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Optimal Plantwide Process Control Applied to the Tennessee Eastman Problem

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ABSTRACT: A new plantwide control (PWC) structure procedure is proposed and tested on the Tennessee Eastman (TE) problem. The goal of developing a plantwide control procedure is to enable control engineers to design a process control structure that will run the plant safely and achieve the economic objective of the process. The control structure developed in this study utilizes the self-optimizing control strategy of Skogestad [*Comput. Chem. Eng.* **2004**, *28*, 219−234], with an emphasis on elucidation of lower layers in the bottom-up section. It is then tested on the TE problem. For the TE problem, the control variables used for optimization are the stripper steam valve, recycle valve, agitation rate, reactor temperature, reactor pressure, reactor level, and composition B in purge. The control structure developed achieved all the control objectives at each stage including self-optimizing control. The procedure uses mathematical tools such as the generalized relative gain array (GRGA) coupled with steady state simulation.

■ INTRODUCTION

Since the late 1970s, research studies in the chemical process industries (CPI) have focused on improvement in energy efficiency, cost efficiency, and reduction in environmental impact of chemical processes. These have led to highly integrated processes resulting in increased complexity of the plants. This has necessitated also changes in designing of process control for the plants. Thus, the control engineer does not have the luxury of setting up the overall control structure for the plant by summing up individual unit operation control configurations as was the case previously. A holistic approach presently known as "plantwide control" (PWC) is now in vogue. By looking at processes as a whole, the degree of freedom to pair control and manipulative variables increases and correspondingly finding an optimal control design has become more difficult.

The genesis of the plantwide control (PWC) studies can be traced to the pioneering work of Buckley,[1]who developed process control structure based on throughput (material) balances. A major boost in PWC studies in the past 20 years can be referenced to the formulation of a "real" process plant control problem,[2] commonly known as the Tennessee Eastman (TE) problem. The TE problem made it possible for PWC researchers to test their various methodologies. Since then many other "real" problems have been studied. Vasuderan et al.[3] has a table of "real" processes that have PWC developed and tested up to 2009. These PWC methodologies can be classified as either heuristic,[4] mathematics based,[5] or integrated framework.[6] The integrated framework (IF) consists of heuristic coupled with simulation (steady state and dynamic) studies. All these approaches result in different ways of achieving decentralized PWC structure to address all the major process control problems such as the effect of recycles and energy integration.

Dynamic theory, constrained optimization, and unconstrained optimization of systems are incorporated in one form or another to develop a PWC structure under the mathematics-based approach. Unfortunately, this approach is very difficult to formulate for a complete process plant, resulting in very intensive computation. Many studies employing the mathematics-based approach try to achieve design by reducing the complexity of the formulation and solution computation. The branch and bound (BAB) algorithm[7] produces a global ranking of all possible inputs and outputs pairing. This results in an efficient stabilizing control, producing decentralized proportional controllers. In a modified branch and bound (BAB)[8] method, the branch pruning involves both upward (the subset size gradually increasing) and downward directions simultaneously. According to this approach, the method greatly reduces the total number of subsets, resulting in efficient handling of large-scale processes. In another study[9] the optimal controller gain matrix from the solution of the output optimum control problem is split into feedback and feed forward parts. From these parts, a decentralized PWC system structure is formulated. This is known as model predictive control (MPC). This involves solving by mixed integer linear programming (MILP)[10] a relationship comprising relative gain array (RGA), internal model control (IMC) concept, and cost coefficients computed from Parseval's theorem.. This result is then used to develop PWC structure.

Some other studies[11,12] developed PWC structure by the combination of the heuristic and mathematics-based approaches. A control structure with self-optimizing characteristics is formulated[13] by selecting control variables as a linear combination of measurements achieved through the minimization of deviation from optimal value. In a recent mathematics-based approach,[14] an extension of the theoretical concept of nonsquare relative gain array (NRGA) is coupled with the generalized relative disturbance gain (GRDG) to develop a PWC system architecture that can be applied to any process where only plant steady state information is available.

In a comparative study,[3] the heuristic, mathematics-based, and integrated framework methodologies are tested on a vinyl

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acetate monomer plant. The three approaches gave good PWC structures, but the mathematics-based (self-optimizing[11] and the integrated framework[6]) methodology produced more robust control structure compared to the heuristic.[4]

It has been suggested[5] that there are essentially two approaches to PWC design. One is based on experience (heuristic rules), generally referred to as the process oriented approach. The second is known as structural decision consisting of two layers. The first layer deals with the decomposition of a large control problem into smaller subproblems. The control structure design serves as the second layer. The process oriented philosophy is based on a time scale. According to this approach, the PWC can be broken down into the following sequence based on the time element required (involved): scheduling (weeks), sitewide (global) optimization (days), local (localized) optimization (hours), supervisory control (minutes), and regulatory control (seconds). Often, PWC studies have focused only on the last three layers. Within this process oriented methodology, the heuristics developed may either be top-down, bottom-up, or a combination of both. In the top-down approach, control objectives are defined and searches for degrees of freedom are carried out to satisfy the objectives. In the bottom-up sequence, important control variables for the stabilization of the process are determined.

Utilizing the structural decision procedure, the following steps are followed to achieve a good control structure design: selection of control variables or control outputs; choice of manipulative variables; selection of measurement variables; formulation of control configuration (i.e., control pairings on measurement, pairing of control variables to manipulative variables), with the controllers able to be assigned hierarchical (vertical) and horizontal (decentralized) control; and finally, choice of controller type (PID, LQG, decoupler, etc). The second aspect of the structural decision is the process decomposition. This procedure can be based on process units, process structure, control objectives, or even on time scale. In a study[15] employing the structural decision methodology, the following sequence is suggested: decompose the plant into individual unit operations, develop the best control structure for each unit, combine these units into a complete one for the plant, and, finally, eliminate conflicts between each unit through adjustment. This approach may not be very effective for present-day highly integrated plants.

Another approach to decomposition is the hierarchical, patterned along the five step sequence of process design.[16] In a study[17] that employed this procedure, design process level 1 is changed to a preliminary analysis step while levels 4 and 5 are combined to form a detail design stage. The hierarchical sequence (also known as tiered sequence) is a bottom-up method. The tiered sequence involves the following:[18] inventory and production rate control, product specification control, equipment and operating constraint control, and economic performance control. In the study,[18] it is observed that an effective control will require that the production rate manipulator be on the "primary process path". Also, the control structure has to be "self-consistent". The "primary process path" is defined as one that directly affects the product rate and quality. Often, this path runs through the reactor (if there is one in the process) to the separation systems and finally to the product stream. Another criterion from the study[17] states that a control structure is "self-consistent", if inventory control actions are not in conflict with the product quality control or product rate control. In another tiered sequence study,[19] nine levels are developed and used. An important aspect of this study is that the control structure is built based on heuristics applied to the nine steps. Also, Skogestad[11] developed an eight point sequence using both top-down and bottom-up approaches to design PWC structure. An important fact is that it is mathematics-based.

In a hierarchical decomposition based on time scale, a four-stage loop speed control strategy is formulated.[21] The four stages are as follows:

i. design of inner cascade loops
ii. design of basic decentralized system without product rate and quality control loops
iii. closing of loops for product rate and quality controls
iv. implementation of higher level control such as model predictive control (MPC) or optimization

Plantwide Control Structure for TE Problem. Almost all these methodologies have been applied to the TE problem. A brief summary of these studies is thus presented.

Lyman et al.[22] utilize the primary process path[18] approach to set up the PWC structure for the TE problem. They first identified the primary path for the throughput manipulator. The primary path is from raw materials to the reactor, condenser, stripper, and finally product flow. Next, they considered inventory variables to be controlled which included columns and reactor pressures, reactor level, separator level, and stripper level. Inventory control variables were then assigned in a "self-consistent structure" fashion. They proposed four control structures and eventually decided to control the production rate with the condenser CW, reactor temperature with the reactor CW, the level with C feed, agitation rate, recycle flow rate with the recycle valve, compositions of A, D, and E in the reactor feed with A, D, and E feeds, composition of B in the purge with the purge rate, and composition of E in product with stripper steam which first controls the stripper temperature and consequently slave controls the composition of E. Using simple decentralized control, their control structure stabilized the TE process under all the specified disturbances and performed all the specified set point changes. Although they discuss process operating cost, they did not implement control variables at optimal steady state condition.

Following the hierarchical decomposition procedure based on loop speed, McAvoy and Ye[21] closed flow loops on the four feed streams, purge stream, stripper bottom, separator bottom, and stripper steam flow. Condenser and reactor cooling water temperatures were also closed.

At stage 2, decentralized control configurations were formed with the assumption that analyzers were not available. Control variables used in stage 2 were subject to the constraints set in stage 3, where product flow or composition manipulators were used. Level loops were closed first since they were the most important. The manipulative variable candidates for stripper level control were product flow set point and steam flow set point. The candidates for reactor level control are cooling water temperature set point and E feed set point. Thus, there were four level control schemes. Eventually, feed E was used to control the reactor level, and stripper bottom flow was used to control the stripper level. For this partially closed system, three 6×6, eighteen 5×5, and fifteen 4×4 systems were considered with the control variables that seemed to be arbitrarily chosen. RGA,[23] Niederlinsk index,[24] and linear valve saturation analysis were employed to screen four possible design scenarios. In the final structure, feed C was used to control the product rate, D and E feeds controlled the product quality ratio between % G and % H, E feed controlled the reactor level, stripper bottom flow set point controlled the stripper level, and separator bottom flow set point controlled the separator level.

Luyben et al.[4,19] applied the nine level approach: In level 3 (energy inventory control), the reactor cooling water was used to control the reactor temperature. In level 5 (product quality and safety control) stripper steam flow was used to control the stripper temperature and also "slave" control product quality. In level 6 (inventory control), the largest feed (C feed) controlled the reactor pressure, D and E feed ratio controlled the reactor level, condenser CW flow controlled the separator level, and separator bottom flow controlled the stripper level. In level 7 (component balances), feed A set point controlled A% in purge and the purge rate controlled B% in purge. Finally, in level 9 the recycle valve position and agitation rate were set at their constraints and also the set points of the reactor pressure, reactor level, separator temperature, stripper temperature, flow of E and D feeds, and compositions of A and B in purge were set.

Ricker[25] identified six control variables that must be controlled, and these included production rate, mole % G in the product, reactor pressure, reactor level, separator level, and stripper level. Based on the optimization study, the production rate was controlled with ratio of the D to E feeds. The following parameters were set at their minimum values: recycle valve position, steam valve position, and reactor level. The controls were reactor level with condenser CW temperature, concentrations of A and A + C with A and C feeds in excess such that D feed became the limiting reactants, reactor pressure with purge valve, separator level with separator bottom flow, and stripper level with stripper bottom flow. Furthermore, override controls were implemented.

Larrson et al.[20] applied Skogestad's[11] self-optimizing design procedure on the TE process. The identified active constraint control variables were reactor pressure, reactor level, recycle valve, stripper steam valve, and agitation rate. The unconstrained control variables were reactor temperature, recycle flow, and % C in purge. The resulting PWC structure is as follows: control the production rate with C feed, separator level with separator liquid flow, stripper level with stripper liquid flow, and reactor cooling water with reactor cooling water temperature. Applying the RGA criterion led to pairing of reactor level with E feed flow, reactor pressure with purge flow, reactor temperature with reactor cooling water temperature set point, % C in purge with A feed flow, recycle flow with condenser cooling water flow, and product ratio with D feed.

■ PRESENT STUDY

This study's design procedure can be categorized as "hierarchical decomposition based on control objectives", similar to the procedures developed by Luyben et al.[4] and Skogestad.[11] At each design stage, new design decisions or control structure settings are implemented on top of the control structure already developed in the previous stage.

This work develops a methodology for decomposition and coordinating the layers in the bottom-up portion of the PWC design procedure.[11] This procedure differs from Luyben et al.'s[4] at which stage to set product rate and quality control and it is not heuristic based. Another difference is that the control variables for optimization are selected first and are reserved until the last stage unless they are significant for stabilization. Also, this is essentially a mathematics-based approach coupled with some simulation.

Similar to Skogestad's[11] design approach, this is a top-down and then a bottom-up procedure. However, the main difference between the two is that in this proposed method emphasis is not placed on how to select control variables that can minimize operating cost. The cost of production is usually very difficult to estimate during the design stages. As has been pointed out by Luyben,[26] the predictive success of marketing analysts is usually lower than that of a meteorologist's success at forecasting tomorrow's weather or a stock market analyst's success at predicting what the stock market will do in the next year. Thus, control variables selected based on the minimization of the operating cost may not be the best or most effective. With this in mind, step 1 in this proposal is similar to the combined steps 1, 2, and 3 of Skogestad.[11] The steps developed in this study also focus more on stabilization of the process than optimization. As part of its philosophy, one should sacrifice a cost variable if it is effective in stabilizing a process. Otherwise, steps 2 and 3 are similar to step 5 of Skogestad and step 8 is equivalent to steps 6 and 7 of Skogestad. Finally, the throughput manipulator is also set at a later stage of the process.

The proposed approach is also similar to the integrated framework (IF) developed by Murthy Konda et al.[6] The major differences are that, in this proposal, mathematics-based analysis is coupled with steady state simulation while the IF is heuristics coupled with simulation (both steady state and dynamics). The proposed design approach can be applied to all processes with or without known process dynamic information. For processes with known dynamic information, the mathematics method would be used. However, for processes with no known dynamic information (black box), steady state simulation would be used. Steady state simulation is performed by varying operating conditions and the variables that have unbounded output responses are considered for stabilization.

Proposed PWC Structure Design Methodology. The design sequence involves nine (9) steps that are essential procedures to decomposition and coordination of layers of control system design:

Step 1. Identify Cost Variables. Cost variables are identified based on operating cost function. Often the economic objective function, which may consist of the total purge cost (including material loss through purge), total product stream cost, raw materials and utilities cost, and total product stream revenue, is analyzed or solved mathematically to determine the minimum total operating cost. Those variables that influence the objective function are selected.

In this procedure, some of the primary variables may be used for plant stabilization. Thus, if at the latter design stage these variables—identified to be cost variables—are found to be good candidates for process stabilization, priority is given to them as stabilization variables, despite the possibility of their being used as cost variables in the process optimization .

Step 2. Stabilize the Plant. Causes of process instability are either derived from pole vector analysis[27] or identified through process insights coupled with steady state simulation. For processes with known dynamics, all unstable poles (RHP eigenvalues) of the process matrix are computed and identified. Starting with the unstable pole that has the largest absolute value (the most unstable pole), one would identify the corresponding manipulative variable that is most easily controlled and the output variable that is most easily observed. This is referred to as the concept of state controllability and observability. When the input−output pairing is closed, one may recalculate the process dynamic with the transfer function of the controller and identify the most unstable pole using the same method that was previously used. The process of vector pole analysis is repeated until there are no more unstable poles in the system.

For processes without dynamic information, energy balance analysis is performed on the system to identify where there may be a unsteady control variable which leads to process instability. The proper manipulative variable is then assigned to the control variable to stabilize the process. Process plants are usually designed based on energy balances throughout the process or unit operations, but if small perturbations in any of the variables lead to energy imbalance, then this may be due to process instability.

Step 3. Close Loops for the Secondary Variables Control. There are two substeps required:

Substep 1. Identify and Close Loops for the Secondary Variables. Secondary variables are output variables selected to stabilize the process and achieve local disturbance rejection. Secondary variables (for example, flow rates) are identified and controlled with manipulative variables located in their proximity (located directly upstream or downstream).

Substep 2. Conduct Steady State Analysis. Conduct small perturbations on the remaining available manipulative variables. For the manipulative variables that are already used to control secondary variables, small set point changes are effected on the secondary variables to generate steady state response for the system. If all the output variables achieve steady state status, one may proceed directly to stage 5. Otherwise, if one or more output variables continue indefinitely without attaining steady state, the next level of design is invoked.

Step 4. Close Loops on Integrating Variables. Substep 1. Identify Integrating Variable. If process dynamic information is available, integrating variables are identified as processes that contain $1/s$ in their transfer functions, and do not settle at steady state. If process dynamic information is not available, these variables can be identified as the control outputs that do not attain steady state during the steady state analysis of step 3. Another approach to identifying the integrating variables is to effect a step change on the inlet flow or the outlet flow of unit operators with accumulators in the process. If the accumulators do not attain steady state, then the unit operators possess integrating variables.

Substep 2. Close Loops on the Integrating Variables. When process dynamic information is available, the Arkun and Downs[28] method is used to determine the proper control pairings for systems with integrating variables. When process dynamic information is not available, all control pairings have to be tested via simulation to identify the best (proper) pairing. The inventory control variables are left at their target values or allowed to attain new steady state values until the next step (step 5).

Step 5. Close Loops for Inventory Control Variables. Substep 1. Inventory Control Inputs or Outputs Selection. Usually inventory variables are the remaining control variables that have operating constraints. For the case where the number of input variables (manipulative variables) is not equal to the number of output variables, the "general relative gain array (GRGA)" is used to select the most effective manipulative variables or the most controllable output variables (inventory variables). Small perturbations on the remaining available manipulative variables or set points of secondary variables are applied if the manipulative variables were already used to control secondary variables. To obtain the steady state gain matrix, the following steps are conducted: record the change of the steady state values of control and manipulative variables and scale the change of control and manipulative variables. The gain value corresponding to a specific input and output variable is calculated by dividing the change of output by the change of input. Mathematically, general RGA can be computed by the following operation $\Lambda^N = G \otimes (G^+)^T$, where G^+ is the pseudoinverse and $\otimes$ is the Hadamard product. G is the open loop steady state gain matrix already obtained from conducting small perturbations on manipulative variables.

The GRGA is computed with the following command in MATLAB:

$$GRGA = G.*pinv(G.')$$

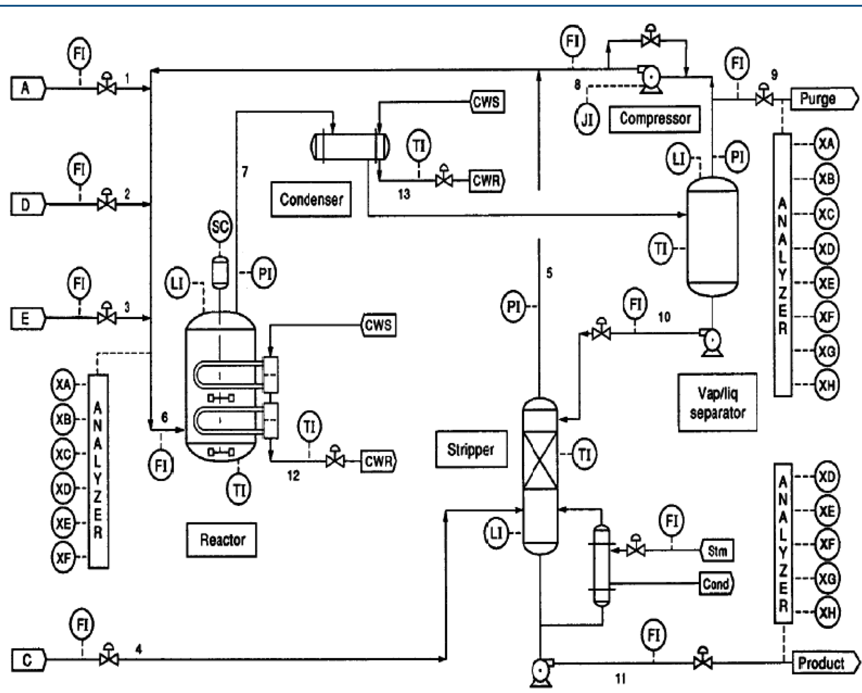

Figure 1. The TE process diagram.

If more than one scenario is generated from stage 4, their GRGA matrix is examined in this stage. Scenarios where the most effective pairing as indicated by GRGA elements but having large lag times are eliminated. The remaining scenarios proceed to the next step of the control design.

There are generally more manipulative variables than inventory variables in chemical processes. Consequently, all inventory variables are controlled. In the rare case where there are more inventory variables than manipulative variables, more manipulative variables can be added by either branching or bypassing of streams to the unit operator. With these additions the entire plantwide control design process will have to start over again.

Substep 2. Assign Control Pairing for the Inventory Control Variables. After selecting manipulative variables, one will need to decide pairing on the inventory variables and the manipulative variables. For chemical processes that are nonlinear, with no process dynamic information, a trial-and-error method is used to determine the proper control pairings from the steady state gain matrix generated in substep 1 of this stage. The sign of the steady state gain for a manipulative and control variable determines the appropriate controller gain for the pair. A positive controller gain is assigned to the pair if the steady state gain is positive, while for negative steady state gain a negative controller gain is assigned. Loops are closed one at a time starting with the pair that has the largest steady state gain in magnitude. After each assignment a new steady state gain matrix between the remaining inventory variables and manipulative variables is generated. This is to ensure that the most effective manipulative variable is paired with its corresponding control variable. The process is repeated until all control loops are closed.

The basic structure of the plantwide control is now in place; the next two steps will focus on disturbance rejection and set point tracking.

Step 6. Close Loops for Disturbance Rejection. Control loops are assigned to achieve disturbance rejection on the remaining primary variables in this stage, since the secondary variables are already controlled in step 3. Thus, the control objective will include control of component compositions in the reactor (if there is any) feed stream to ensure the component compositions do not fluctuate. In addition, advanced control strategies are employed for rejection of all possible disturbances.

Step 7. Close Loops for Set Point Changes. Control loops for product rate and quality control are assigned first because they are the most important variables that determine the process economics. These two control variables are considered together because they are highly correlated with each other. The product rate and quality can be controlled by controlling the feed rates and sometimes with feed compositions.

It is the choice of control engineers to decide which control output (product rate or quality) is the priority after evaluation. The control output (product rate or quality) given the priority should have its control loops assigned first by controlling either the feed rates or feed compositions. After control loops are assigned to control product rate and quality, other output variables for specific set point changes are then identified and controlled.

One can use material balance to select the most effective manipulative variables to perform set point changes on the product rate and product quality.

$$A_{(g)} + C_{(g)} + D_{(g)} \rightarrow G_{(l)}\,(product\ \ 1)$$
$$A_{(g)} + C_{(g)} + E_{(g)} \rightarrow H_{(l)}\,(product\ \ 2)$$
$$A_{(g)} + E_{(g)} \rightarrow F_{(l)}\,(byproduct\ \ )$$
$$3D_{(g)} \rightarrow 2F_{(l)}\,(byproduct\ \ )$$

Figure 2. TE reaction process.

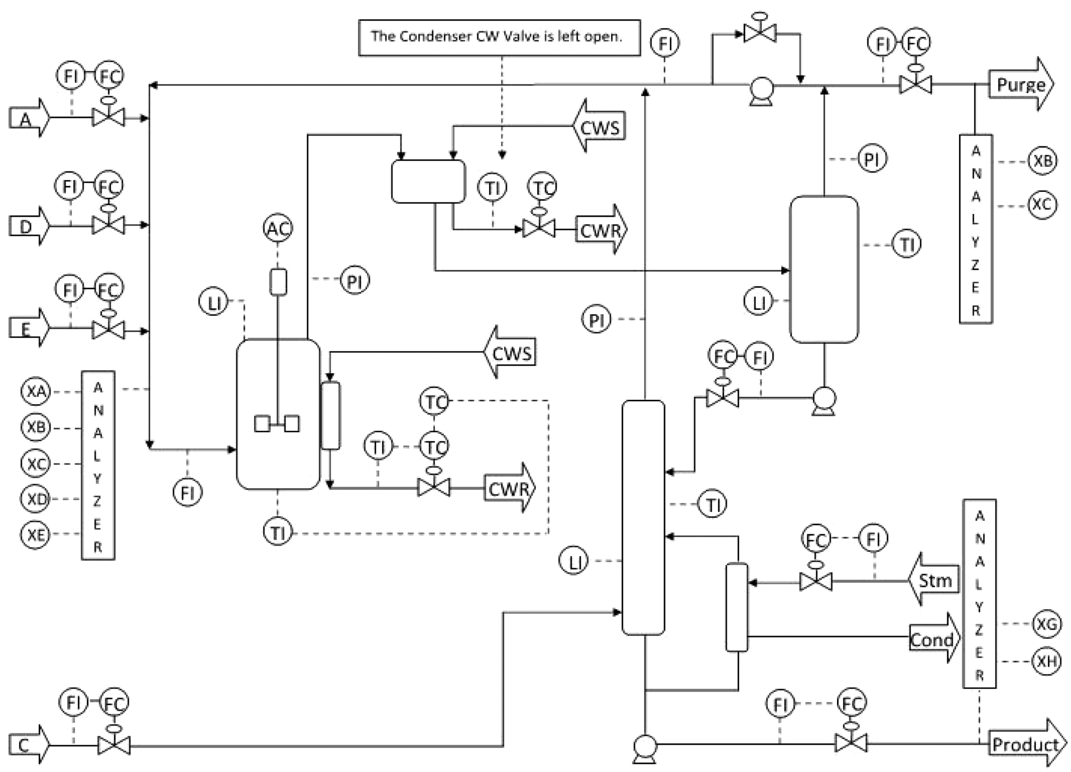

Figure 3. TE control structure with flow loops closed.

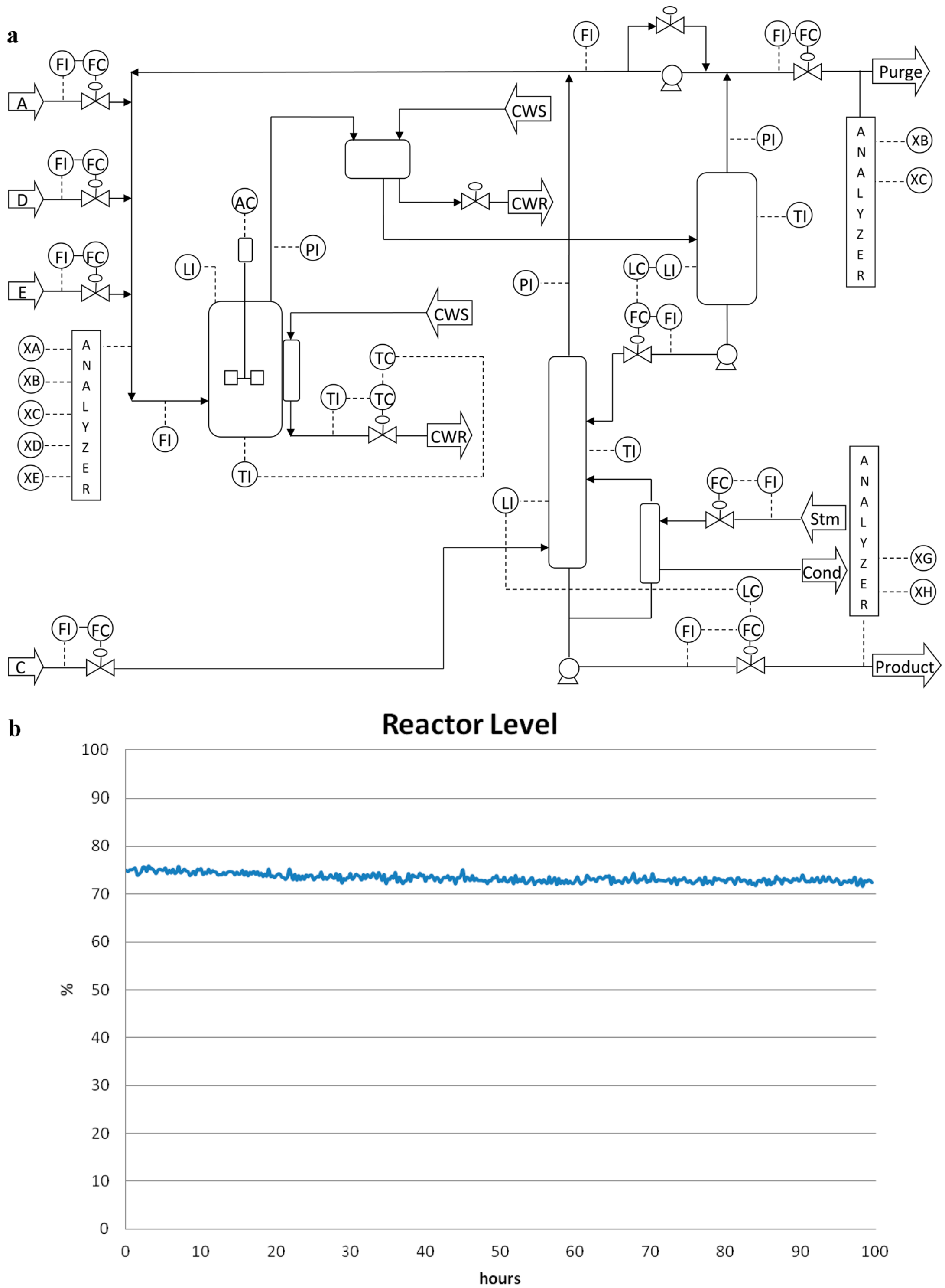

Figure 4. (a) Scenario 1 level control configuration. (b) Reactor level response, 5% increase in a feed (level control mode 1).

Step 8. Close Loops for Process Optimization. Substep 1. The variables identified for optimization in stage 1 that have control loops assigned to them are set at their optimal operating values.

Substep 2. If the variables identified for optimization in stage 1 have not been controlled, they are paired with appropriate manipulative variables and set at their optimal operating values.

Step 9. Validation. The final PWC structure is tested under various disturbances to determine the effectiveness of the control system on stabilization, self-optimization, and operating cost of the process.

This new strategy is now applied to the Eastman Chemical Co. (TE) project.[2]

Process Description. The TE problem is based on a real process developed by the Eastman Chemical Co. which is written in FORTRAN and consists of five unit operations. These are a reactor, a partial condenser, a vapor/liquid separator, a product stripper, and a recycle compressor. The process has a total of

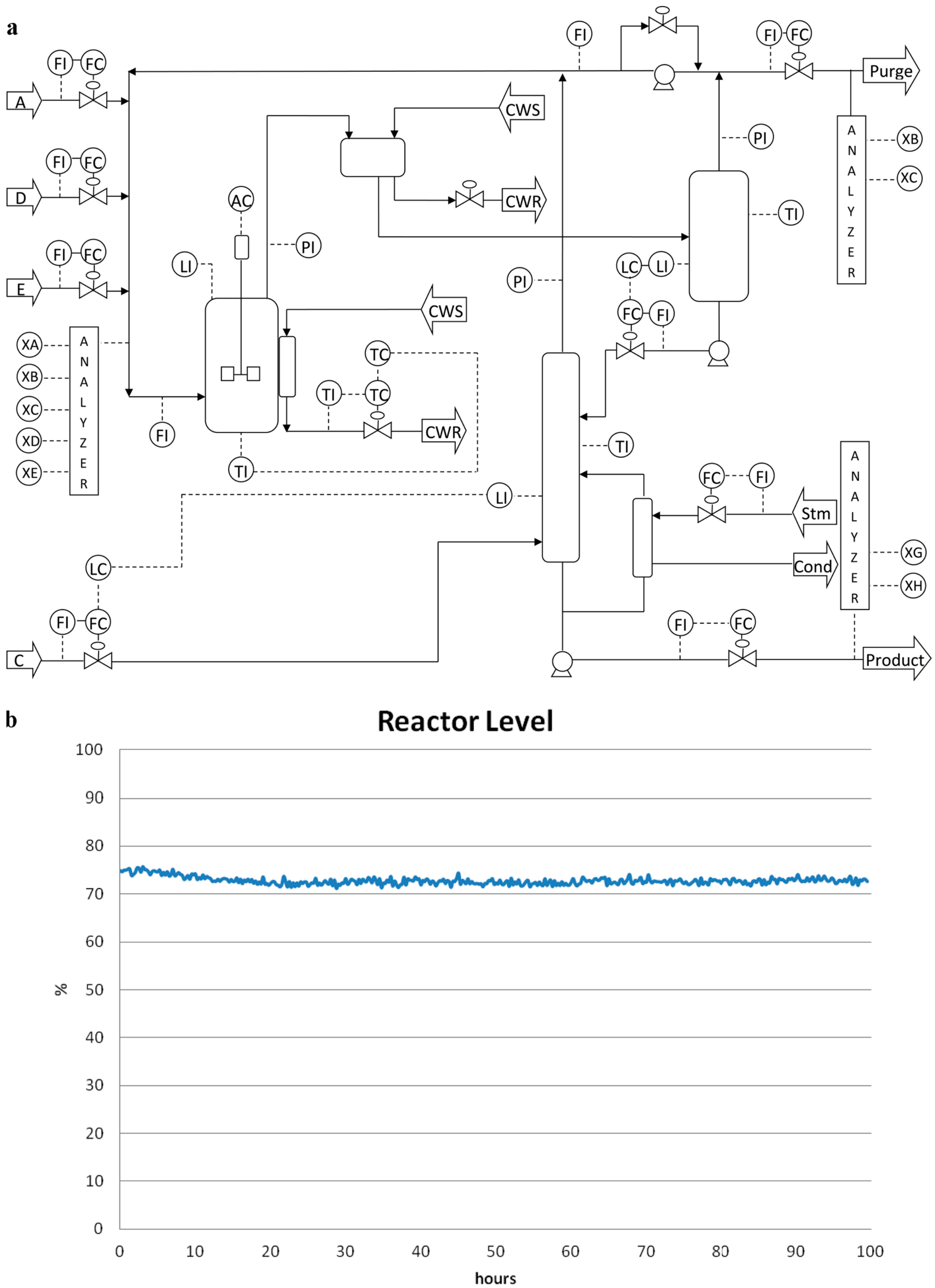

Figure 5. (a) Scenario 2 level control configuration. (b) Reactor level response, 5% increase in a feed (level control mode 2).

eight components making up the reactants, products, by-products, and inert gas. Components A, C, D, and E are the reactants. Components G and H are the products. Component B is the inert gas, and component F is the byproduct. Figure 1 represents the flow sheet for the overall TE process.

The process has the reactions in Figure 2 taking place in the reactor:

The TE process is hard to control for the following reasons:

1. It contains a recycle loop.
2. It is a nonlinear process.
3. It is open loop unstable.
4. It contains an integrator.
5. Its process variables have strong interactions.

Control Structure Formulation and Application. The control structure is developed for a process without dynamic information. The PWC design procedure proposed in this study is applied. Simulation is used to verify if a control objective is achieved, and mathematical tools are utilized to aid in assigning

Table 1. GRGA Analysis for Direct Control on Condenser CW Valve (Mode 1 Level Control)

SS gain	set pt 4, A feed	set pt 14, D feed	set pt 15, E feed	set pt 16, C feed	XMV11, sep CW valve	set pt 18, purge rate	set pt 19, steam flow
reactor level	−96.28	4488.88	4357.84	−7038.16	−89 971.98	97.05	32.91
reactor press.	−797.45	28 148.20	29 455.12	−46 807.04	−4832.11	200.19	250.81
GRGA	set pt 4, A feed	set pt 14, D feed	set pt 15, E feed	set pt 16, C feed	XMV11, sep CW valve	set pt 18, purge rate	set pt 19, steam flow
reactor level	0	−0.0017	−0.0019	−0.0047	1.0082	0	0
reactor press.	0.0002	0.2072	0.2272	0.5736	−0.0082	0	0
sum	0.0002	0.2055	0.2253	0.5689	1	0	0

Table 2. GRGA Analysis for Direct Control on the Condenser CW Valve (Mode 2 Level Control)

SS gain	set pt 4, A feed	set pt 14, D feed	set pt 15, E feed	XMV11, sep CW valve	set pt 18, purge rate	set pt 19, steam flow	set pt 21, product flow
reactor level	−52 191	−6.99	−7.69	1013.96	−107.11	−0.11	−5628.27
reactor press.	3 955 833.80	18 817.87	15 315.35	5 485 181.57	2 935 488.74	1075.05	12 022 641.08
GRGA	set pt 4, A feed	set pt 14, D feed	set pt 15, E feed	XMV11, sep CW valve	set pt 18, purge rate	set pt 19, steam flow	set pt 21, product flow
reactor level	−0.076	0	0	−0.0404	−0.0245	0	1.141
reactor press.	0.2589	0	0	0.7031	0.1859	0	−0.1478
sum	0.1829	0	0	0.6627	0.1614	0	0.9932

Table 3. Steady State Gain Matrix of Inventory and Manipulative Variables

SS gain	set pt 16, C feed	XMV11, sep CW valve
reactor level	−7038.16	−89 971.98
reactor press.	−46 807.04	−4832.11

appropriate control loops. The process is simulated each time for 200 h with positive and negative perturbations.

Step 1. Identify Cost Variable.

cost function of the TE process:

$$\text{(purge costs)(purge rate)} + \text{(product stream costs)} \\ \text{(product rate)} + \text{(compressor costs)(compressor work)} \\ + \text{(steam costs)(steam rate)} = \text{total cost} \quad (1)$$

From the operating cost function of the TE process (eq 1), the following are cost variables that need to be controlled at their optimal values: purge cost, purge rate, product stream cost, product rate, compressor work, and steam rate. All these cost variables are controlled directly with the exception of purge cost and product stream cost. To minimize purge cost, increase in composition of B in the purge stream is required, since inert gas B does not have an associated cost. To minimize the product stream cost, reactor pressure, reactor level, and reactor temperature are set at their optimal values to improve reaction yield. It is also known from Ricker's optimization study[29] that active constraint control variables for the TE process are reactor pressure (maximum), reactor level (minimum), recycle valve (closed), steam valve (closed), and agitation rate (maximum). These variables are included as the variables for optimization.

In summary, the variables selected for optimization are composition of B purge, purge rate, reactor pressure, reactor level, reactor temperature, compressor work, recycle valve, steam valve, and agitation rate. This agrees closely with what Larsson[20] found.

Step 2. Close Loops for Energy Balances as Part of Process Stabilization. The reaction in the TE process is known to be exothermic. Exothermic reactions are inherently unstable, so a stabilization sequence is applied. There are possibly two ways to remove the excess heat produced from the reaction: control of the reactor temperature and the reactor's cooling water temperature. The TE process is successfully stabilized by closing a cascade loop (the reactor temperature has an inner slave loop which controls the cooling water temperature) on the reactor temperature.

Step 3. Close Flow Loops for Secondary Variables Control. With the process stabilized now, all flow loops are closed except the condenser cooling water stream. The condenser cooling water stream is not closed because it is considered an important manipulative variable to be later used for inventory control in step 5 due to its proximity to the reactor. The flow loops that are closed are A, D, E, and C feeds, purge stream, product stream, stripper steam stream, and separator bottom stream (Figure 3). Each stream is controlled by the control valve that directly limits the flow rate of that stream. The steady state gain matrix is generated by making perturbations on A, D, E, and C feed rates, purge rate, product rate, steam rate, condenser cooling water rate, and separator bottom stream rate. This is used to identify integrating variables in the next design stage.

Step 4. Close Loops on Integrating Variables. From the steady state gain matrix generated in step 3, the separator and stripper level are identified as integrating variables since they do not attain steady state after small perturbation of manipulative variables. With no available dynamic information of the process, series of simulations are performed based on probable control pairings to identify manipulative variables that can most effectively control the integrating variables (separator and stripper levels).

To control the separator level, possible manipulative variables include condenser cooling water and separator bottom flow. For stripper level, the possible candidates are C feed rate, product flow, and separator bottom flow. The control of these integrating variables results in five possible scenarios of control structure, but only two are used in this study.

Scenario 1. The stripper level is regulated by a product flow valve and the separator level is regulated by a separator bottom flow valve on stream 10 (Figure 4).

Scenario 2. The stripper level is regulated by the C feed, and the separator level is regulated by a separator bottom flow valve on stream 10 (Figure 5).

Based on simulation with all available manipulative variables, only scenarios 1 and 2 are successful with the screening test since

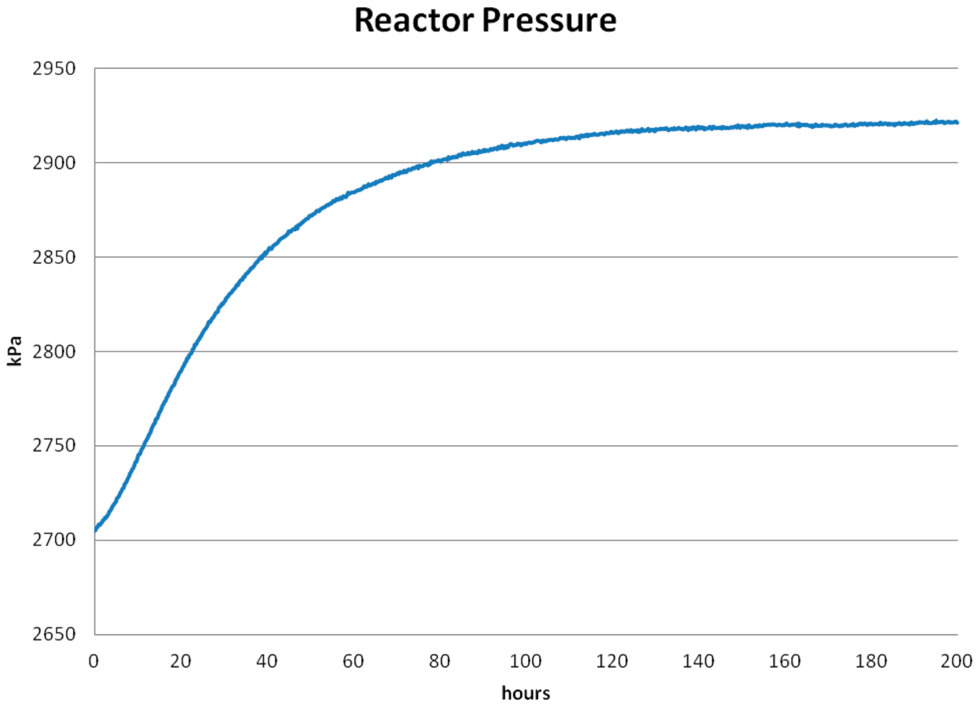

Figure 6. Reactor pressure response, 1% increase in C feed.

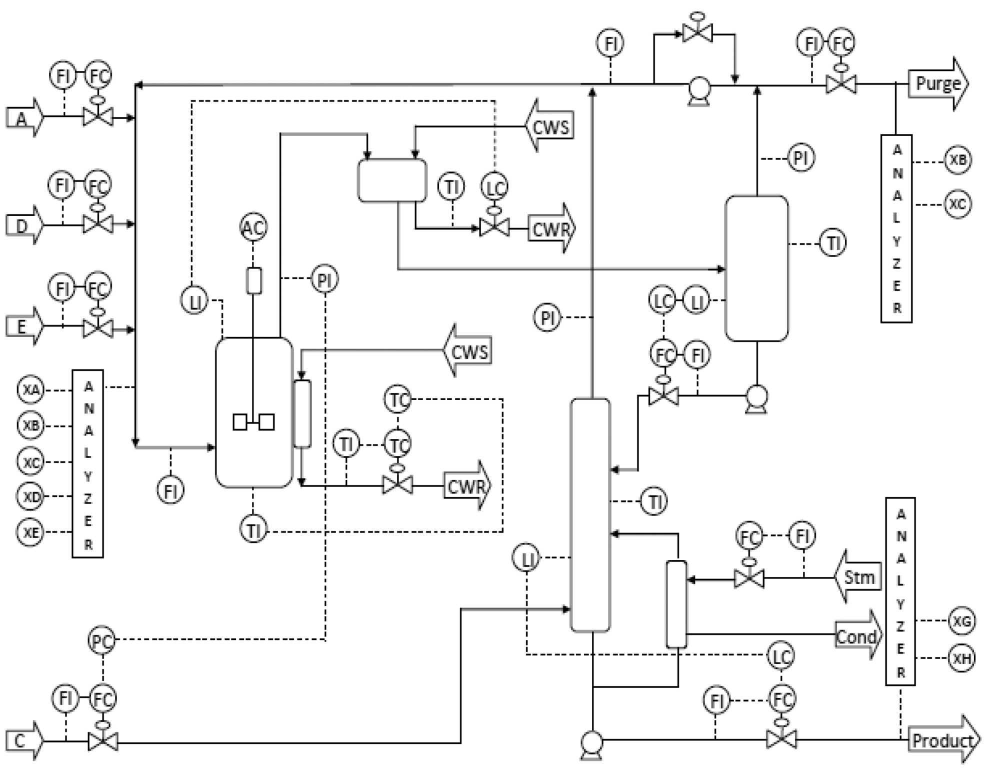

Figure 7. TE control structure after inventory variables are closed.

they control the integrating variables and do not cause instability to the remaining inventory variables (reactor level and reactor pressure).

Step 5. Inventory Control. The reactor level and pressure are the two inventory variables that are to be controlled. The reactor pressure is controlled primarily for the purpose of optimization. This is because—from the aspect of process stabilization—there is really no point in controlling the reactor pressure directly since it can be controlled indirectly with reactor temperature and level and may incur risk on the system to be unstable if one attempts to close the control loop on reactor pressure. Therefore, this reemphasizes the importance of conducting top-down analysis before conducting the bottom-up portion of the design procedure.

The GRGA results show that, in scenario 1, C feed rate and condenser CW valve are the manipulative variables (Table 1).

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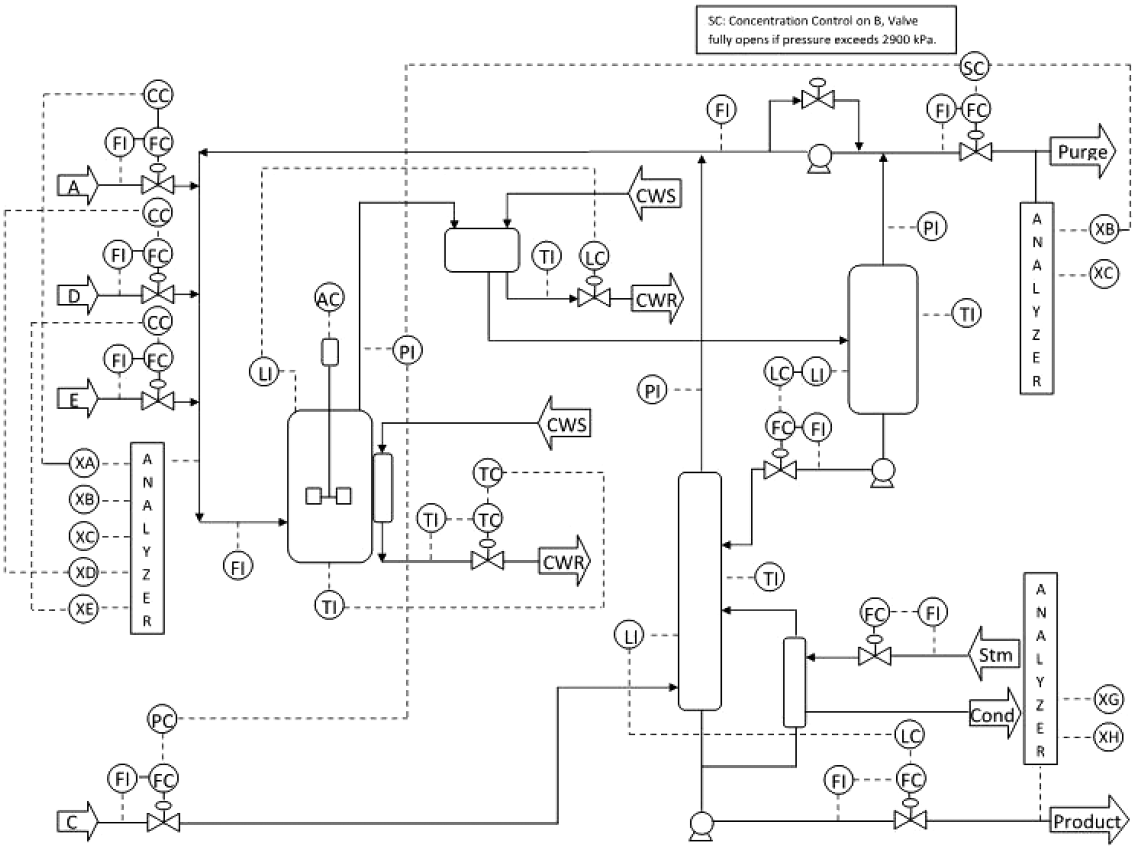

Figure 8. TE control structure after loops are closed for disturbance rejection.

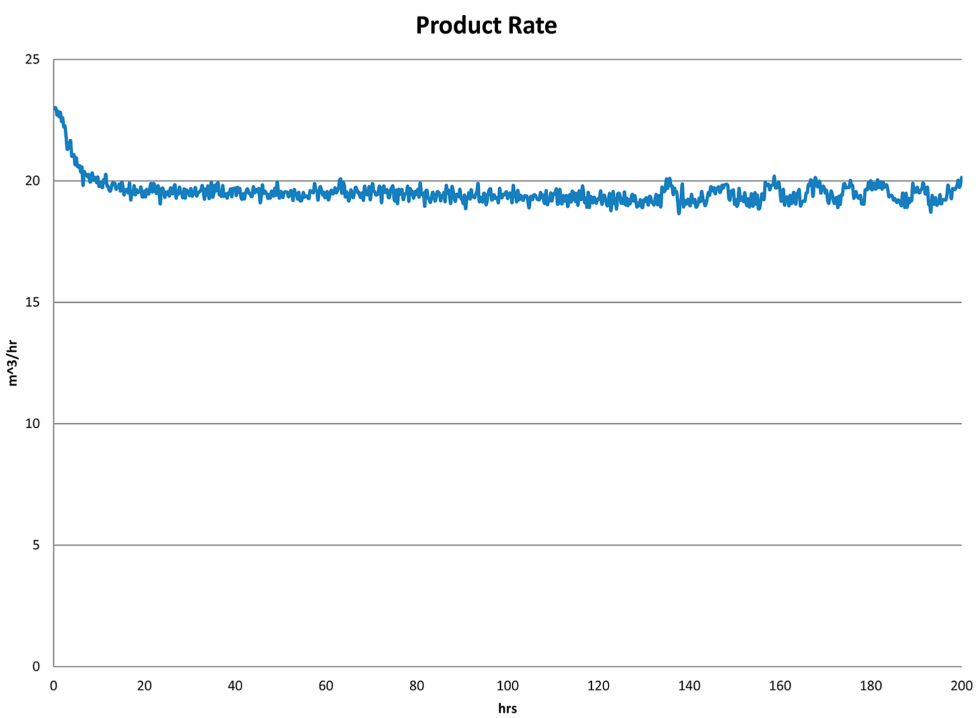

Figure 9. Product rate response (product rate change).

The GRGA results show that, in scenario 2, condenser CW valve and product flow are the manipulative variables (Table 2).

Control pairings presented in scenario 2 were eliminated based on the fact that there is a large dead time between product flow (one of the manipulative variables) and both inventory variables. Furthermore, it is found through simulation that this control pairing makes for unstable control structure.

For scenario 1, steady state gain matrix (Table 3) is generated to select proper control pairings for the inventory and manipulative variables.

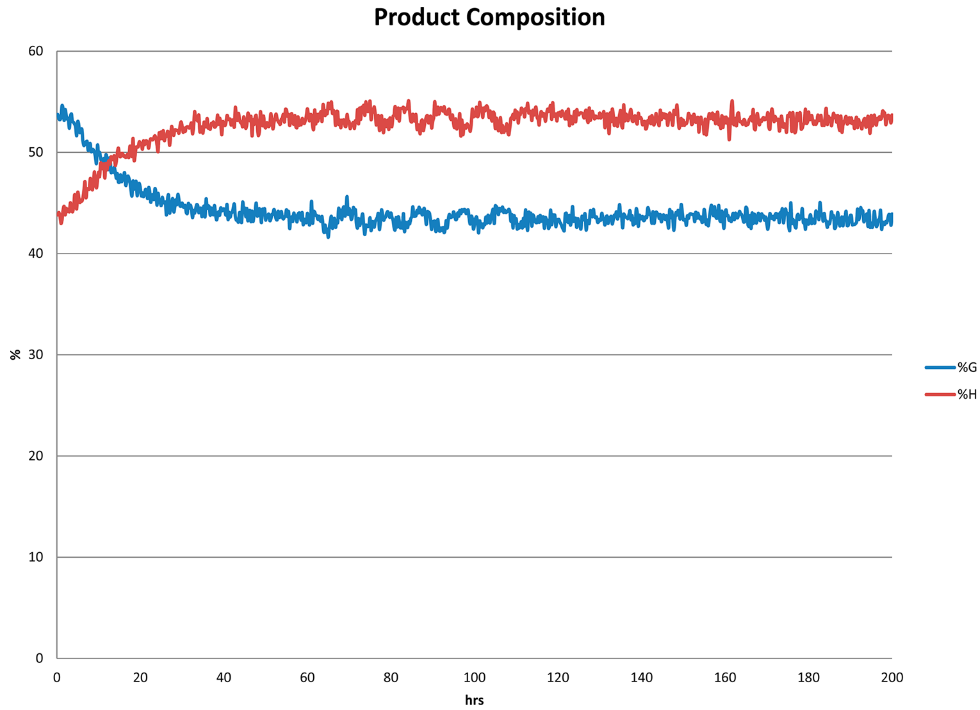

Figure 10. Product composition response (product quality change).

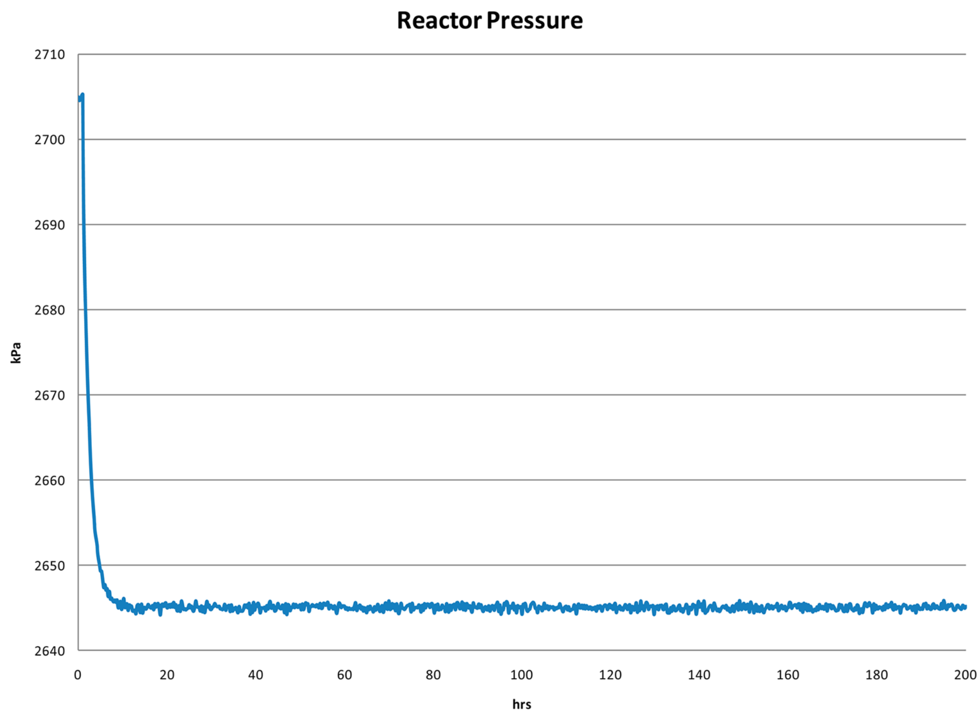

Figure 11. Reactor pressure change.

Based on the analysis of the steady state gain matrix of manipulative and control variables, the condenser CW valve and reactor level pairing loop is closed first as it has the highest steady state gain magnitude (absolute). Then steady state response from the updated system is generated. The steady state response shows that the steady state gain between C feed and reactor pressure is positive, so a positive controller gain is assigned to close the control loop (Figure 6). Therefore, it is determined that the best control candidate for reactor pressure is C feed and that for reactor level is condenser CW valve.

Figure 7 is the control structure after implementation of step 5, Inventory Control.

Step 6. Close Loops for Disturbance Rejection. The control objective at this stage is to close loops for output variables to reject all possible disturbances that may destabilize the process. Downs and Vogel[2] proposed 20 disturbances, some with known causes and others with unknown causes that could most likely occur in the process plant. By closing all loops for secondary variables control with the exception of condenser cooling water temperature in stage 3, the effect of 3 of the 15 known

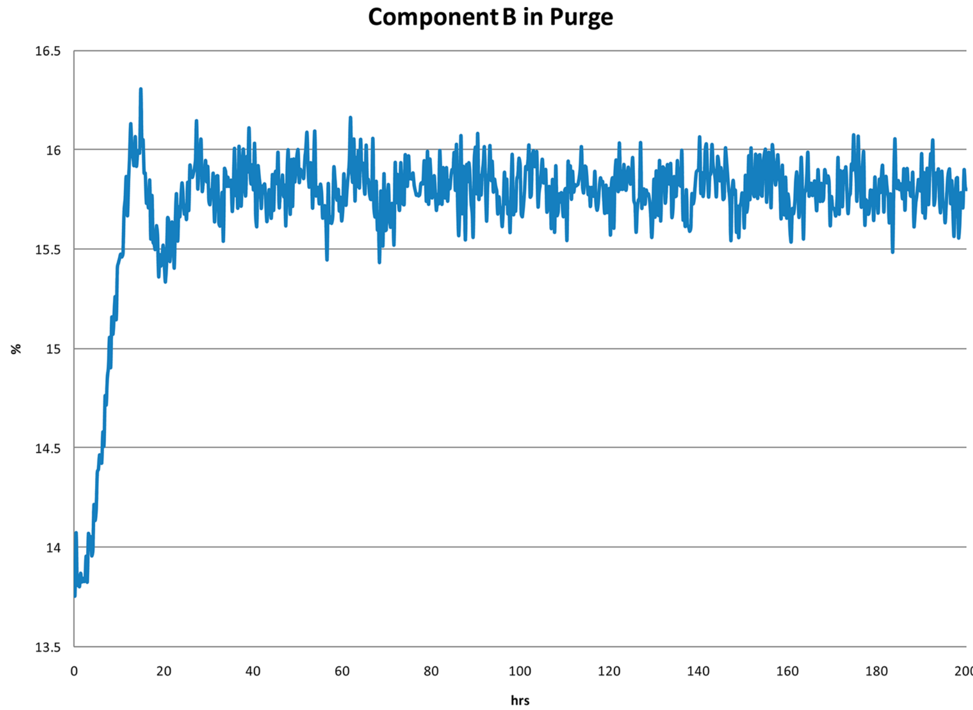

Figure 12. Composition B in purge change.

Table 4. Optimal Operating Condition

reactor press., kPa	2800
reactor level, %	60
reactor temp, °C	122.8
separator press., kPa	2706
separator temp, °C	91.7
stripper press., kPa	3326
stripper temp, °C	66.7
recycle valve, %	0
purge rate, kscmh	0.206
purge % B, mol %	22.37
product % E, mol %	0.55
purge losses, $/h	71.3
product losses, $/h	24.51
compression, $/h	15.02
total cost, $/h	110.98

Table 5. Operating Output Results (Base Case)

reactor press., kPa	2800.004
reactor level, %	60
reactor temp, °C	122.8
separator press., kPa	2704.6
separator temp, °C	92.364
stripper press., kPa	3331.774
stripper temp, °C	66.7
recycle valve, %	1
purge rate, kscmh	0.2052
purge % B, mol %	22.325
product % E, mol %	0.544
purge losses, $/h	71.28
product losses, $/h	24.30
compression, $/h	14.83
total cost, $/h	110.41

disturbances (IDV 4, 11, 14) is eliminated. By closing the composition A, D, and E master cascade loops employing A, D, and E feeds and composition B in purge on purge rate, respectively, the process can reject all the disturbances except for disturbances 6, 8, and 13. Since feed A is completely lost in disturbance 6, a new strategy to deal with disturbance 6 is to increase the C feed rate coupled with an override control on the purge valve that will fully open the purge valve when the reactor pressure exceeds 2900 kPa. For disturbances 8 and 13, the cause of instability is the fluctuation of component composition in the reactor feed. Therefore, an override control is used to ensure that the percent composition of A + C is within a certain range, and if it is out of range, C feed will be used to control the percent composition C in reactor feed instead of reactor pressure. C feed will be used to control reactor pressure once the percent composition of A + C is within range. With the control strategies discussed above, the control system is able to stabilize the process under all 20 disturbances.

Figure 8 is the control structure after implementing steps 1−6.

Step 7. Close Loops for Set Point Change. In this study, it is decided that product rate is the priority, thus manipulative variables for this control output are first assigned. Based on mass balance, one can conclude that changing D and E feeds together can effectively control product rate without incurring too much change on product mix. To achieve product rate and mix change, an override control is used to ensure that both product rate and quality are within a specified range from the set points. The override control logic will respond to either product rate or quality when it is out of the range and adjust D feed and E feeds. For product flow, D and E feeds are adjusted together to control the flow rate. For product quality, % G composition in the product stream is the master loop for D feed and % H composition in the product stream is the master loop for the E feed.

The control system is tested by the four set point change requirements for the TE process: product rate and quality, reactor pressure, and component B in the purge stream.

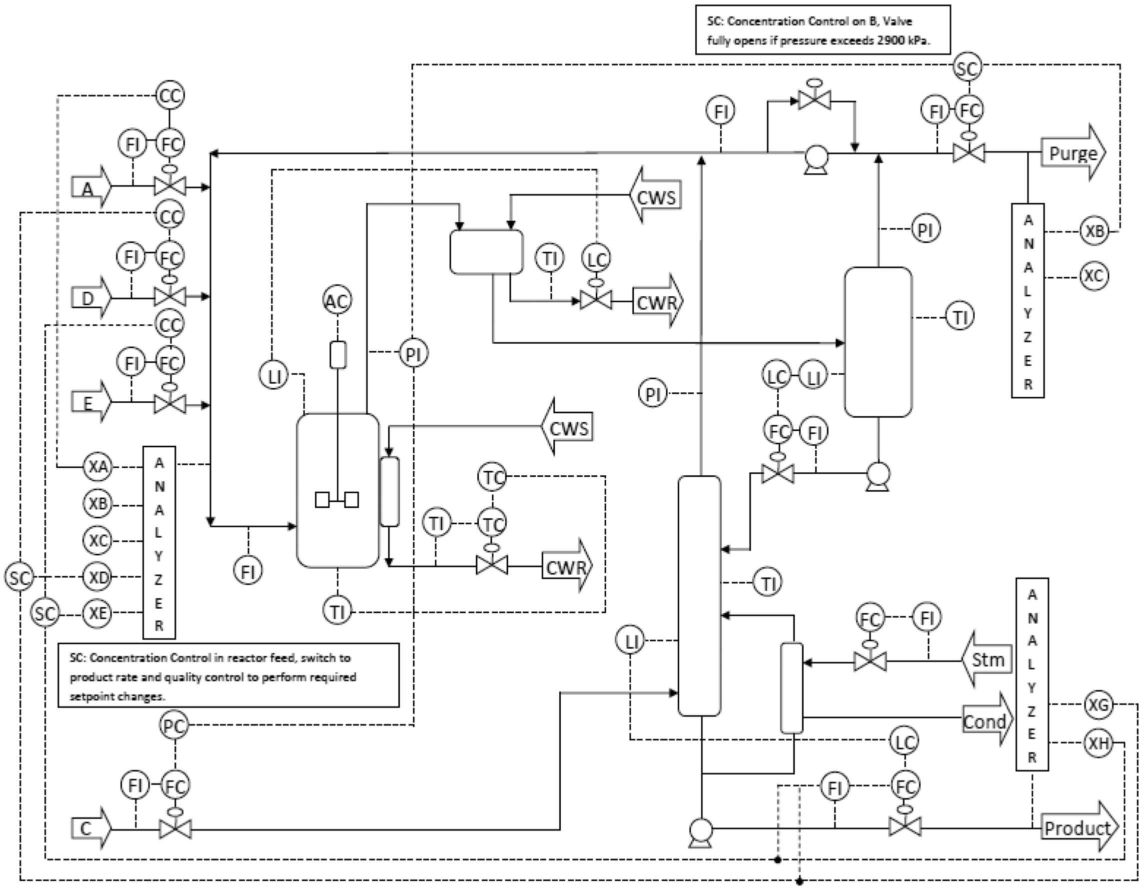

Figure 13. Final control structure.

Product Rate Change. The product rate change requires a 15% decrease in production rate (from 22.949 to 19.5 m^3). To achieve the product flow rate change, this can be achieved by changing the set point value of product rate to 19.5 m^3. Figure 9 shows that the process reaches the full effect of the set point change in about 30 h.

Product Quality Change. To perform product quality change, one can change the set point on % G and % H directly to change product quality. From mass balance calculation, in order for the process to achieve 40 G/60 H molar ratio production, the composition of H has to be about 53.7% while the composition of G is about 46%. This successfully changes the product composition while keeping the product rate at its original set point value. Figure 10 shows that the process reaches the full effect of the set point change in about 40 h.

Set Point Changes for Reactor Pressure and Composition B in the Purge Stream. The control pairings for reactor pressure and composition B in the purge stream have already been assigned. No additional control pairings are necessary to perform set point changes for these two variables. The set point changes are performed by changing the reactor pressure and reactor level set point (change reactor pressure from 2705 to 2645 kPa and change composition B in the purge stream from 13.82 to 15.82%). Figures 11 and 12 show the processes reach the full effect of the reactor pressure and composition B set point changes in about 20 and 30 h, respectively.

Step 8. Close Loops for Process Optimization. The cost variables that are already controlled are identified to be purge rate, composition of B in purge stream, reactor pressure, reactor level, reactor temperature, and steam rate (steam valve).

Table 6. Optimal Operating Cost under Disturbances

optimizn simuln result	purge loss ($)	product loss ($)	compressor ($)	total cost ($)
base case with no optimal setting	113.98	28.44	18.59	161.01
base case with optimal setting	70.95	23.68	14.85	109.48
disturbance 1	67.60	24.66	14.71	106.97
disturbance 2	*137.86*	*16.86*	*15.15*	*169.87*
disturbance 3	70.93	23.68	14.85	109.46
disturbance 4	71.03	23.85	14.85	109.73
disturbance 5	70.93	23.68	14.85	109.46
disturbance 6	*290.61*	*28.01*	*12.73*	*331.35*
disturbance 7	70.96	23.74	14.85	109.55
disturbance 8	*130.75*	*11.96*	*16.64*	*159.35*
disturbance 9	71.01	23.82	14.85	109.68
disturbance 10	71.02	23.82	14.85	109.69
disturbance 11	71.10	23.68	$14.85	09.64
disturbance 12	71.94	24.82	14.94	111.70
disturbance 13	*121.05*	*15.31*	*15.98*	*152.34*
disturbance 14	70.96	23.72	14.85	109.53
disturbance 15	70.95	23.52	14.87	109.34
disturbance 16	70.93	23.68	$14.85	109.46
disturbance 17	72.10	24.74	4.80	111.65
disturbance 18	71.05	23.44	14.93	109.42
disturbance 19	70.91	23.63	14.85	109.40
disturbance 20	70.97	23.17	14.75	108.88

The other cost variable identified in stage 1 but which does not have control pairing assigned is compressor work. No available manipulative variable is left to control compressor work, so compressor work is allowed to float.

Stripper steam valve and recycle valve are closed and agitation speed is set at its maximum based on Ricker's suggestion.[29] The set points of the rest of the cost are changed to the optimal operating condition in Table 4 given by Ricker.[29]

All the cost variables loops are then closed; the system is able to operate close to the optimal condition in Table 4 and achieves an operating cost close to the minimal operating cost in Ricker's result. The operating condition is shown in Table 5.

Figure 13 is the final control structure after implementing steps 1−8.

Step 9. Validation. The TE process with the final control structure (Figure 13) is simulated for the given 20 disturbance cases. The operating cost for these cases is shown in Table 6. As can be observed, the process is at its optimal operating condition. The control system is able to stabilize the process in all the cases and achieve self-optimization control for almost all of them except for disturbances 2, 6, 8, and 13. These disturbances are considered as special cases because the priority under these disturbances is process stabilization, which is satisfied. Thus, the control structure is found to be complete and successful.

■ CONCLUSION

The plantwide control methodology developed in this study simplified the decomposition and coordination of layers in the bottom-up portion of Skogestad's methodology.[11] It was tested on the TE problem. The variables found in this study for optimization agree with those of Larson[20] with the exception of composition B in purge. In addition, the optimal values are just like Ricker's.[29]

The developed structure is stable for all 20 disturbances and also achieves the four set point change cases suggested by Downs and Vogel. Furthermore, the control system is able to stabilize the process in all cases and achieve self-optimization control for almost all of them except for disturbances 2, 6, 8, and 13.

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Notes

The authors declare no competing financial interest.

■ REFERENCES

(1) Buckley, P. S. *Techniques of Process Control*; John Wiley & Sons: New York, 1964; Chapter 13.

(2) Downs, J. J.; Vogel, E. F. A plant-wide industrial process control problem. *Comput. Chem. Eng.* **1993**, *17*, 245−255.

(3) Vasudevan, S.; Rangaiah, G. P.; Murthy Konda, N. V. S. N.; Tay, W. H. Application and evaluation of three methodologies for plantwide control of the styrene monomer plant. *Ind. Eng. Chem. Res.* **2009**, *48*, 10941−10961.

(4) Luyben, W. L.; Tyreus, B. D.; Luyben, M. L. *Plant-wide Process Control*; McGraw-Hill: New York, 1998.

(5) Larsson, T.; Skogestad, S. Plant-Wide Control—A Review and a new design procedure. *Model., Identif. Control* **2000**, *21* (4), 209−240.

(6) Murthy Konda, N. V. S. N.; Rangaiah, G. P.; Krishnaswamy, P. R. Plant-wide control of industrial processes: An integrated frame work of simulation and heuristics. *Ind. Eng. Chem. Res.* **2005**, *44*, 8300−8313.

(7) Cao, Y.; Saha, P. Improved branch and bound method for control structure screening. *Chem. Eng. Sci.* **2005**, *66*, 1555−1564.

(8) Cao, Y.; Kariwala, V. Bidirectional branch and bound for controlled variable selection Part 1. Principles and minimum singular value criterion. *Comput. Chem. Eng.* **2008**, *32*, 2306−2319.

(9) Robinson, D.; Chen, R.; McAvoy, T.; Schenelle, P. D. An optimal based approach to designing plant-wide control system architectures. *J. Process Control* **2001**, *11*, 223−236.

(10) Jorgensen, J. B.; Jorgensen, S. B. Towards automatic decentralized control structure selection. *Comput. Chem. Eng.* **2000**, *24*, 841−846.

(11) Skogestad, S. Control structure design for complete chemical plants. *Comput. Chem. Eng.* **2004**, *28*, 219−234.

(12) Skogestad, S. Plant-wide control: The search for the self-optimizing control structure. *J. Process Control* **2000**, *10*, 487−507.

(13) Alstad, V.; Skogestad, S. Null space method for selecting optimal measurement combinations as control variables. *Ind. Eng. Chem. Res.* **2007**, *46*, 846−853.

(14) Molina, G. D.; Zumoffen, D. A. R.; Basualdo, M. S. Plant-wide control strategy applied to the Tennessee Eastman process at two operating points. *Comput. Chem. Eng.* **2011**, *35*, 281−2097.

(15) Umeda, T.; Kuriyama, T.; Ichikawa, A. A logical structure for process control synthesis. *Proceedings of the Seventh IFAC Congress, Helsinki, Finland, 1978*; Pergamon: Oxford, U.K., 1979.

(16) Douglas, J. M. *Conceptual Design of Chemical Processes*; McGraw-Hill: New York, 1988.

(17) Ng, C.; Stephanopoulos, G. Plant-wide control structures and strategies. *Preprints DYCOPS-5*; International Federation of Automatic Control: Laxenburg, Austria, 1988; pp 1−6.

(18) Price, R. M.; Georgakis, C. Plant-wide regulatory control design procedure using a tiered framework. *Ind. Eng. Chem. Res.* **1993**, *32*, 2693−2705.

(19) Luyben, M. L.; Tyreus, B. D.; Luyben, W. L. Plantwide control design procedure. *AIChE J.* **1997**, *43*, 3161−3174.

(20) Larsson, T.; Hestetun, K.; Hovland, E.; Skogestad, S. Self-optimizing control of a large-scale plant: The Tennessee Eastman Process. *Ind. Eng. Chem. Res.* **2001**, *40*, 4889−4901.

(21) McAvoy, T. J.; Ye, N. Base control for the Tennessee Eastman Problem. *Comput. Chem. Eng.* **1994**, *18*, 383−413.

(22) Lyman, P. R.; Georgakis, C. Plant-wide control of the Tennessee Eastman Problem. *Comput. Chem. Eng.* **1995**, *19*, 321−331.

(23) Bristol, E. H. On a new measure of interaction for multivariable process control. *IEEE Trans. Autom. Control* **1966**, *AC-11*, 133−134.

(24) Niederlinski, A. A heuristic approach to the design of linear multivariable control problem. *Automatica* **1972**, *7*, 691−701.

(25) Ricker, N. L. Decentralized control of the Tennessee Eastman challenge problem. *J. Process Control* **1996**, *6*, 205−221.

(26) Luyben, W. L. *Principles and Case Studies of Simultaneous Design*; John Wiley & Sons: New York, 2010; p 23.

(27) Havre, K.; Skogestad, S. Selection of variables for regulatory control using pole-vectors. *Proceedings, IFAC Symposium DYCOPS-5, Corfu, Greece, 1998*; Pergamon: Oxford, U.K., 1998; pp 614−619.

(28) Arkun, Y.; Downs, J. A generalized method to calculate input-output gains and the relative gain array for integrating processes. *Comput. Chem. Eng.* **1990**, *14*, 1101−1110.

(29) Ricker, N. L. Optimal Steady-State Operation of the Tennessee Eastman Challenge Process. *Comput. Chem. Eng.* **1995**, *19*, 949−959.