active constraints.

overhead methane product from the stabilizer column by allowing for a larger benzene contents. However, the flow rate of this distillate stream is very small so this would not change the results of this paper.

7. Conclusions

This paper has discussed the selection of controlled variables for the HDA process using the self-optimizing control procedure. The large number of variable combinations makes it a challenging problem, and a local (linear) analysis based on the SVD of the linearized model of the plant was used to select good candidate sets for the unconstrained controlled variables. Specifically, 16 candidate sets were found to be suitable to select from. Aspen Plus™ proved to be a valuable tool for the evaluation of self-optimizing control structures for large-scale processes.

Appendix A

This appendix outlines the steps taken to compute the steady-state linear matrix G and the Hessian J_{uu} of the unconstrained inputs as well as the optimal variation for the candidate variables $span(c_i)$.

Optimization of the entire plant in Aspen Plus™ was used to identify the active constraints. For the local analysis (calculation of $\Delta c_{opt}(d)$, G, and J_{uu}), several auxiliary blocks were used, including a calculator block to compute the value

of the cost function; design specification blocks were used to close feedback loops for the active constraints; and a sensitivity block was used to perform auxiliary computations. Finally, Aspen Plus^{TM} was used to compute the "nonlinear" loss imposed by keeping the selected sets of controlled variables constant at their setpoints.

A.1. Calculation of the linear matrix G and the Hessian J_{uu}

G and J_{uu} are calculated with respect to the nominal optimal operating point, i.e., for $d = 0$. The matrix G is calculated by the usual approximation:

$$\frac{\partial c_i(u)}{\partial u_j} = \lim_{h \to 0} \frac{c(u + e_j h) - c(u)}{h_j}, \tag{20}$$

where $i = 1, \ldots, n_c$ is the index set of candidate variables, $j = 1, \ldots, n_u$ is the index set of unconstrained inputs, h is the vector of increments for each input u_j, and $e_j = [000 \ldots 1 \ldots 0]$ is the zero vector except for the j-element which is 1.

In Aspen Plus^{TM}, $c(u)$ and $c(u + e_j h)$ are evaluated by adding the step $e_j h$ to the vector u for each input j in a calculator block and then taken the resulting vectors to a MatLab^{TM} code that numerically calculates the terms $G_{ij} = \partial c_i(u)/\partial u_j$.

The Hessian J_{uu} is evaluate similarly. The following simple approximation was used:

$$\frac{\partial^2 J(u)}{\partial u_j^2}|_i$$
$$= \lim_{h \to 0} \frac{J(u + E_{ii}h + E_{jj}h) - J(u + E_{ii}h) - J(u + E_{jj}h) + J(u)}{[hh^T]_{ij}}, \tag{21}$$

where E_{ij} is the zero matrix except for the ij-element which is 1. The several functions of J in the denominator of (21) are evaluated in a Calculator block in Aspen Plus^{TM} and taken to MatLab^{TM} for the numerical calculation of $H_{ij} = \partial^2 J(u)/\partial u_j^2|_i$.

A.2. Optimal variation for the candidate variables

The optimal variation for the candidate variables ($span(c_i)$) is used to scale the linear matrix G obtained by linearizing the nonlinear model of the process. In this work, it was used direct calculations from the nonlinear model of the HDA process in Aspen Plus^{TM}.

For each candidate controlled variable c_i, it is obtained its maximum optimal variation $\Delta c_{i,opt}(d)$ due to variation in disturbances. From the nonlinear model, the optimal parameters (inputs and outputs) for various conditions (disturbances and operating points) are computed. This yields a "lookup" table of optimal parameter values as a function of the operating conditions. From this, one can identify

$$\Delta c_{i,opt}(d) = \max_{j \in D}(|c_{i,opt}^j - c_{i,opt}^{nom}|), \tag{22}$$

where D is the set of disturbances, $c_{i,opt}^j$ is the optimal value of c_i due to disturbance j and $c_{i,opt}^{nom}$ is the nominal optimal value of c_i.

For each candidate controlled variable c_i, its expected implementation error n_i (sum of measurement error and control error) is obtained. Then, the candidate controlled variables are scaled such that for each variable i the sum of the magnitudes of $\Delta c_{i,opt}(d)$ and the implementation error n_i is similar, which corresponds to selecting the scaling

$$span(c_i) = \Delta c_{i,opt}(d) + n_i. \tag{23}$$

Then, the scaling matrix S_1 can be computed as $S_1 = diag\{1/span(c_i)\}$. All data were retrieved from nonlinear simulations in Aspen Plus^{TM} and the calculations were performed in a dedicated MatLab^{TM} code.

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